wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2025 – 02:36 PM EDT

PDB ID	:	9NTE / pdb_00009nte
Title	:	Helix pomatia AMP deaminase (HPAMPD) apoenzyme
Authors	:	Kaur, G.; Horton, J.R.; Cheng, X.
Deposited on	:	2025-03-18
Resolution	:	1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

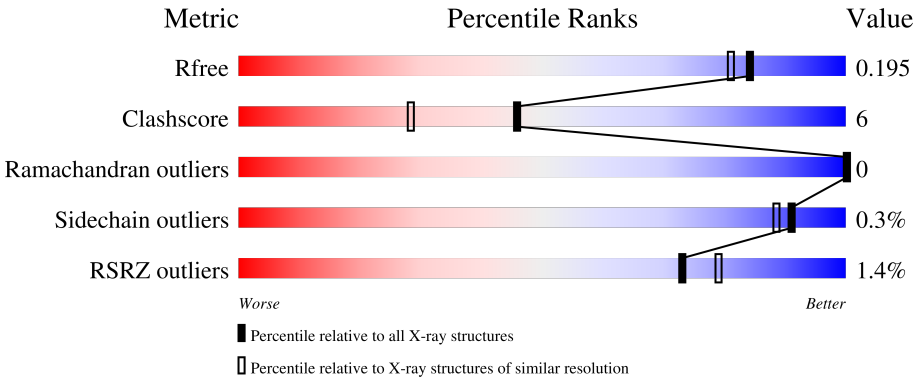
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	541	82% 10% 8%
1	B	541	85% 8% 7%
1	C	541	83% 8% 8%
1	D	541	85% 6% 8%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	624	-	-	X	-
3	EDO	A	627	-	-	X	-
3	EDO	C	630	-	-	X	-
3	EDO	D	626	-	-	X	-
6	GOL	C	602	-	-	X	-
6	GOL	C	603	-	-	X	-
6	GOL	C	624	-	-	X	-
6	GOL	C	631	-	-	X	-
7	PEG	A	646	-	-	X	-
7	PEG	C	627	-	-	X	-
9	PGE	B	643	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 19110 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.

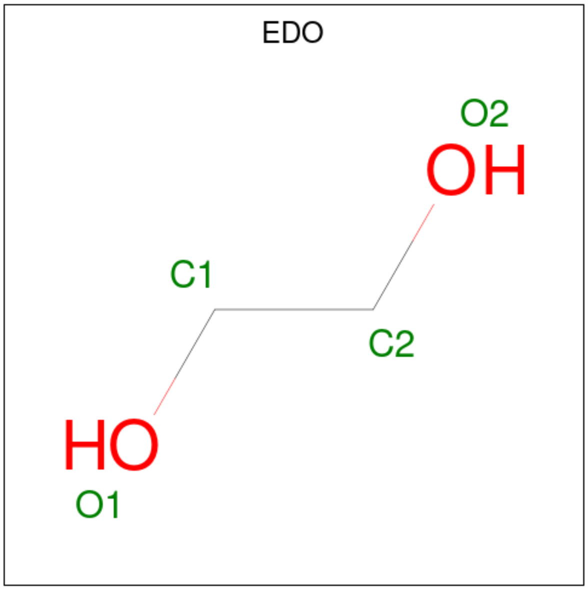
- Molecule 1 is a protein called Helix pomatia AMP deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	6	0
			4025	2577	683	753	12			
1	B	505	Total	C	N	O	S	0	10	0
			4102	2628	697	765	12			
1	C	496	Total	C	N	O	S	0	9	0
			4036	2584	685	755	12			
1	D	497	Total	C	N	O	S	0	4	0
			4012	2570	681	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
			29	16	2	11			
2	F	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

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

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

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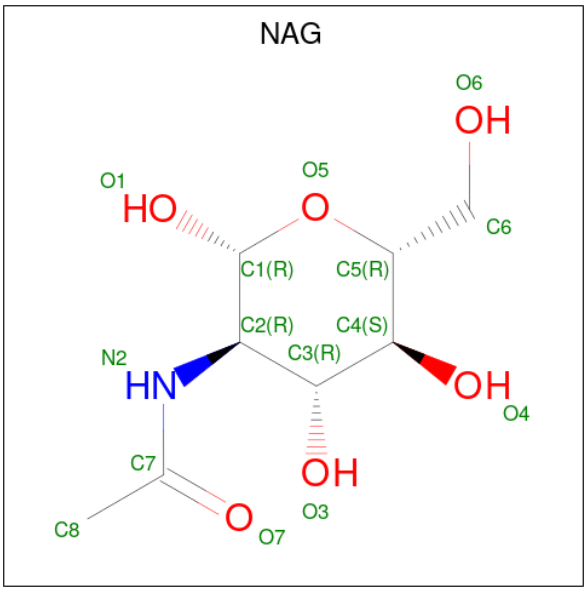
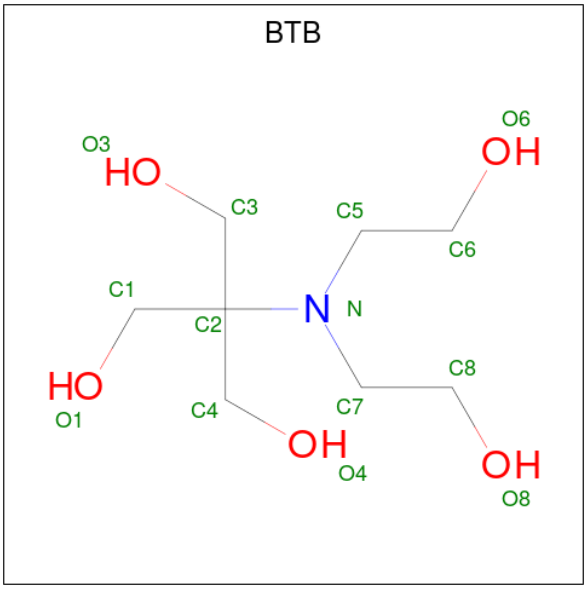
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



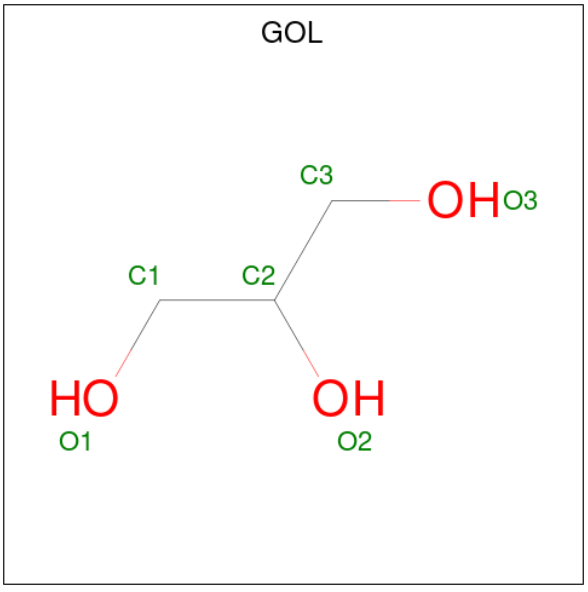
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 15 8 1 6	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



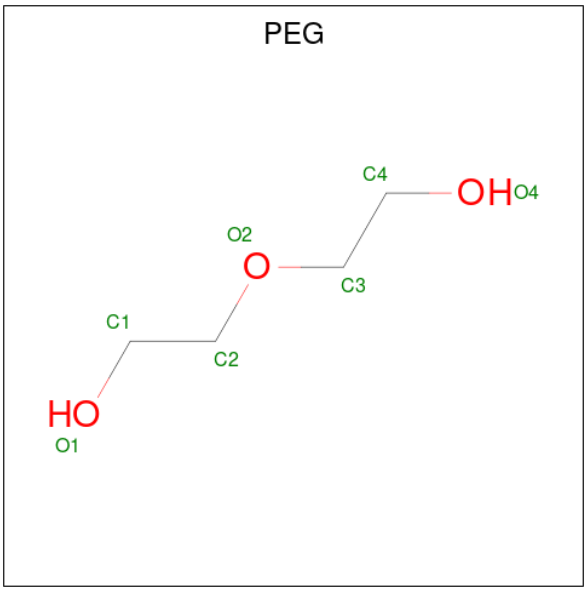
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	C	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0
7	D	1	Total C O 7 4 3	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0
8	B	1	Total Zn 1 1	0	0

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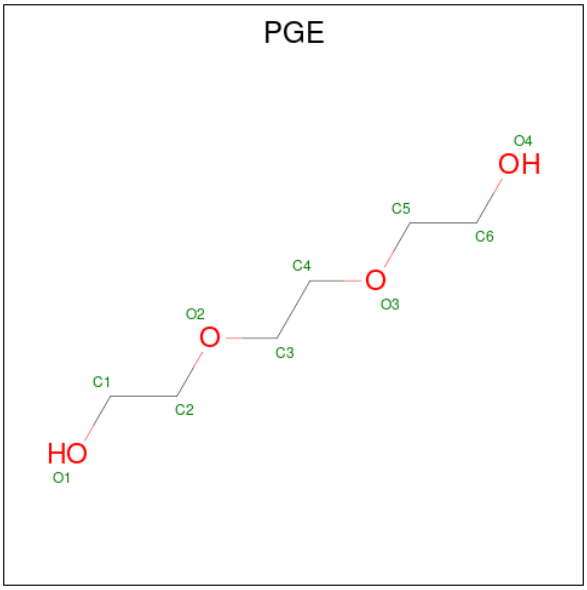
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Zn 1 1	0	0
8	D	1	Total Zn 1 1	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 10 6 4	0	0
9	C	1	Total C O 10 6 4	0	0

- Molecule 10 is water.

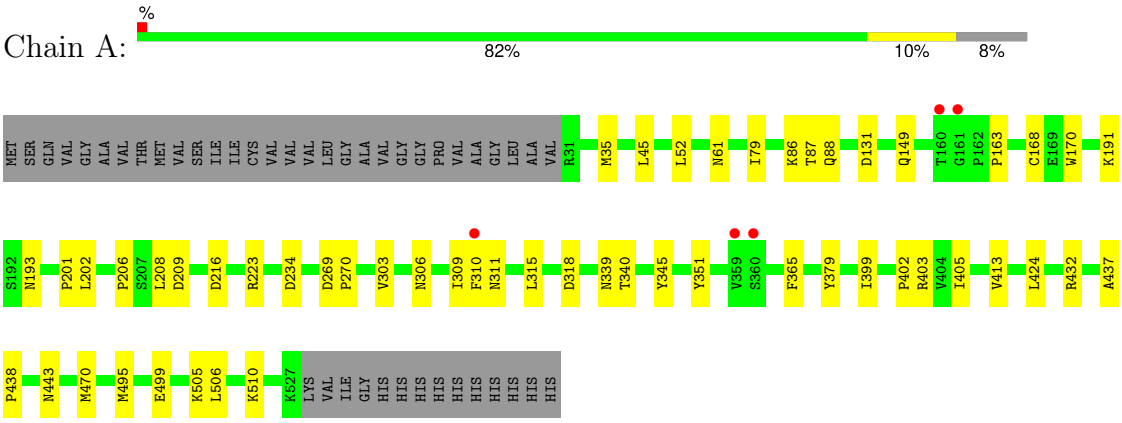
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	494	Total O 494 494	0	0
10	B	545	Total O 545 545	0	0
10	C	517	Total O 517 517	0	0
10	D	440	Total O 440 440	0	0

3 Residue-property plots (i)

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

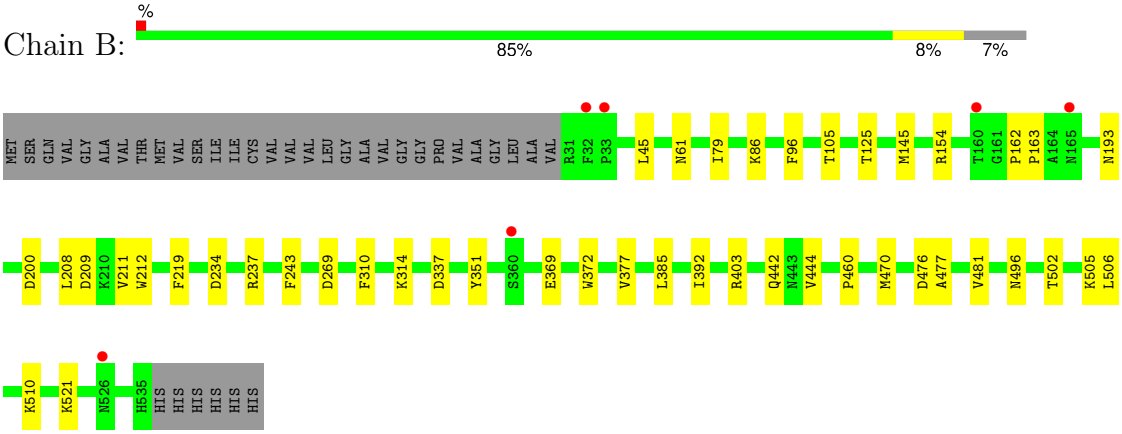
• Molecule 1: Helix pomatia AMP deaminase

Chain A:



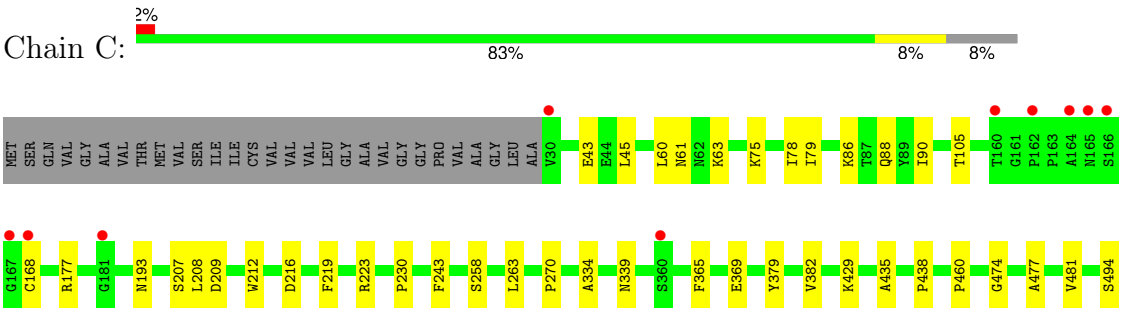
• Molecule 1: Helix pomatia AMP deaminase

Chain B:



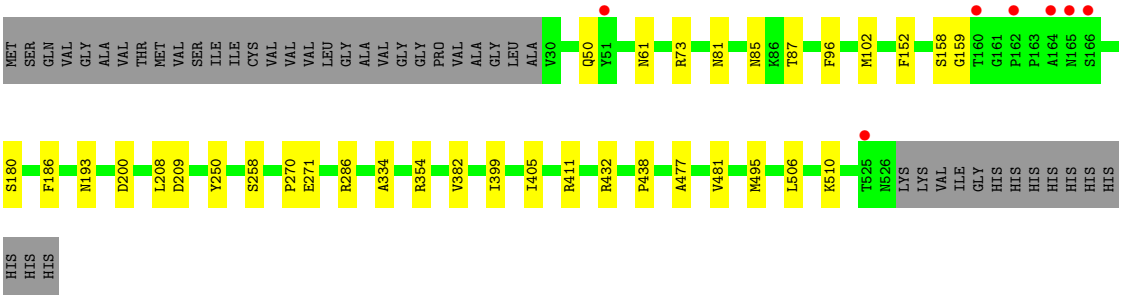
• Molecule 1: Helix pomatia AMP deaminase

Chain C:



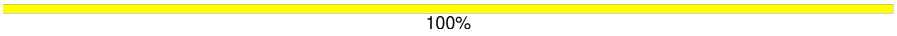
• Molecule 1: Helix pomatia AMP deaminase

Chain D:



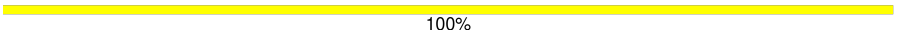
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.23Å 82.43Å 211.42Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	19.95 – 1.75 19.95 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.95-1.75) 91.3 (19.95-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.163 , 0.195 0.163 , 0.195	Depositor DCC
R_{free} test set	13145 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19110	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PGE, EDO, NAG, ZN, BTB, PEG, 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	0.44	0/4143	0.60	0/5626
1	B	0.45	0/4233	0.61	0/5751
1	C	0.46	0/4148	0.61	0/5636
1	D	0.42	0/4121	0.56	0/5600
All	All	0.44	0/16645	0.59	0/22613

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	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	365	PHE	Peptide
1	C	365	PHE	Peptide

5.2 Too-close contacts (i)

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	4025	0	3992	48	0
1	B	4102	0	4061	46	0
1	C	4036	0	3996	49	0
1	D	4012	0	3977	31	0
2	E	29	0	26	0	0
2	F	29	0	26	0	0
3	A	140	0	210	27	0
3	B	152	0	228	18	0
3	C	88	0	132	16	0
3	D	92	0	138	15	0
4	A	42	0	39	0	0
4	B	71	0	67	2	0
4	C	28	0	26	0	0
4	D	56	0	52	0	0
5	A	14	0	19	0	0
5	B	14	0	19	0	0
6	A	24	0	32	6	0
6	B	30	0	40	3	0
6	C	36	0	48	25	0
7	A	21	0	30	8	0
7	B	21	0	30	5	0
7	C	7	0	10	4	0
7	D	21	0	30	6	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	10	0	14	8	0
9	C	10	0	14	5	0
10	A	494	0	0	5	0
10	B	545	0	0	8	0
10	C	517	0	0	5	0
10	D	440	0	0	7	0
All	All	19110	0	17256	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 196 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD12	3:A:605:EDO:H11	1.50	0.94
1:B:212:TRP:HH2	9:B:643:PGE:H5	1.32	0.91
7:A:646:PEG:H31	1:D:432:ARG:HH22	1.35	0.88
1:B:79:ILE:HD11	6:B:651:GOL:H31	1.57	0.87
7:B:646:PEG:H41	1:C:208:LEU:HD23	1.54	0.87

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/541 (93%)	486 (97%)	16 (3%)	0	100	100
1	B	513/541 (95%)	493 (96%)	20 (4%)	0	100	100
1	C	503/541 (93%)	489 (97%)	14 (3%)	0	100	100
1	D	499/541 (92%)	483 (97%)	16 (3%)	0	100	100
All	All	2017/2164 (93%)	1951 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	446/474 (94%)	445 (100%)	1 (0%)	92	90
1	B	455/474 (96%)	453 (100%)	2 (0%)	89	86
1	C	447/474 (94%)	445 (100%)	2 (0%)	89	86
1	D	444/474 (94%)	443 (100%)	1 (0%)	92	90
All	All	1792/1896 (94%)	1786 (100%)	6 (0%)	91	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	168	CYS
1	C	193	ASN
1	D	193	ASN
1	B	193	ASN
1	A	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	151	ASN
1	D	355	GLN
1	D	484	GLN
1	D	373	GLN
1	B	443	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	1,2	14,14,15	0.68	0	17,19,21	1.46	2 (11%)
2	NAG	E	2	2	15,15,15	0.51	0	21,21,21	1.98	4 (19%)
2	NAG	F	1	1,2	14,14,15	0.72	0	17,19,21	1.19	2 (11%)
2	NAG	F	2	2	15,15,15	0.61	0	21,21,21	2.13	8 (38%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/26/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	NAG	C1-C2-C3	5.82	118.48	110.54
2	E	2	NAG	C1-O5-C5	4.83	123.00	113.65
2	F	2	NAG	C1-O5-C5	4.20	121.78	113.65
2	E	2	NAG	C1-C2-C3	4.17	116.22	110.54
2	E	2	NAG	O5-C1-C2	3.80	113.34	109.52

There are no chirality outliers.

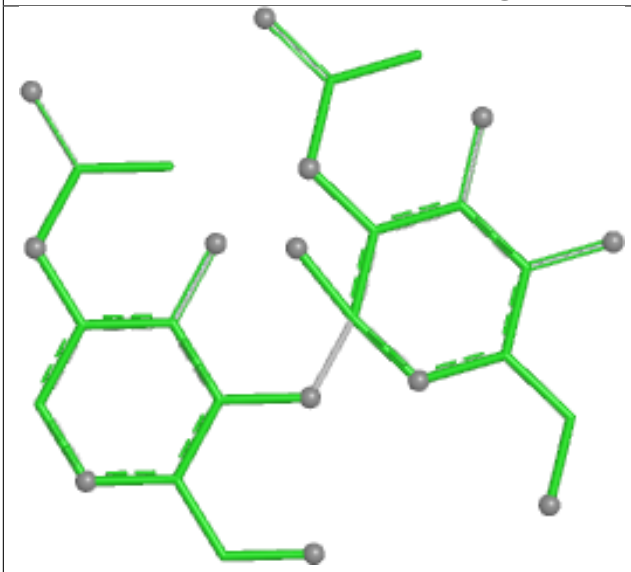
There are no torsion outliers.

There are no ring outliers.

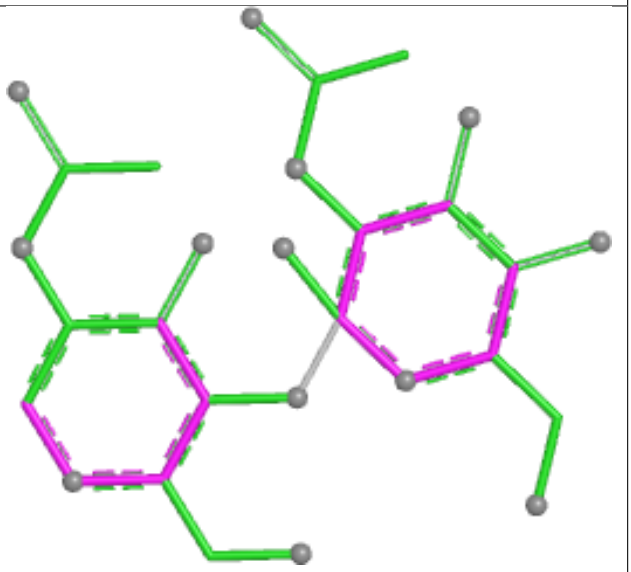
No monomer is involved in short contacts.

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

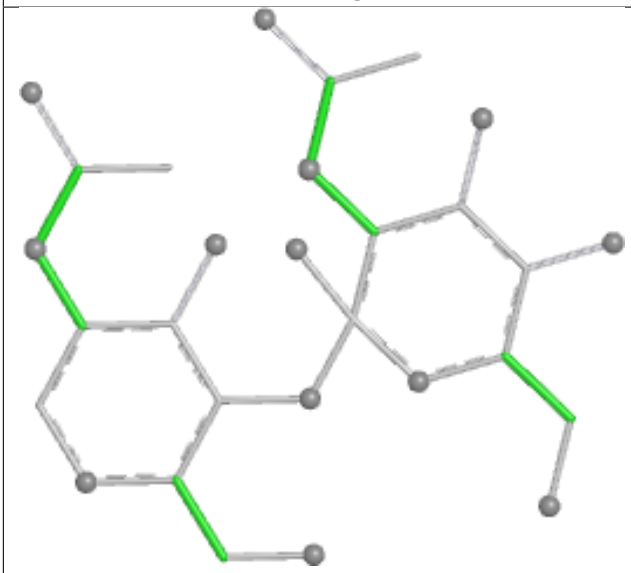
Oligosaccharide Chain E



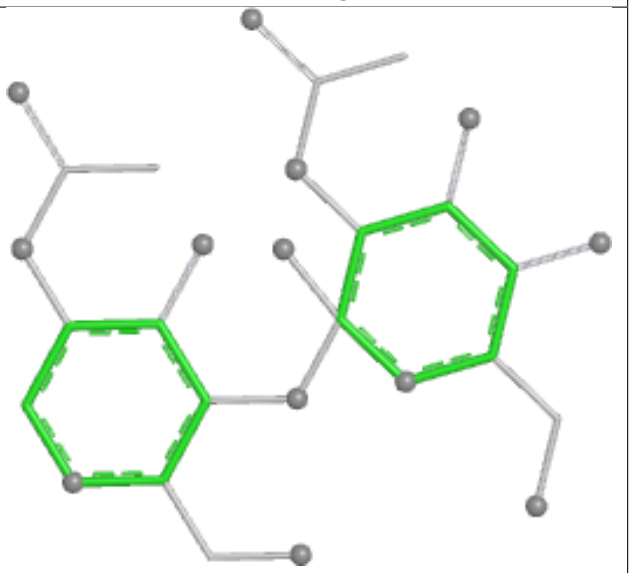
Bond lengths



Bond angles

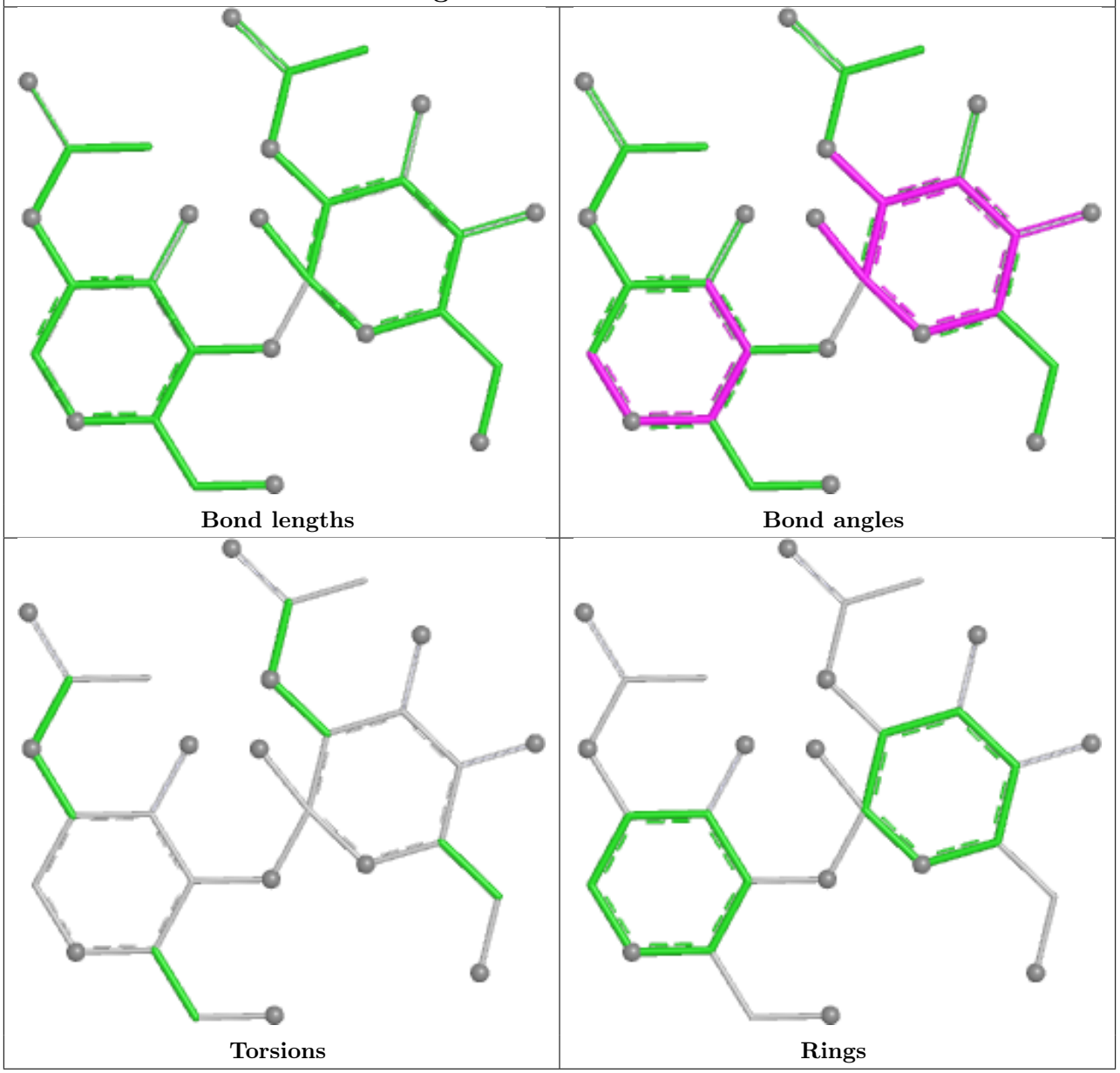


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 165 ligands modelled in this entry, 4 are monoatomic - leaving 161 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	$\#\|Z\|>2$
9	PGE	C	625	-	9,9,9	0.49	0	8,8,8	0.95	0
6	GOL	C	601	-	5,5,5	0.32	0	5,5,5	0.48	0
3	EDO	C	633	-	3,3,3	0.27	0	2,2,2	0.28	0
7	PEG	B	644	-	6,6,6	0.21	0	5,5,5	0.41	0
3	EDO	A	627	-	3,3,3	0.16	0	2,2,2	0.37	0
3	EDO	C	622	-	3,3,3	0.26	0	2,2,2	0.23	0
3	EDO	B	634	-	3,3,3	0.23	0	2,2,2	0.33	0
3	EDO	C	608	-	3,3,3	0.30	0	2,2,2	0.80	0
3	EDO	D	609	-	3,3,3	0.32	0	2,2,2	0.42	0
3	EDO	B	653	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	C	621	-	3,3,3	0.22	0	2,2,2	0.12	0
4	NAG	B	604	1	14,14,15	0.79	1 (7%)	17,19,21	2.18	4 (23%)
3	EDO	D	629	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	D	622	-	3,3,3	0.21	0	2,2,2	0.31	0
3	EDO	B	602	-	3,3,3	0.27	0	2,2,2	0.23	0
3	EDO	D	625	-	3,3,3	0.26	0	2,2,2	0.17	0
3	EDO	B	617	-	3,3,3	0.27	0	2,2,2	0.13	0
3	EDO	C	619	-	3,3,3	0.28	0	2,2,2	0.16	0
3	EDO	C	613	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	A	609	-	3,3,3	0.23	0	2,2,2	0.42	0
3	EDO	A	617	-	3,3,3	0.24	0	2,2,2	0.30	0
6	GOL	A	623	-	5,5,5	0.29	0	5,5,5	0.22	0
3	EDO	B	632	-	3,3,3	0.24	0	2,2,2	0.47	0
3	EDO	B	636	-	3,3,3	0.26	0	2,2,2	0.14	0
3	EDO	A	625	-	3,3,3	0.22	0	2,2,2	0.41	0
3	EDO	C	612	-	3,3,3	0.15	0	2,2,2	0.22	0
3	EDO	A	632	-	3,3,3	0.27	0	2,2,2	0.18	0
4	NAG	B	606	1	14,14,15	0.72	0	17,19,21	1.20	2 (11%)
7	PEG	D	614	-	6,6,6	0.27	0	5,5,5	0.35	0
4	NAG	D	603	1	14,14,15	0.73	0	17,19,21	1.14	2 (11%)
3	EDO	B	640	-	3,3,3	0.31	0	2,2,2	0.12	0
3	EDO	A	610	-	3,3,3	0.23	0	2,2,2	0.32	0
3	EDO	B	622	-	3,3,3	0.26	0	2,2,2	0.06	0
3	EDO	B	649	-	3,3,3	0.23	0	2,2,2	0.28	0
7	PEG	A	636	-	6,6,6	0.26	0	5,5,5	0.70	0
3	EDO	B	642	-	3,3,3	0.38	0	2,2,2	0.32	0
3	EDO	D	621	-	3,3,3	0.25	0	2,2,2	0.28	0
3	EDO	C	609	-	3,3,3	0.29	0	2,2,2	0.35	0
3	EDO	B	620	-	3,3,3	0.25	0	2,2,2	0.41	0
3	EDO	C	604	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	A	644	-	3,3,3	0.25	0	2,2,2	0.21	0
7	PEG	B	641	-	6,6,6	0.25	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	617	-	3,3,3	0.26	0	2,2,2	0.38	0
3	EDO	B	609	-	3,3,3	0.30	0	2,2,2	0.25	0
6	GOL	B	630	-	5,5,5	0.42	0	5,5,5	1.01	0
3	EDO	A	601	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	A	640	-	3,3,3	0.26	0	2,2,2	0.19	0
6	GOL	A	630	-	5,5,5	0.32	0	5,5,5	0.42	0
3	EDO	B	645	-	3,3,3	0.30	0	2,2,2	0.13	0
3	EDO	B	625	-	3,3,3	0.27	0	2,2,2	0.13	0
3	EDO	B	618	-	3,3,3	0.27	0	2,2,2	0.17	0
3	EDO	B	626	-	3,3,3	0.27	0	2,2,2	0.09	0
3	EDO	B	637	-	3,3,3	0.29	0	2,2,2	0.22	0
3	EDO	B	603	-	3,3,3	0.27	0	2,2,2	0.74	0
3	EDO	A	643	-	3,3,3	0.23	0	2,2,2	0.16	0
3	EDO	A	619	-	3,3,3	0.28	0	2,2,2	0.13	0
3	EDO	B	611	-	3,3,3	0.30	0	2,2,2	0.19	0
4	NAG	D	602	1	14,14,15	0.74	0	17,19,21	1.11	2 (11%)
3	EDO	C	616	-	3,3,3	0.24	0	2,2,2	0.48	0
6	GOL	C	631	-	5,5,5	0.45	0	5,5,5	1.39	1 (20%)
3	EDO	A	612	-	3,3,3	0.33	0	2,2,2	0.32	0
7	PEG	D	617	-	6,6,6	0.28	0	5,5,5	0.38	0
3	EDO	D	619	-	3,3,3	0.27	0	2,2,2	0.30	0
3	EDO	A	621	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	D	623	-	3,3,3	0.25	0	2,2,2	0.30	0
4	NAG	B	607	1	14,14,15	0.77	0	17,19,21	1.10	1 (5%)
6	GOL	B	601	-	5,5,5	0.37	0	5,5,5	0.28	0
3	EDO	A	614	-	3,3,3	0.23	0	2,2,2	0.12	0
3	EDO	A	638	-	3,3,3	0.28	0	2,2,2	0.21	0
4	NAG	C	606	1	14,14,15	0.78	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	D	604	1	14,14,15	0.86	0	17,19,21	1.37	2 (11%)
3	EDO	A	613	-	3,3,3	0.26	0	2,2,2	0.52	0
6	GOL	A	645	-	5,5,5	0.34	0	5,5,5	0.83	0
6	GOL	B	635	-	5,5,5	0.17	0	5,5,5	0.39	0
3	EDO	D	627	-	3,3,3	0.25	0	2,2,2	0.38	0
3	EDO	A	618	-	3,3,3	0.28	0	2,2,2	0.16	0
6	GOL	A	634	-	5,5,5	0.39	0	5,5,5	0.50	0
3	EDO	C	629	-	3,3,3	0.29	0	2,2,2	0.03	0
3	EDO	C	623	-	3,3,3	0.22	0	2,2,2	0.65	0
3	EDO	A	637	-	3,3,3	0.26	0	2,2,2	0.20	0
3	EDO	B	633	-	3,3,3	0.27	0	2,2,2	0.22	0
3	EDO	C	618	-	3,3,3	0.27	0	2,2,2	0.26	0
3	EDO	B	631	-	3,3,3	0.30	0	2,2,2	0.43	0
3	EDO	D	610	-	3,3,3	0.33	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	607	-	3,3,3	0.35	0	2,2,2	0.14	0
3	EDO	D	601	-	3,3,3	0.24	0	2,2,2	0.21	0
3	EDO	A	624	-	3,3,3	0.28	0	2,2,2	0.12	0
3	EDO	A	635	-	3,3,3	0.25	0	2,2,2	0.29	0
3	EDO	A	642	-	3,3,3	0.26	0	2,2,2	0.45	0
6	GOL	C	602	-	5,5,5	0.47	0	5,5,5	0.57	0
3	EDO	B	612	-	3,3,3	0.27	0	2,2,2	0.18	0
3	EDO	B	628	-	3,3,3	0.24	0	2,2,2	0.17	0
3	EDO	B	629	-	3,3,3	0.22	0	2,2,2	0.32	0
3	EDO	D	607	-	3,3,3	0.27	0	2,2,2	0.28	0
3	EDO	A	639	-	3,3,3	0.30	0	2,2,2	0.24	0
3	EDO	B	616	-	3,3,3	0.25	0	2,2,2	0.20	0
3	EDO	B	614	-	3,3,3	0.23	0	2,2,2	0.31	0
7	PEG	B	646	-	6,6,6	0.22	0	5,5,5	0.88	0
3	EDO	D	612	-	3,3,3	0.22	0	2,2,2	0.50	0
3	EDO	C	614	-	3,3,3	0.24	0	2,2,2	0.17	0
7	PEG	A	646	-	6,6,6	0.34	0	5,5,5	0.67	0
4	NAG	A	604	1	14,14,15	0.73	0	17,19,21	1.17	1 (5%)
7	PEG	A	626	-	6,6,6	0.22	0	5,5,5	0.46	0
3	EDO	B	647	-	3,3,3	0.24	0	2,2,2	0.51	0
6	GOL	B	627	-	5,5,5	0.26	0	5,5,5	0.63	0
3	EDO	B	621	-	3,3,3	0.22	0	2,2,2	0.47	0
3	EDO	A	616	-	3,3,3	0.24	0	2,2,2	0.26	0
3	EDO	D	608	-	3,3,3	0.23	0	2,2,2	0.50	0
3	EDO	B	654	-	3,3,3	0.28	0	2,2,2	0.41	0
3	EDO	B	615	-	3,3,3	0.22	0	2,2,2	0.61	0
4	NAG	A	602	1	14,14,15	1.02	2 (14%)	17,19,21	1.83	4 (23%)
3	EDO	D	618	-	3,3,3	0.29	0	2,2,2	0.31	0
7	PEG	C	627	-	6,6,6	0.36	0	5,5,5	1.04	0
9	PGE	B	643	-	9,9,9	0.42	0	8,8,8	1.26	1 (12%)
3	EDO	D	626	-	3,3,3	0.27	0	2,2,2	0.61	0
3	EDO	D	616	-	3,3,3	0.23	0	2,2,2	0.35	0
3	EDO	A	631	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	A	633	-	3,3,3	0.22	0	2,2,2	0.73	0
3	EDO	A	629	-	3,3,3	0.29	0	2,2,2	0.32	0
3	EDO	D	606	-	3,3,3	0.24	0	2,2,2	0.47	0
3	EDO	D	613	-	3,3,3	0.17	0	2,2,2	0.48	0
3	EDO	B	610	-	3,3,3	0.19	0	2,2,2	0.42	0
3	EDO	A	605	-	3,3,3	0.37	0	2,2,2	0.47	0
3	EDO	A	641	-	3,3,3	0.27	0	2,2,2	0.31	0
3	EDO	B	638	-	3,3,3	0.24	0	2,2,2	0.38	0
3	EDO	C	628	-	3,3,3	0.28	0	2,2,2	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PEG	D	624	-	6,6,6	0.27	0	5,5,5	0.43	0
5	BTB	B	613	-	13,13,13	0.99	0	7,16,16	0.86	0
6	GOL	B	651	-	5,5,5	0.48	0	5,5,5	0.96	0
6	GOL	C	626	-	5,5,5	0.52	0	5,5,5	1.30	0
3	EDO	A	606	-	3,3,3	0.34	0	2,2,2	0.39	0
3	EDO	B	623	-	3,3,3	0.28	0	2,2,2	0.35	0
3	EDO	C	620	-	3,3,3	0.19	0	2,2,2	0.59	0
4	NAG	B	605	1	14,14,15	0.81	0	17,19,21	1.07	2 (11%)
3	EDO	D	628	-	3,3,3	0.26	0	2,2,2	0.42	0
3	EDO	B	619	-	3,3,3	0.24	0	2,2,2	0.47	0
3	EDO	C	615	-	3,3,3	0.31	0	2,2,2	0.15	0
3	EDO	C	611	-	3,3,3	0.21	0	2,2,2	0.34	0
3	EDO	A	622	-	3,3,3	0.26	0	2,2,2	0.35	0
3	EDO	D	611	-	3,3,3	0.22	0	2,2,2	0.40	0
5	BTB	A	607	-	13,13,13	0.98	1 (7%)	7,16,16	0.84	0
6	GOL	C	624	-	5,5,5	0.61	0	5,5,5	1.87	1 (20%)
3	EDO	A	620	-	3,3,3	0.26	0	2,2,2	0.29	0
3	EDO	B	608	-	3,3,3	0.32	0	2,2,2	0.57	0
3	EDO	A	628	-	3,3,3	0.27	0	2,2,2	0.32	0
4	NAG	B	648	-	15,15,15	0.49	0	21,21,21	2.85	8 (38%)
3	EDO	B	650	-	3,3,3	0.30	0	2,2,2	0.29	0
3	EDO	A	611	-	3,3,3	0.19	0	2,2,2	0.33	0
3	EDO	D	615	-	3,3,3	0.27	0	2,2,2	0.38	0
3	EDO	C	610	-	3,3,3	0.26	0	2,2,2	0.22	0
3	EDO	A	608	-	3,3,3	0.33	0	2,2,2	0.46	0
3	EDO	B	624	-	3,3,3	0.26	0	2,2,2	0.50	0
3	EDO	D	620	-	3,3,3	0.26	0	2,2,2	0.10	0
3	EDO	D	631	-	3,3,3	0.29	0	2,2,2	0.57	0
3	EDO	C	630	-	3,3,3	0.23	0	2,2,2	0.18	0
4	NAG	A	603	1	14,14,15	0.73	0	17,19,21	1.30	2 (11%)
4	NAG	D	605	1	14,14,15	0.78	0	17,19,21	0.94	1 (5%)
6	GOL	C	603	-	5,5,5	1.15	1 (20%)	5,5,5	0.56	0
3	EDO	B	639	-	3,3,3	0.26	0	2,2,2	0.16	0
4	NAG	C	605	1	14,14,15	0.82	1 (7%)	17,19,21	1.11	1 (5%)
3	EDO	A	615	-	3,3,3	0.24	0	2,2,2	0.25	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
9	PGE	C	625	-	-	3/7/7/7	-
6	GOL	C	601	-	-	2/4/4/4	-
3	EDO	C	633	-	-	0/1/1/1	-
7	PEG	B	644	-	-	0/4/4/4	-
3	EDO	A	627	-	-	1/1/1/1	-
3	EDO	C	622	-	-	0/1/1/1	-
3	EDO	B	634	-	-	0/1/1/1	-
3	EDO	C	608	-	-	0/1/1/1	-
3	EDO	D	609	-	-	1/1/1/1	-
3	EDO	B	653	-	-	0/1/1/1	-
3	EDO	C	621	-	-	0/1/1/1	-
4	NAG	B	604	1	-	2/6/23/26	0/1/1/1
3	EDO	D	629	-	-	0/1/1/1	-
3	EDO	D	622	-	-	0/1/1/1	-
3	EDO	B	602	-	-	1/1/1/1	-
3	EDO	D	625	-	-	0/1/1/1	-
3	EDO	B	617	-	-	1/1/1/1	-
3	EDO	C	619	-	-	1/1/1/1	-
3	EDO	C	613	-	-	1/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	A	617	-	-	1/1/1/1	-
6	GOL	A	623	-	-	2/4/4/4	-
3	EDO	B	632	-	-	1/1/1/1	-
3	EDO	B	636	-	-	1/1/1/1	-
3	EDO	A	625	-	-	0/1/1/1	-
3	EDO	C	612	-	-	0/1/1/1	-
3	EDO	A	632	-	-	0/1/1/1	-
4	NAG	B	606	1	-	0/6/23/26	0/1/1/1
7	PEG	D	614	-	-	1/4/4/4	-
4	NAG	D	603	1	-	0/6/23/26	0/1/1/1
3	EDO	B	640	-	-	0/1/1/1	-
3	EDO	A	610	-	-	0/1/1/1	-
3	EDO	B	622	-	-	0/1/1/1	-
3	EDO	B	649	-	-	1/1/1/1	-
7	PEG	A	636	-	-	3/4/4/4	-
3	EDO	B	642	-	-	1/1/1/1	-
3	EDO	D	621	-	-	1/1/1/1	-
3	EDO	C	609	-	-	0/1/1/1	-
3	EDO	B	620	-	-	1/1/1/1	-
3	EDO	C	604	-	-	0/1/1/1	-
3	EDO	A	644	-	-	0/1/1/1	-
7	PEG	B	641	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	617	-	-	1/1/1/1	-
3	EDO	B	609	-	-	0/1/1/1	-
6	GOL	B	630	-	-	2/4/4/4	-
3	EDO	A	601	-	-	0/1/1/1	-
3	EDO	A	640	-	-	1/1/1/1	-
6	GOL	A	630	-	-	0/4/4/4	-
3	EDO	B	645	-	-	1/1/1/1	-
3	EDO	B	625	-	-	1/1/1/1	-
3	EDO	B	618	-	-	0/1/1/1	-
3	EDO	B	626	-	-	1/1/1/1	-
3	EDO	B	637	-	-	1/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	A	643	-	-	0/1/1/1	-
3	EDO	A	619	-	-	1/1/1/1	-
3	EDO	B	611	-	-	0/1/1/1	-
4	NAG	D	602	1	-	0/6/23/26	0/1/1/1
3	EDO	C	616	-	-	0/1/1/1	-
6	GOL	C	631	-	-	2/4/4/4	-
3	EDO	A	612	-	-	0/1/1/1	-
7	PEG	D	617	-	-	2/4/4/4	-
3	EDO	D	619	-	-	0/1/1/1	-
3	EDO	A	621	-	-	0/1/1/1	-
3	EDO	D	623	-	-	0/1/1/1	-
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1
6	GOL	B	601	-	-	4/4/4/4	-
3	EDO	A	614	-	-	1/1/1/1	-
3	EDO	A	638	-	-	0/1/1/1	-
4	NAG	C	606	1	-	0/6/23/26	0/1/1/1
4	NAG	D	604	1	-	0/6/23/26	0/1/1/1
3	EDO	A	613	-	-	1/1/1/1	-
6	GOL	A	645	-	-	2/4/4/4	-
6	GOL	B	635	-	-	4/4/4/4	-
3	EDO	D	627	-	-	1/1/1/1	-
3	EDO	A	618	-	-	1/1/1/1	-
6	GOL	A	634	-	-	2/4/4/4	-
3	EDO	C	629	-	-	0/1/1/1	-
3	EDO	C	623	-	-	1/1/1/1	-
3	EDO	A	637	-	-	0/1/1/1	-
3	EDO	B	633	-	-	0/1/1/1	-
3	EDO	C	618	-	-	1/1/1/1	-
3	EDO	B	631	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	610	-	-	0/1/1/1	-
3	EDO	C	607	-	-	0/1/1/1	-
3	EDO	D	601	-	-	1/1/1/1	-
3	EDO	A	624	-	-	1/1/1/1	-
3	EDO	A	635	-	-	0/1/1/1	-
3	EDO	A	642	-	-	1/1/1/1	-
6	GOL	C	602	-	-	2/4/4/4	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	B	628	-	-	1/1/1/1	-
3	EDO	B	629	-	-	0/1/1/1	-
3	EDO	D	607	-	-	0/1/1/1	-
3	EDO	A	639	-	-	1/1/1/1	-
3	EDO	B	616	-	-	1/1/1/1	-
3	EDO	B	614	-	-	0/1/1/1	-
7	PEG	B	646	-	-	2/4/4/4	-
3	EDO	D	612	-	-	1/1/1/1	-
3	EDO	C	614	-	-	1/1/1/1	-
7	PEG	A	646	-	-	1/4/4/4	-
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	PEG	A	626	-	-	3/4/4/4	-
3	EDO	B	647	-	-	1/1/1/1	-
6	GOL	B	627	-	-	3/4/4/4	-
3	EDO	B	621	-	-	0/1/1/1	-
3	EDO	A	616	-	-	1/1/1/1	-
3	EDO	D	608	-	-	0/1/1/1	-
3	EDO	B	654	-	-	0/1/1/1	-
3	EDO	B	615	-	-	1/1/1/1	-
4	NAG	A	602	1	-	4/6/23/26	0/1/1/1
3	EDO	D	618	-	-	1/1/1/1	-
7	PEG	C	627	-	-	3/4/4/4	-
9	PGE	B	643	-	-	5/7/7/7	-
3	EDO	D	626	-	-	0/1/1/1	-
3	EDO	D	616	-	-	0/1/1/1	-
3	EDO	A	631	-	-	1/1/1/1	-
3	EDO	A	633	-	-	1/1/1/1	-
3	EDO	A	629	-	-	0/1/1/1	-
3	EDO	D	606	-	-	0/1/1/1	-
3	EDO	D	613	-	-	0/1/1/1	-
3	EDO	B	610	-	-	0/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	641	-	-	0/1/1/1	-
3	EDO	B	638	-	-	0/1/1/1	-
3	EDO	C	628	-	-	1/1/1/1	-
7	PEG	D	624	-	-	3/4/4/4	-
5	BTB	B	613	-	-	1/21/21/21	-
6	GOL	B	651	-	-	0/4/4/4	-
6	GOL	C	626	-	-	1/4/4/4	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	B	623	-	-	1/1/1/1	-
3	EDO	C	620	-	-	0/1/1/1	-
4	NAG	B	605	1	-	0/6/23/26	0/1/1/1
3	EDO	D	628	-	-	1/1/1/1	-
3	EDO	B	619	-	-	1/1/1/1	-
3	EDO	C	615	-	-	1/1/1/1	-
3	EDO	C	611	-	-	1/1/1/1	-
3	EDO	A	622	-	-	0/1/1/1	-
3	EDO	D	611	-	-	1/1/1/1	-
5	BTB	A	607	-	-	4/21/21/21	-
6	GOL	C	624	-	-	4/4/4/4	-
3	EDO	A	620	-	-	1/1/1/1	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	A	628	-	-	0/1/1/1	-
4	NAG	B	648	-	-	6/6/26/26	0/1/1/1
3	EDO	B	650	-	-	0/1/1/1	-
3	EDO	A	611	-	-	0/1/1/1	-
3	EDO	D	615	-	-	1/1/1/1	-
3	EDO	C	610	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	B	624	-	-	1/1/1/1	-
3	EDO	D	620	-	-	1/1/1/1	-
3	EDO	D	631	-	-	0/1/1/1	-
3	EDO	C	630	-	-	1/1/1/1	-
4	NAG	A	603	1	-	2/6/23/26	0/1/1/1
4	NAG	D	605	1	-	0/6/23/26	0/1/1/1
6	GOL	C	603	-	-	2/4/4/4	-
3	EDO	B	639	-	-	0/1/1/1	-
4	NAG	C	605	1	-	0/6/23/26	0/1/1/1
3	EDO	A	615	-	-	1/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	NAG	C1-C2	2.50	1.55	1.52
5	A	607	BTB	C3-C2	2.48	1.56	1.53
4	C	605	NAG	C1-C2	2.18	1.55	1.52
6	C	603	GOL	O2-C2	-2.14	1.37	1.43
4	B	604	NAG	C2-N2	-2.06	1.42	1.46

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	648	NAG	C1-C2-N2	7.54	119.46	110.73
4	B	604	NAG	C1-C2-N2	-7.01	99.39	110.43
4	B	648	NAG	C4-C3-C2	5.61	118.58	110.40
4	B	648	NAG	C2-N2-C7	5.18	135.24	123.11
4	A	602	NAG	C1-C2-N2	-4.65	103.10	110.43

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	648	NAG	C1-C2-N2-C7
5	A	607	BTB	O1-C1-C2-C3
5	A	607	BTB	N-C2-C3-O3
6	A	645	GOL	O1-C1-C2-C3
6	B	601	GOL	O1-C1-C2-O2

There are no ring outliers.

74 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	625	PGE	5	0
6	C	601	GOL	1	0
7	B	644	PEG	1	0
3	A	627	EDO	5	0
3	B	653	EDO	1	0
3	C	621	EDO	3	0
3	D	622	EDO	3	0
3	D	625	EDO	1	0
3	C	619	EDO	1	0
3	A	609	EDO	1	0
6	A	623	GOL	1	0
3	A	625	EDO	1	0
4	B	606	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	614	PEG	2	0
3	B	640	EDO	1	0
3	B	622	EDO	1	0
7	A	636	PEG	2	0
3	B	642	EDO	2	0
3	D	621	EDO	1	0
3	B	620	EDO	1	0
3	C	604	EDO	1	0
7	B	641	PEG	1	0
3	A	601	EDO	1	0
3	B	645	EDO	1	0
3	B	618	EDO	1	0
3	A	643	EDO	3	0
6	C	631	GOL	5	0
3	A	612	EDO	1	0
7	D	617	PEG	2	0
3	D	619	EDO	1	0
4	B	607	NAG	1	0
3	A	638	EDO	1	0
6	A	645	GOL	3	0
3	D	627	EDO	1	0
3	A	618	EDO	1	0
6	A	634	GOL	2	0
3	C	629	EDO	1	0
3	C	623	EDO	1	0
3	A	637	EDO	1	0
3	B	633	EDO	1	0
3	C	618	EDO	1	0
3	A	624	EDO	7	0
6	C	602	GOL	4	0
3	B	612	EDO	1	0
3	B	628	EDO	2	0
3	B	616	EDO	3	0
7	B	646	PEG	3	0
3	C	614	EDO	2	0
7	A	646	PEG	5	0
7	A	626	PEG	1	0
3	A	616	EDO	1	0
3	B	654	EDO	1	0
3	D	618	EDO	1	0
7	C	627	PEG	4	0
9	B	643	PGE	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	626	EDO	4	0
3	A	631	EDO	1	0
3	A	633	EDO	1	0
3	B	610	EDO	1	0
3	A	605	EDO	3	0
3	C	628	EDO	1	0
7	D	624	PEG	2	0
6	B	651	GOL	3	0
6	C	626	GOL	1	0
3	D	628	EDO	1	0
3	C	615	EDO	1	0
3	D	611	EDO	1	0
6	C	624	GOL	4	0
4	B	648	NAG	1	0
3	B	650	EDO	1	0
3	A	611	EDO	1	0
3	D	615	EDO	1	0
3	C	630	EDO	4	0
6	C	603	GOL	12	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

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, 95^{th} 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%)	-0.53	5 (1%)	79	84	9, 21, 41, 63	6 (1%)
1	B	505/541 (93%)	-0.58	6 (1%)	76	82	11, 20, 38, 61	10 (1%)
1	C	496/541 (91%)	-0.55	10 (2%)	64	71	8, 19, 38, 72	9 (1%)
1	D	497/541 (91%)	-0.26	7 (1%)	73	79	14, 25, 40, 91	4 (0%)
All	All	1995/2164 (92%)	-0.48	28 (1%)	73	79	8, 21, 40, 91	29 (1%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	PRO	4.0
1	C	166	SER	3.8
1	C	167	GLY	3.6
1	C	160	THR	3.6
1	A	160	THR	3.5

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	2	15/15	0.65	0.16	47,61,75,77	0
2	NAG	E	2	15/15	0.68	0.15	45,60,73,74	0

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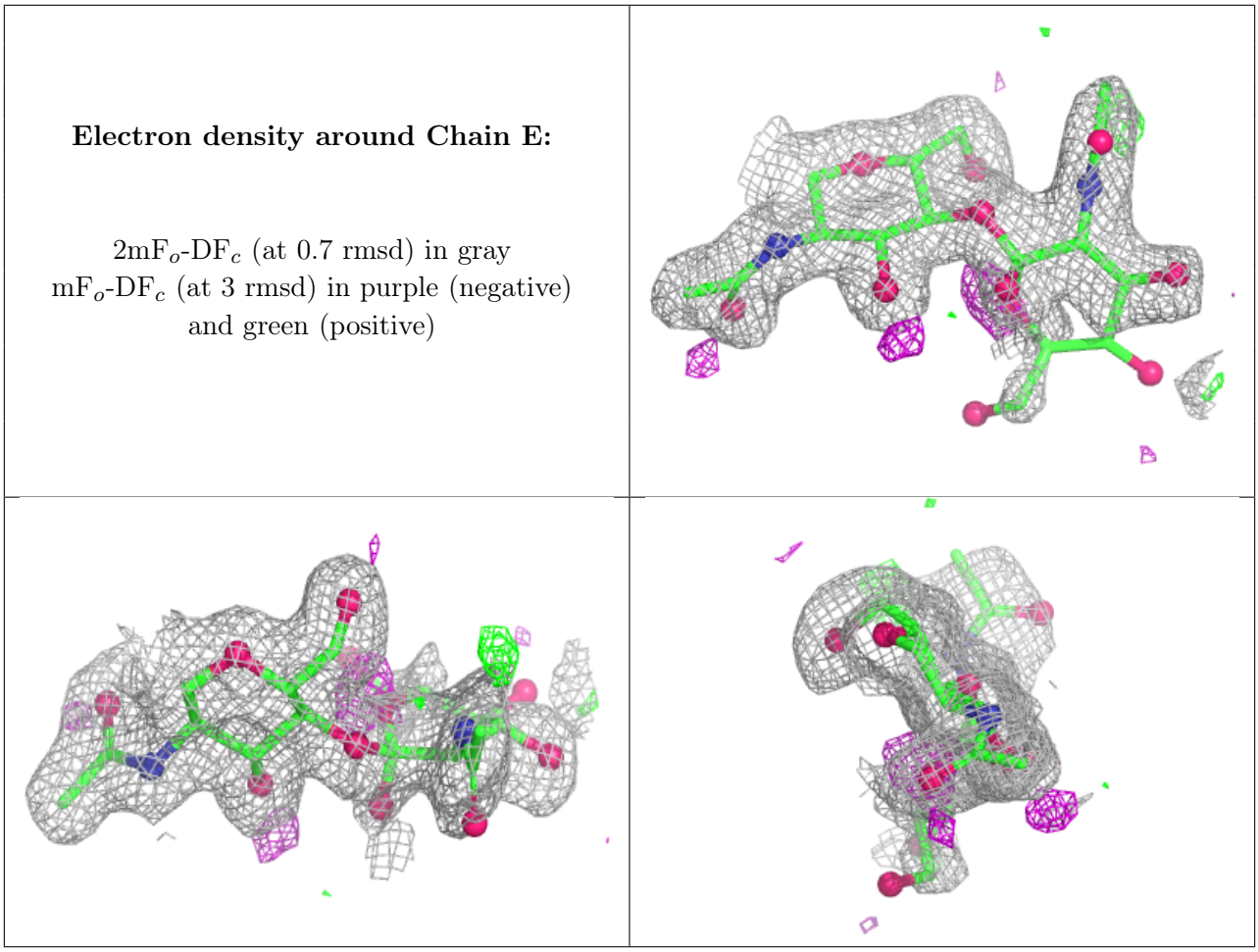
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	1	14/15	0.94	0.08	23,30,38,39	0
2	NAG	E	1	14/15	0.96	0.07	20,25,31,37	0

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

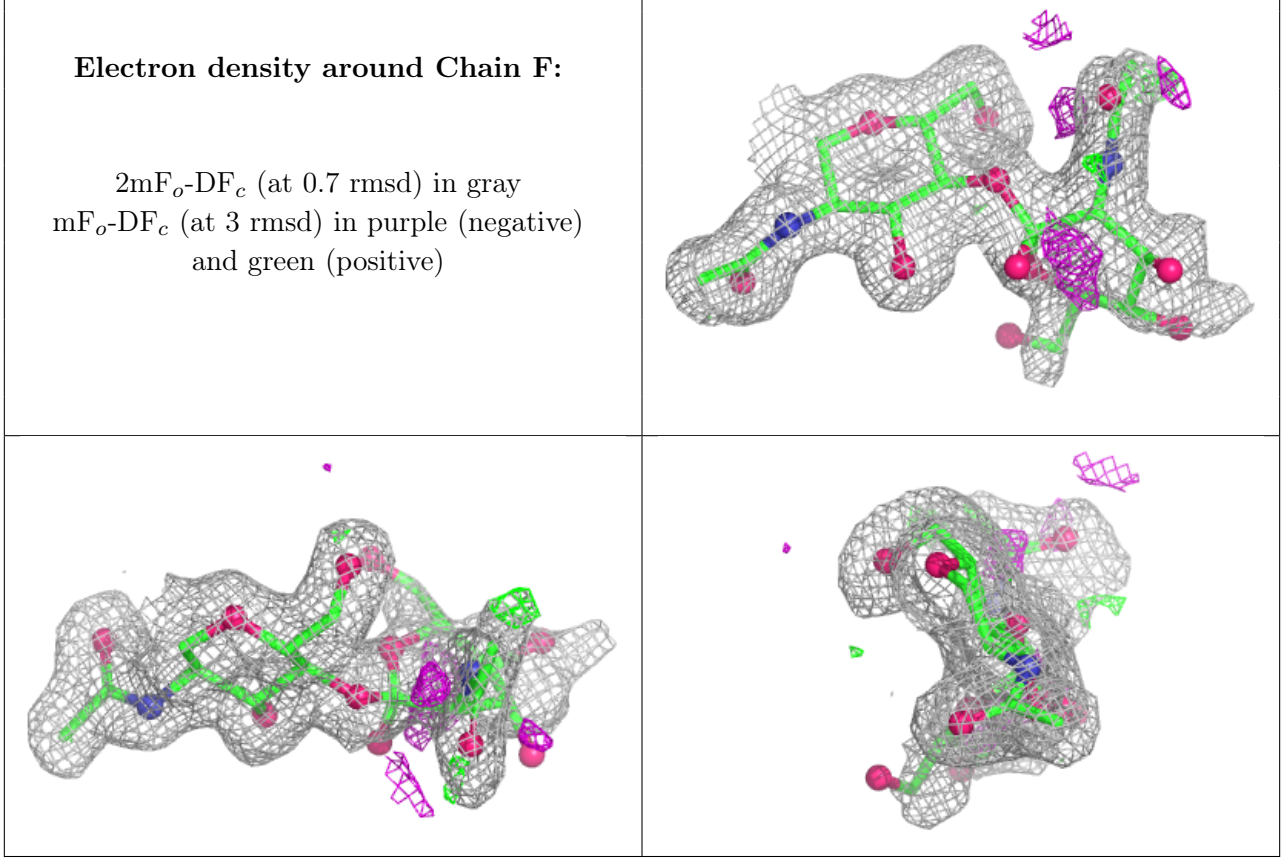
Electron density around Chain E:

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



Electron density around Chain F:

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



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, 95^{th} 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
4	NAG	B	648	15/15	0.64	0.19	41,68,90,91	0
3	EDO	D	625	4/4	0.66	0.15	51,62,62,64	0
3	EDO	B	638	4/4	0.71	0.16	56,57,58,62	0
3	EDO	C	613	4/4	0.71	0.13	46,48,54,63	0
3	EDO	C	619	4/4	0.72	0.21	43,45,48,55	0
7	PEG	A	626	7/7	0.72	0.17	46,54,58,67	0
4	NAG	A	604	14/15	0.73	0.12	34,59,73,78	0
3	EDO	B	650	4/4	0.73	0.20	47,50,67,76	0
3	EDO	C	617	4/4	0.73	0.16	37,38,47,50	0
3	EDO	D	613	4/4	0.74	0.19	40,46,48,48	0
3	EDO	A	640	4/4	0.74	0.14	50,57,58,59	0
3	EDO	A	620	4/4	0.74	0.17	41,44,48,59	0
3	EDO	A	622	4/4	0.74	0.20	37,43,44,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	601	6/6	0.74	0.12	54,65,68,73	0
3	EDO	C	633	4/4	0.74	0.17	53,62,64,64	0
7	PEG	B	641	7/7	0.74	0.18	52,57,69,74	0
3	EDO	B	624	4/4	0.75	0.19	40,43,51,55	0
3	EDO	A	617	4/4	0.75	0.19	35,45,47,48	0
7	PEG	D	617	7/7	0.75	0.15	36,47,57,60	0
3	EDO	D	612	4/4	0.76	0.21	46,48,55,59	0
3	EDO	B	647	4/4	0.77	0.18	39,46,54,58	0
3	EDO	D	631	4/4	0.77	0.17	40,44,55,64	0
3	EDO	B	633	4/4	0.77	0.14	57,57,59,62	0
3	EDO	D	623	4/4	0.77	0.12	51,54,56,57	0
6	GOL	A	630	6/6	0.78	0.12	64,67,69,76	0
3	EDO	C	615	4/4	0.78	0.20	36,41,49,58	0
3	EDO	A	615	4/4	0.78	0.19	41,44,53,55	0
3	EDO	B	649	4/4	0.78	0.15	52,53,55,55	0
7	PEG	B	644	7/7	0.78	0.16	43,52,57,58	0
3	EDO	C	622	4/4	0.78	0.13	52,58,62,62	0
4	NAG	B	607	14/15	0.79	0.12	33,50,70,71	0
3	EDO	B	639	4/4	0.79	0.22	48,50,51,54	0
3	EDO	B	640	4/4	0.79	0.19	33,44,44,46	0
3	EDO	C	623	4/4	0.79	0.15	40,44,48,49	0
3	EDO	D	627	4/4	0.79	0.18	41,44,46,68	0
3	EDO	B	620	4/4	0.79	0.18	33,42,45,46	0
3	EDO	B	632	4/4	0.79	0.23	39,44,52,56	0
4	NAG	B	604	14/15	0.79	0.13	31,42,57,62	0
3	EDO	D	607	4/4	0.80	0.16	41,47,49,50	0
3	EDO	C	616	4/4	0.80	0.15	36,42,43,50	0
3	EDO	A	624	4/4	0.80	0.25	29,43,47,55	0
4	NAG	D	605	14/15	0.80	0.12	38,54,65,76	0
3	EDO	A	642	4/4	0.80	0.22	43,47,48,51	0
3	EDO	A	613	4/4	0.81	0.15	38,38,42,46	0
3	EDO	B	602	4/4	0.81	0.15	50,50,51,54	0
6	GOL	B	630	6/6	0.81	0.14	42,44,47,52	0
3	EDO	B	626	4/4	0.81	0.23	36,43,47,56	0
3	EDO	D	608	4/4	0.82	0.14	33,38,50,51	0
6	GOL	C	631	6/6	0.82	0.12	39,42,45,52	0
3	EDO	B	617	4/4	0.82	0.12	34,35,44,49	0
3	EDO	A	621	4/4	0.82	0.13	43,51,53,65	0
3	EDO	D	620	4/4	0.82	0.12	45,53,55,60	0
3	EDO	C	611	4/4	0.82	0.13	41,41,42,46	0
9	PGE	C	625	10/10	0.82	0.14	21,33,44,45	0
6	GOL	B	601	6/6	0.83	0.13	48,51,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	632	4/4	0.83	0.14	43,46,56,58	0
4	NAG	A	602	14/15	0.83	0.12	25,40,51,55	0
3	EDO	A	639	4/4	0.83	0.14	33,33,41,54	0
3	EDO	C	629	4/4	0.83	0.17	41,42,44,45	0
3	EDO	B	619	4/4	0.83	0.21	51,52,53,55	0
3	EDO	A	605	4/4	0.83	0.19	37,37,44,47	0
3	EDO	A	631	4/4	0.83	0.14	35,44,45,55	0
7	PEG	D	624	7/7	0.83	0.14	34,47,55,66	0
3	EDO	D	628	4/4	0.83	0.15	35,49,54,61	0
3	EDO	A	609	4/4	0.84	0.16	39,43,47,48	0
6	GOL	B	635	6/6	0.84	0.13	41,43,48,50	0
3	EDO	C	628	4/4	0.84	0.19	38,41,49,51	0
3	EDO	B	625	4/4	0.84	0.13	41,44,45,50	0
3	EDO	A	619	4/4	0.84	0.14	40,41,47,47	0
7	PEG	A	646	7/7	0.84	0.15	25,28,40,50	0
3	EDO	A	637	4/4	0.84	0.16	47,47,52,53	0
4	NAG	C	605	14/15	0.84	0.12	26,29,35,35	0
3	EDO	A	616	4/4	0.84	0.18	38,39,48,49	0
3	EDO	D	629	4/4	0.84	0.13	45,57,57,61	0
3	EDO	A	625	4/4	0.84	0.14	42,46,50,51	0
3	EDO	B	645	4/4	0.85	0.18	43,44,48,48	0
3	EDO	B	616	4/4	0.85	0.16	30,42,49,54	0
3	EDO	A	643	4/4	0.85	0.17	36,39,40,64	0
3	EDO	A	627	4/4	0.85	0.41	33,33,40,43	0
3	EDO	D	615	4/4	0.85	0.20	33,43,47,50	0
4	NAG	C	606	14/15	0.85	0.10	24,42,53,57	0
4	NAG	D	603	14/15	0.85	0.10	27,41,60,69	0
3	EDO	D	619	4/4	0.85	0.15	31,42,43,59	0
7	PEG	B	646	7/7	0.85	0.14	23,33,38,40	0
3	EDO	B	603	4/4	0.85	0.14	28,31,38,44	0
6	GOL	A	634	6/6	0.85	0.12	35,46,47,53	0
9	PGE	B	643	10/10	0.85	0.14	26,37,45,47	0
4	NAG	A	603	14/15	0.85	0.11	33,48,73,76	0
3	EDO	D	611	4/4	0.86	0.13	35,47,47,52	0
3	EDO	B	612	4/4	0.86	0.14	37,41,44,44	0
7	PEG	A	636	7/7	0.86	0.12	34,43,48,52	0
3	EDO	B	642	4/4	0.86	0.22	31,32,34,47	0
3	EDO	B	622	4/4	0.86	0.17	38,39,40,44	0
3	EDO	D	618	4/4	0.86	0.12	31,44,44,49	0
3	EDO	C	630	4/4	0.86	0.16	35,41,46,54	0
7	PEG	D	614	7/7	0.86	0.13	30,35,52,61	0
3	EDO	A	628	4/4	0.86	0.17	35,40,49,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	621	4/4	0.86	0.17	30,34,41,42	0
3	EDO	C	614	4/4	0.86	0.14	30,37,47,48	0
3	EDO	D	626	4/4	0.86	0.27	36,37,37,38	0
3	EDO	A	611	4/4	0.87	0.16	33,40,42,50	0
3	EDO	B	629	4/4	0.87	0.12	37,39,43,51	0
6	GOL	A	623	6/6	0.87	0.11	38,44,50,62	0
3	EDO	A	629	4/4	0.87	0.14	26,29,34,42	0
3	EDO	C	610	4/4	0.87	0.16	39,47,50,51	0
3	EDO	B	621	4/4	0.87	0.14	38,41,43,66	0
3	EDO	B	636	4/4	0.87	0.14	42,48,49,56	0
3	EDO	B	628	4/4	0.88	0.17	36,47,53,64	0
3	EDO	C	604	4/4	0.88	0.20	34,44,50,74	0
6	GOL	C	626	6/6	0.88	0.13	29,37,38,58	0
3	EDO	D	616	4/4	0.88	0.14	38,40,45,46	0
3	EDO	A	641	4/4	0.88	0.10	38,39,49,51	0
6	GOL	C	624	6/6	0.89	0.17	21,29,32,37	0
6	GOL	A	645	6/6	0.89	0.15	29,34,37,37	0
7	PEG	C	627	7/7	0.89	0.11	24,28,44,49	0
3	EDO	B	653	4/4	0.89	0.20	36,38,44,53	0
3	EDO	C	618	4/4	0.89	0.14	29,36,39,55	0
4	NAG	B	605	14/15	0.89	0.10	27,40,57,69	0
3	EDO	D	622	4/4	0.89	0.12	36,45,49,57	0
6	GOL	C	603	6/6	0.89	0.16	23,36,43,48	0
3	EDO	C	620	4/4	0.90	0.11	36,40,48,52	0
6	GOL	B	651	6/6	0.90	0.21	24,31,35,42	0
5	BTB	A	607	14/14	0.90	0.10	26,34,39,42	0
6	GOL	C	602	6/6	0.90	0.23	25,32,41,49	0
3	EDO	B	637	4/4	0.90	0.14	25,31,33,50	0
3	EDO	B	611	4/4	0.90	0.10	37,37,39,41	0
3	EDO	A	614	4/4	0.90	0.13	26,30,35,49	0
3	EDO	B	615	4/4	0.90	0.12	26,26,33,39	0
4	NAG	D	602	14/15	0.90	0.09	33,37,47,50	0
3	EDO	B	623	4/4	0.90	0.10	36,38,45,51	0
3	EDO	B	618	4/4	0.91	0.12	26,27,35,41	0
3	EDO	B	610	4/4	0.91	0.10	28,34,34,37	0
3	EDO	A	635	4/4	0.91	0.10	39,44,44,58	0
4	NAG	D	604	14/15	0.92	0.08	26,28,35,35	0
3	EDO	D	621	4/4	0.92	0.13	39,44,48,51	0
6	GOL	B	627	6/6	0.92	0.18	19,36,40,43	0
3	EDO	A	618	4/4	0.93	0.10	46,47,48,49	0
3	EDO	C	612	4/4	0.93	0.09	21,27,28,37	0
5	BTB	B	613	14/14	0.93	0.08	24,30,35,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	638	4/4	0.93	0.12	28,30,32,42	0
3	EDO	B	631	4/4	0.93	0.11	34,36,36,38	0
3	EDO	D	610	4/4	0.94	0.09	25,26,27,29	0
3	EDO	A	612	4/4	0.94	0.12	27,28,32,34	0
3	EDO	A	608	4/4	0.94	0.07	20,23,25,27	0
3	EDO	B	634	4/4	0.94	0.08	30,36,38,41	0
3	EDO	C	608	4/4	0.94	0.10	17,20,24,26	0
3	EDO	A	610	4/4	0.95	0.10	22,26,37,44	0
3	EDO	A	601	4/4	0.95	0.08	29,31,32,33	0
3	EDO	D	601	4/4	0.95	0.10	29,40,40,42	0
3	EDO	D	606	4/4	0.95	0.06	27,27,29,30	0
4	NAG	B	606	14/15	0.95	0.06	19,23,29,32	0
3	EDO	B	654	4/4	0.95	0.10	30,34,34,37	0
3	EDO	A	606	4/4	0.96	0.07	22,26,31,35	0
3	EDO	A	633	4/4	0.96	0.11	22,28,34,35	0
3	EDO	D	609	4/4	0.96	0.07	25,26,28,31	0
3	EDO	A	644	4/4	0.96	0.07	31,31,32,34	0
3	EDO	B	608	4/4	0.97	0.06	21,21,22,24	0
3	EDO	C	607	4/4	0.97	0.06	22,23,25,29	0
3	EDO	B	614	4/4	0.97	0.06	23,26,27,29	0
3	EDO	B	609	4/4	0.98	0.06	22,24,25,29	0
3	EDO	C	609	4/4	0.98	0.05	21,23,26,32	0
8	ZN	C	632	1/1	1.00	0.01	16,16,16,16	0
8	ZN	D	630	1/1	1.00	0.02	22,22,22,22	0
8	ZN	A	647	1/1	1.00	0.01	18,18,18,18	0
8	ZN	B	652	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.