



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2020 – 12:16 PM EDT

PDB ID : 7JWF
Title : Crystal structure of PdGH110B D344N in complex with alpha-(1,3)-galactobi
ose
Authors : Hettle, A.G.; Boraston, A.B.
Deposited on : 2020-08-25
Resolution : 2.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

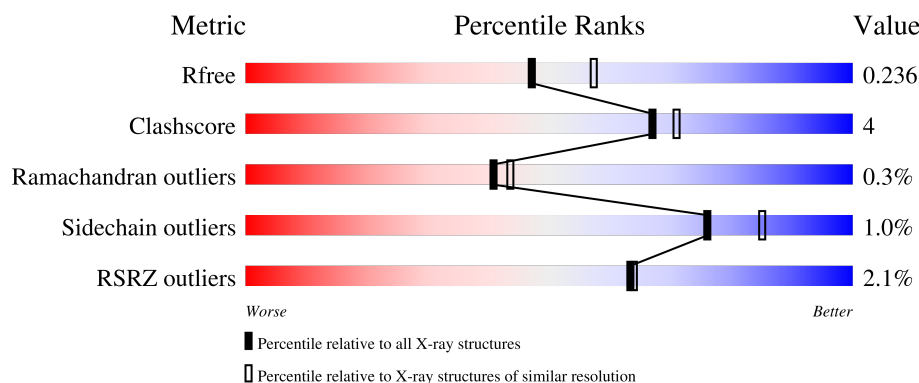
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on 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	620	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	B	620	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	620	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	620	<div> <div>0%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 50% 50%
2	H	2	 50% 50%

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
12	EPE	D	748	-	-	-	X
4	EDO	D	702	-	-	X	-
5	IOD	A	723	-	-	X	-
5	IOD	D	722	-	-	X	-

2 Entry composition

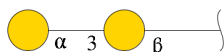
There are 13 unique types of molecules in this entry. The entry contains 20631 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside hydrolase family 110.

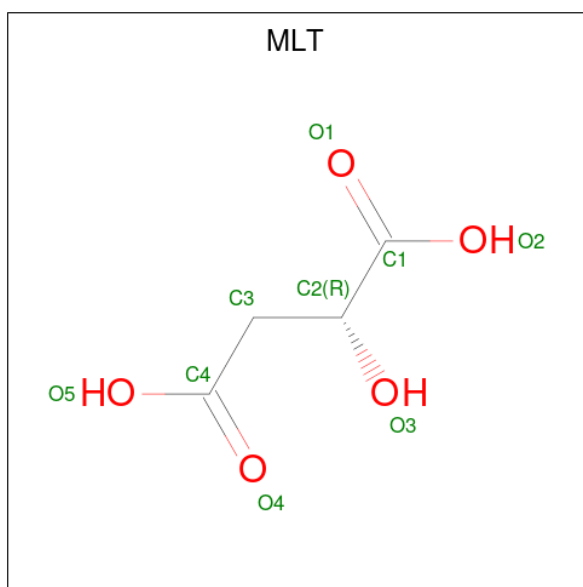
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4625	2950	793	877	5			
1	B	582	Total	C	N	O	S	0	1	0
			4613	2947	786	875	5			
1	C	582	Total	C	N	O	S	0	1	0
			4612	2947	781	879	5			
1	D	582	Total	C	N	O	S	0	1	0
			4594	2928	783	878	5			

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	C	1	Total	C	O	0	0
			9	4	5		
3	D	1	Total	C	O	0	0
			9	4	5		
3	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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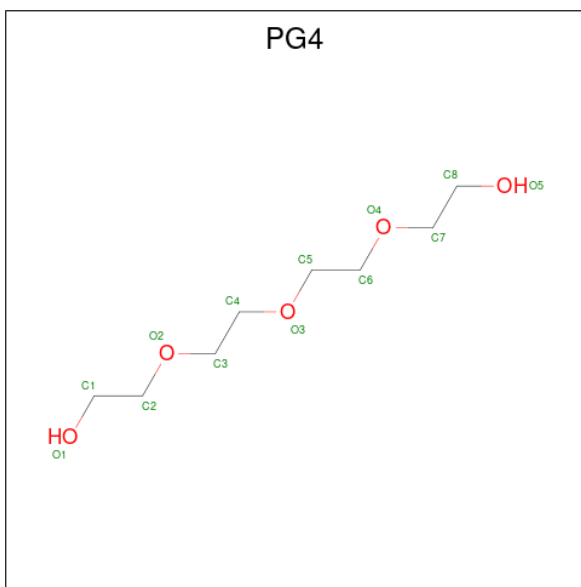
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	29	Total I 29 29	0	0
5	A	31	Total I 32 32	0	1
5	D	32	Total I 32 32	0	0
5	C	27	Total I 27 27	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).

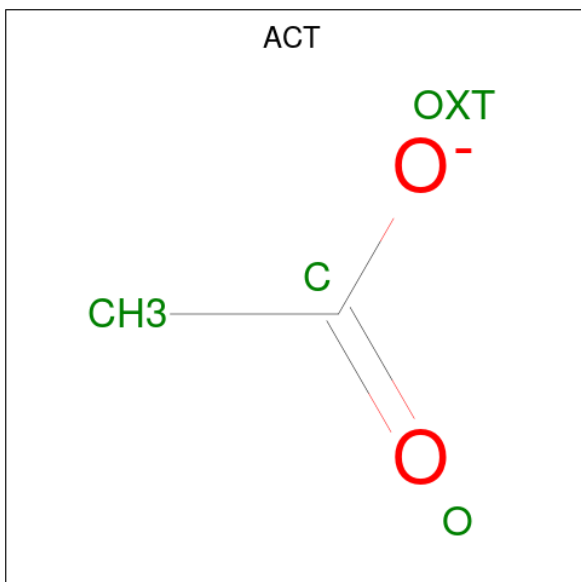


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

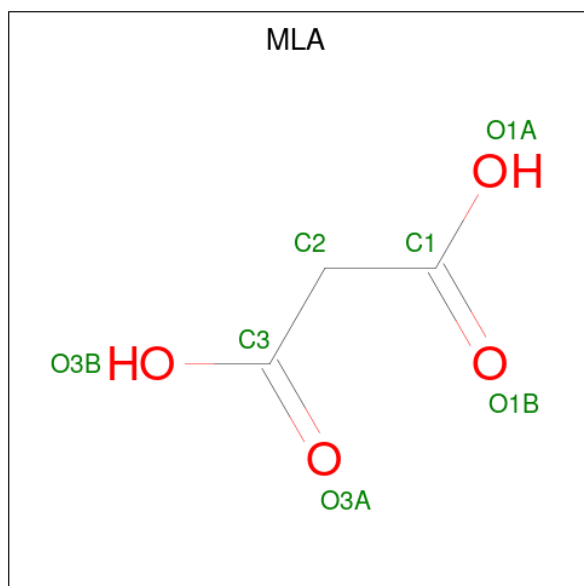


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

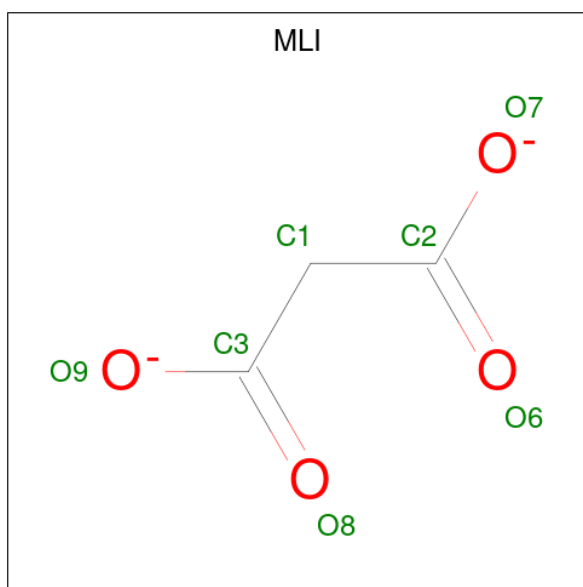
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	4	Total Cl 4 4	0	0
9	A	3	Total Cl 3 3	0	0
9	D	1	Total Cl 1 1	0	0
9	C	2	Total Cl 2 2	0	0

- Molecule 10 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



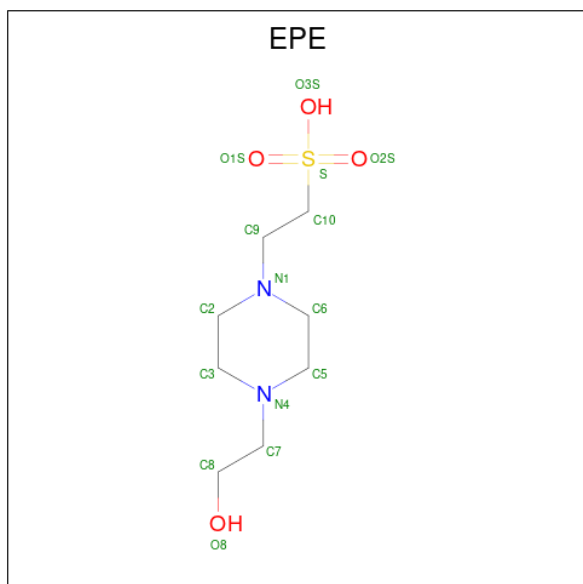
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C O 7 3 4	0	0

- Molecule 11 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



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

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

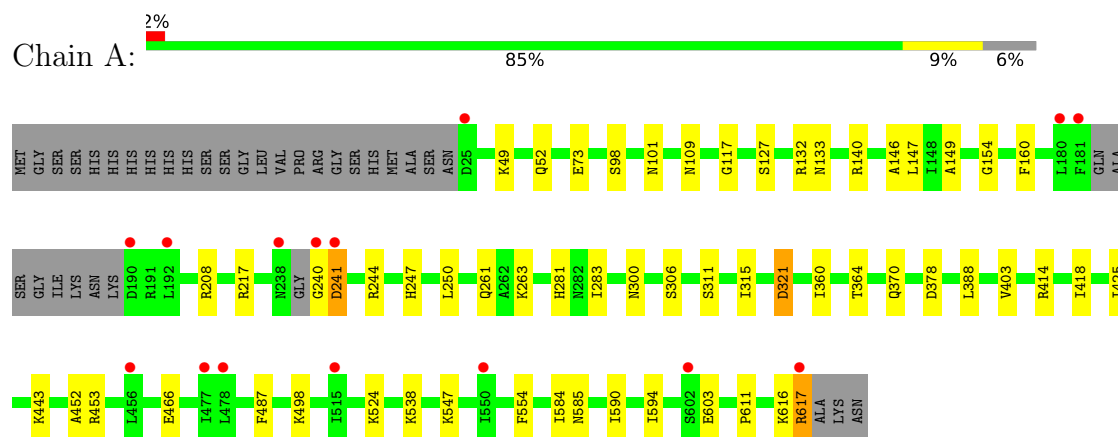
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	418	Total 418	O 418	0	0
13	B	406	Total 406	O 406	0	0
13	C	408	Total 408	O 408	0	0
13	D	429	Total 429	O 429	0	0

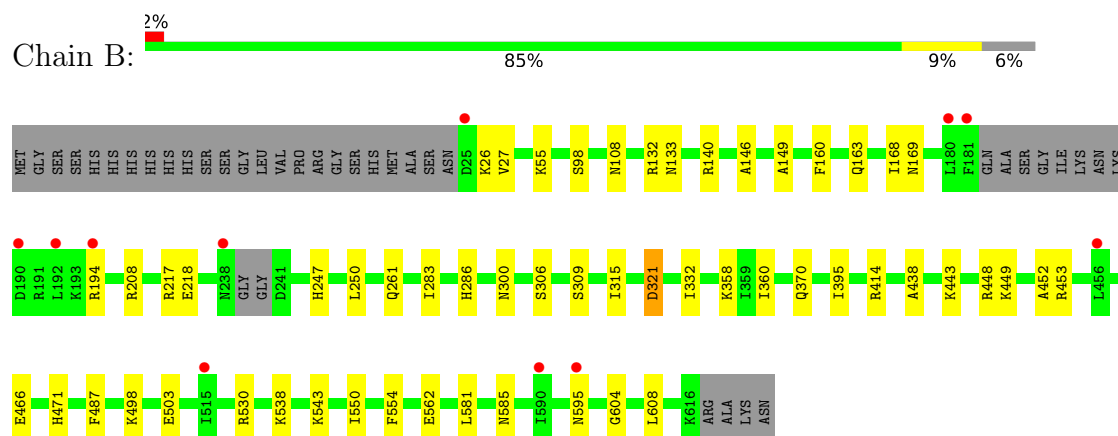
3 Residue-property plots [i](#)

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.

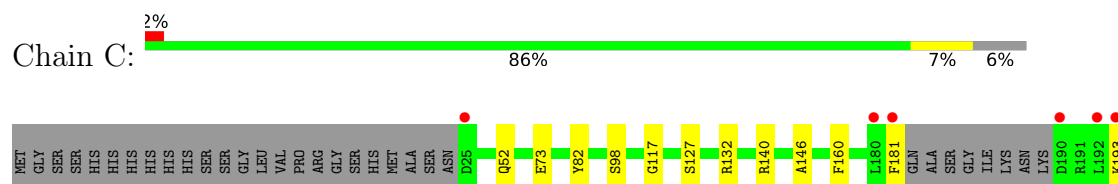
• Molecule 1: Glycoside hydrolase family 110

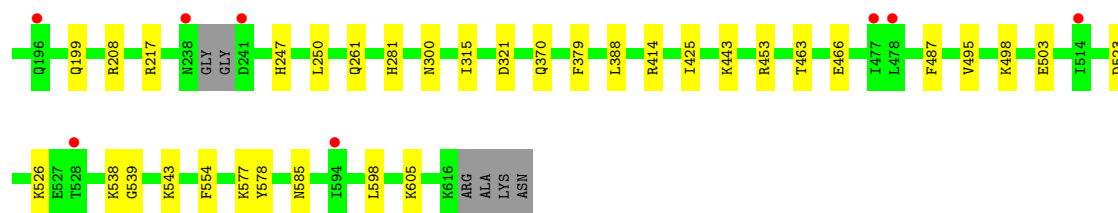


• Molecule 1: Glycoside hydrolase family 110

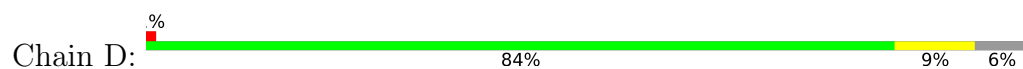


• Molecule 1: Glycoside hydrolase family 110





- Molecule 1: Glycoside hydrolase family 110



- Molecule 2: alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.52Å 124.76Å 142.42Å 90.00° 93.86° 90.00°	Depositor
Resolution (Å)	29.76 – 2.19 29.76 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.76-2.19) 97.4 (29.76-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.15.2 _3472	Depositor
R, R_{free}	0.205 , 0.237 0.204 , 0.236	Depositor DCC
R_{free} test set	8679 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20631	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, CL, GLA, CA, MLI, EDO, PG4, GAL, MLT, ACT, EPE, MLA

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	0.25	0/4717	0.45	0/6370
1	B	0.25	0/4708	0.44	0/6358
1	C	0.26	0/4707	0.45	0/6360
1	D	0.25	0/4689	0.44	0/6339
All	All	0.25	0/18821	0.45	0/25427

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4625	0	4543	41	0
1	B	4613	0	4526	36	0
1	C	4612	0	4501	24	0
1	D	4594	0	4464	38	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	4	0	0
3	D	18	0	8	2	0
4	A	48	0	72	10	0
4	B	56	0	84	8	0
4	C	52	0	78	2	0
4	D	44	0	66	7	0
5	A	32	0	0	9	0
5	B	29	0	0	6	0
5	C	27	0	0	4	0
5	D	32	0	0	5	0
6	A	13	0	18	0	0
6	D	13	0	18	0	0
7	A	1	0	0	0	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
8	C	4	0	3	0	0
9	A	3	0	0	0	0
9	B	4	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
10	D	7	0	2	0	0
11	D	7	0	2	0	0
12	D	15	0	17	3	0
13	A	418	0	0	1	0
13	B	406	0	0	1	0
13	C	408	0	0	1	0
13	D	429	0	0	1	0
All	All	20631	0	18500	145	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 4.

All (145) 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:101:ASN:H	4:A:706:EDO:H21	1.42	0.84
1:A:547:LYS:HE2	5:A:723:IOD:I	2.59	0.72
1:D:524:LYS:HG3	5:D:744:IOD:I	2.63	0.68
1:B:530:ARG:H	4:B:709:EDO:H22	1.60	0.67
1:A:443:LYS:HB3	4:A:707:EDO:H21	1.77	0.66
1:A:149:ALA:HA	4:A:712:EDO:H11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:HA	4:A:702:EDO:H11	1.77	0.65
5:A:723:IOD:I	5:A:726:IOD:I	3.55	0.64
1:C:598:LEU:HD13	1:C:605:LYS:HB2	1.78	0.64
1:A:247:HIS:HB3	1:A:250:LEU:HG	1.80	0.63
1:B:247:HIS:HB3	1:B:250:LEU:HG	1.80	0.63
1:A:98:SER:HB3	5:A:730:IOD:I	2.69	0.62
1:C:217:ARG:HA	1:C:315:ILE:HD11	1.82	0.62
1:D:418:ILE:HA	4:D:702:EDO:H22	1.82	0.61
1:C:523:ASP:HA	1:C:526:LYS:HD2	1.82	0.60
1:B:98:SER:HB3	5:B:730:IOD:I	2.71	0.60
1:A:244:ARG:HH12	4:A:703:EDO:H12	1.66	0.60
1:C:247:HIS:HB3	1:C:250:LEU:HG	1.81	0.60
1:D:247:HIS:HB3	1:D:250:LEU:HG	1.81	0.60
1:C:82:TYR:HB2	4:C:708:EDO:H21	1.85	0.59
1:A:603:GLU:HB2	5:A:723:IOD:I	2.73	0.58
1:D:403:VAL:HG23	1:D:404:THR:HG23	1.86	0.58
5:D:714:IOD:I	5:D:722:IOD:I	3.61	0.58
1:A:524:LYS:HB2	5:A:740:IOD:I	2.73	0.58
1:D:307:LYS:HG3	1:D:338:LEU:HB3	1.86	0.58
5:A:719:IOD:I	5:A:725:IOD:I	3.61	0.58
1:A:49:LYS:HA	1:A:49:LYS:HE2	1.86	0.57
1:C:539:GLY:HA3	4:C:703:EDO:H22	1.84	0.57
1:B:217:ARG:HA	1:B:315:ILE:HD11	1.86	0.57
5:C:718:IOD:I	5:C:728:IOD:I	3.63	0.57
1:A:594:ILE:HG22	5:A:738[B]:IOD:I	2.74	0.56
1:D:422:ASP:HB3	1:D:425:ILE:HD12	1.88	0.56
1:A:403:VAL:HG12	4:A:710:EDO:H11	1.86	0.56
1:A:263:LYS:HE3	5:A:743:IOD:I	2.77	0.55
1:B:27:VAL:HG21	4:B:711:EDO:H22	1.86	0.55
1:A:244:ARG:HH22	4:A:703:EDO:H21	1.71	0.55
1:B:208:ARG:HG2	1:B:261:GLN:HB3	1.89	0.55
1:A:217:ARG:HA	1:A:315:ILE:HD11	1.88	0.54
1:D:241:ASP:N	4:D:708:EDO:HO1	2.04	0.54
1:A:240:GLY:O	1:A:241:ASP:HB2	2.07	0.54
1:D:170:GLU:N	3:D:701:MLT:O1	2.39	0.54
1:D:52:GLN:NE2	13:D:806:HOH:O	2.36	0.53
1:A:616:LYS:HB3	1:A:617:ARG:HH11	1.74	0.53
1:B:168:ILE:H	4:B:704:EDO:H21	1.72	0.53
1:D:388:LEU:HD22	1:D:425:ILE:HD13	1.90	0.53
1:B:149:ALA:HA	4:B:714:EDO:H21	1.91	0.52
1:B:395:ILE:HG12	4:B:709:EDO:H21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:PHE:CZ	12:D:748:EPE:H21	2.45	0.52
1:A:418:ILE:HA	4:D:702:EDO:H12	1.92	0.52
1:A:584:ILE:HD13	1:A:590:ILE:HG21	1.92	0.52
1:D:525:PHE:HZ	12:D:748:EPE:H21	1.75	0.52
1:C:208:ARG:HG2	1:C:261:GLN:HB3	1.92	0.51
1:A:498:LYS:HD3	1:A:538:LYS:HE3	1.92	0.51
1:D:443:LYS:HA	1:D:466:GLU:O	2.11	0.50
1:A:208:ARG:HG2	1:A:261:GLN:HB3	1.92	0.50
1:A:73:GLU:OE2	1:A:117:GLY:N	2.40	0.50
1:D:208:ARG:HG2	1:D:261:GLN:HB3	1.92	0.50
1:B:108:ASN:HD21	4:B:712:EDO:H11	1.76	0.50
1:A:52:GLN:NE2	13:A:803:HOH:O	2.33	0.49
1:A:360:ILE:HB	1:A:364:THR:HB	1.94	0.49
1:C:498:LYS:HA	1:C:538:LYS:O	2.12	0.49
1:C:52:GLN:NE2	13:C:805:HOH:O	2.31	0.49
1:D:132:ARG:HA	1:D:281:HIS:O	2.13	0.49
1:B:169:ASN:HA	4:B:703:EDO:H11	1.95	0.48
1:D:530:ARG:H	4:D:704:EDO:HO2	1.59	0.48
1:A:443:LYS:HA	1:A:466:GLU:O	2.14	0.48
1:A:311:SER:HA	4:A:704:EDO:H22	1.96	0.48
1:B:448:ARG:HG3	1:B:449:LYS:HG3	1.95	0.48
1:C:554:PHE:HA	1:C:585:ASN:O	2.13	0.48
1:B:146:ALA:HB2	1:B:160:PHE:CE1	2.49	0.48
1:D:498:LYS:HA	1:D:538:LYS:O	2.13	0.47
1:B:554:PHE:HA	1:B:585:ASN:O	2.13	0.47
1:C:132:ARG:HA	1:C:281:HIS:O	2.15	0.47
1:C:98:SER:HB3	5:C:732:IOD:I	2.84	0.47
1:B:498:LYS:HA	1:B:538:LYS:O	2.14	0.47
1:B:414:ARG:HD2	5:B:732:IOD:I	2.85	0.47
1:D:403:VAL:HG21	4:D:702:EDO:H11	1.96	0.47
1:C:443:LYS:HA	1:C:466:GLU:O	2.15	0.47
1:A:132:ARG:HA	1:A:281:HIS:O	2.15	0.46
1:A:554:PHE:HA	1:A:585:ASN:O	2.14	0.46
1:C:503:GLU:HA	1:C:543:LYS:HB2	1.97	0.46
1:B:443:LYS:HA	1:B:466:GLU:O	2.14	0.46
1:C:577:LYS:HE3	1:C:578:TYR:CZ	2.50	0.46
1:A:146:ALA:HB2	1:A:160:PHE:CE1	2.50	0.46
1:C:370:GLN:HG3	1:C:487:PHE:CZ	2.51	0.46
1:D:146:ALA:HB2	1:D:160:PHE:CE1	2.50	0.46
1:D:466:GLU:HA	1:D:498:LYS:O	2.16	0.45
1:D:152:GLY:HA2	4:D:711:EDO:H22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LYS:HE3	5:D:739:IOD:I	2.87	0.45
1:D:227:PHE:HB2	5:D:722:IOD:I	2.86	0.45
1:C:181:PHE:CE1	1:C:193:LYS:HD3	2.52	0.45
1:C:414:ARG:HG2	5:C:730:IOD:I	2.87	0.45
1:D:606:SER:HA	5:D:721:IOD:I	2.87	0.45
1:D:538:LYS:HA	1:D:562:GLU:O	2.17	0.45
1:D:217:ARG:HA	1:D:315:ILE:HD11	1.98	0.45
1:D:533:LYS:HG2	1:D:557:SER:HB3	1.99	0.45
1:D:554:PHE:HA	1:D:585:ASN:O	2.16	0.44
1:B:163:GLN:HB3	5:B:738:IOD:I	2.87	0.44
1:B:414:ARG:HG2	5:B:727:IOD:I	2.87	0.44
1:D:404:THR:OG1	1:D:416:GLN:HB3	2.17	0.44
1:A:466:GLU:HA	1:A:498:LYS:O	2.17	0.44
1:D:584:ILE:HD13	1:D:590:ILE:HG21	1.99	0.44
1:A:321:ASP:OD2	1:A:321:ASP:N	2.51	0.44
1:B:332:ILE:HG12	1:B:438:ALA:HB1	1.99	0.44
1:B:283:ILE:O	1:B:306:SER:HB3	2.18	0.44
1:A:414:ARG:HD2	5:A:734:IOD:I	2.88	0.43
1:A:147:LEU:HD21	4:A:712:EDO:H12	2.01	0.43
1:B:503:GLU:HA	1:B:543:LYS:HB2	2.00	0.43
1:D:169:ASN:HA	3:D:701:MLT:H32	2.00	0.43
1:D:370:GLN:HG3	1:D:487:PHE:CZ	2.54	0.43
1:B:55:LYS:HG3	5:B:724:IOD:I	2.89	0.43
1:B:538:LYS:HA	1:B:562:GLU:O	2.19	0.43
4:B:705:EDO:H12	5:B:739:IOD:I	2.89	0.43
1:C:73:GLU:OE2	1:C:117:GLY:N	2.43	0.43
1:A:283:ILE:O	1:A:306:SER:HB3	2.19	0.42
1:C:146:ALA:HB2	1:C:160:PHE:CE1	2.54	0.42
1:D:109:ASN:H	1:D:133:ASN:HB3	1.84	0.42
1:C:379:PHE:HB2	5:C:716:IOD:I	2.88	0.42
1:C:463:THR:HB	1:C:495:VAL:HG22	2.00	0.42
1:A:418:ILE:HG13	4:D:702:EDO:H12	2.00	0.42
1:A:154:GLY:HA3	4:A:711:EDO:H21	2.00	0.42
1:B:218:GLU:OE1	1:B:471:HIS:NE2	2.51	0.42
1:B:370:GLN:HG3	1:B:487:PHE:CZ	2.55	0.42
1:D:360:ILE:HB	1:D:364:THR:HB	2.01	0.42
1:D:73:GLU:HA	1:D:118:LEU:HD21	2.01	0.42
1:B:466:GLU:HA	1:B:498:LYS:O	2.19	0.42
1:A:370:GLN:HG3	1:A:487:PHE:CZ	2.55	0.41
1:B:26[A]:LYS:HB2	1:B:26[A]:LYS:HE2	1.94	0.41
1:D:385:GLU:HG2	1:D:434:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:LEU:HB3	1:C:425:ILE:HD11	2.02	0.41
1:B:286:HIS:HA	1:B:309:SER:O	2.20	0.41
12:D:748:EPE:H51	12:D:748:EPE:H81	1.89	0.41
1:B:194:ARG:HG2	1:B:194:ARG:HH21	1.85	0.41
1:B:550:ILE:N	1:B:581:LEU:O	2.50	0.41
1:B:595:ASN:OD1	13:B:801:HOH:O	2.22	0.41
1:C:466:GLU:HA	1:C:498:LYS:O	2.21	0.41
1:D:321:ASP:OD1	1:D:321:ASP:N	2.53	0.41
1:A:584:ILE:HD12	1:A:611:PRO:HB3	2.02	0.40
1:A:109:ASN:H	1:A:133:ASN:HB3	1.87	0.40
1:A:388:LEU:HB3	1:A:425:ILE:HD11	2.04	0.40
1:B:604:GLY:O	1:B:608:LEU:HD12	2.21	0.40
1:B:132:ARG:HG2	1:B:133:ASN:CG	2.41	0.40
1:B:321:ASP:N	1:B:321:ASP:OD1	2.54	0.40
1:B:360:ILE:N	1:B:360:ILE:HD12	2.36	0.40
1:D:304:LYS:HA	1:D:335:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	578/620 (93%)	544 (94%)	31 (5%)	3 (0%)	29	28
1	B	577/620 (93%)	544 (94%)	31 (5%)	2 (0%)	41	43
1	C	577/620 (93%)	549 (95%)	27 (5%)	1 (0%)	47	52
1	D	577/620 (93%)	547 (95%)	29 (5%)	1 (0%)	47	52
All	All	2309/2480 (93%)	2184 (95%)	118 (5%)	7 (0%)	41	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	B	300	ASN
1	C	300	ASN
1	D	300	ASN
1	B	452	ALA
1	A	241	ASP
1	A	452	ALA

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	499/541 (92%)	494 (99%)	5 (1%)	76	85
1	B	496/541 (92%)	492 (99%)	4 (1%)	81	89
1	C	493/541 (91%)	488 (99%)	5 (1%)	76	85
1	D	492/541 (91%)	487 (99%)	5 (1%)	76	85
All	All	1980/2164 (92%)	1961 (99%)	19 (1%)	76	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	140	ARG
1	A	321	ASP
1	A	453	ARG
1	A	617	ARG
1	B	140	ARG
1	B	321	ASP
1	B	358	LYS
1	B	453	ARG
1	C	127	SER
1	C	140	ARG
1	C	199	GLN
1	C	321	ASP
1	C	453	ARG
1	D	140	ARG

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Mol	Chain	Res	Type
1	D	190	ASP
1	D	198	SER
1	D	321	ASP
1	D	453	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	GAL	E	1	2	12,12,12	0.30	0	17,17,17	0.74	0
2	GLA	E	2	2	11,11,12	1.79	3 (27%)	15,15,17	0.67	0
2	GAL	F	1	2	12,12,12	0.31	0	17,17,17	0.75	0
2	GLA	F	2	2	11,11,12	1.80	3 (27%)	15,15,17	0.58	0
2	GAL	G	1	2	12,12,12	0.34	0	17,17,17	0.74	0
2	GLA	G	2	2	11,11,12	1.82	3 (27%)	15,15,17	0.64	0
2	GAL	H	1	2	12,12,12	0.38	0	17,17,17	0.74	0
2	GLA	H	2	2	11,11,12	1.81	3 (27%)	15,15,17	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	E	1	2	-	0/2/22/22	0/1/1/1
2	GLA	E	2	2	-	0/2/19/22	0/1/1/1
2	GAL	F	1	2	-	0/2/22/22	0/1/1/1
2	GLA	F	2	2	-	1/2/19/22	0/1/1/1
2	GAL	G	1	2	-	0/2/22/22	0/1/1/1
2	GLA	G	2	2	-	0/2/19/22	0/1/1/1
2	GAL	H	1	2	-	0/2/22/22	0/1/1/1
2	GLA	H	2	2	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GLA	O5-C1	4.65	1.51	1.43
2	H	2	GLA	O5-C1	4.65	1.51	1.43
2	F	2	GLA	O5-C1	4.65	1.51	1.43
2	E	2	GLA	O5-C1	4.59	1.51	1.43
2	G	2	GLA	C2-C3	-2.63	1.48	1.52
2	F	2	GLA	C2-C3	-2.61	1.48	1.52
2	E	2	GLA	C2-C3	-2.61	1.48	1.52
2	H	2	GLA	C2-C3	-2.59	1.48	1.52
2	G	2	GLA	O5-C5	2.24	1.48	1.43
2	H	2	GLA	O5-C5	2.19	1.47	1.43
2	E	2	GLA	O5-C5	2.19	1.47	1.43
2	F	2	GLA	O5-C5	2.18	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

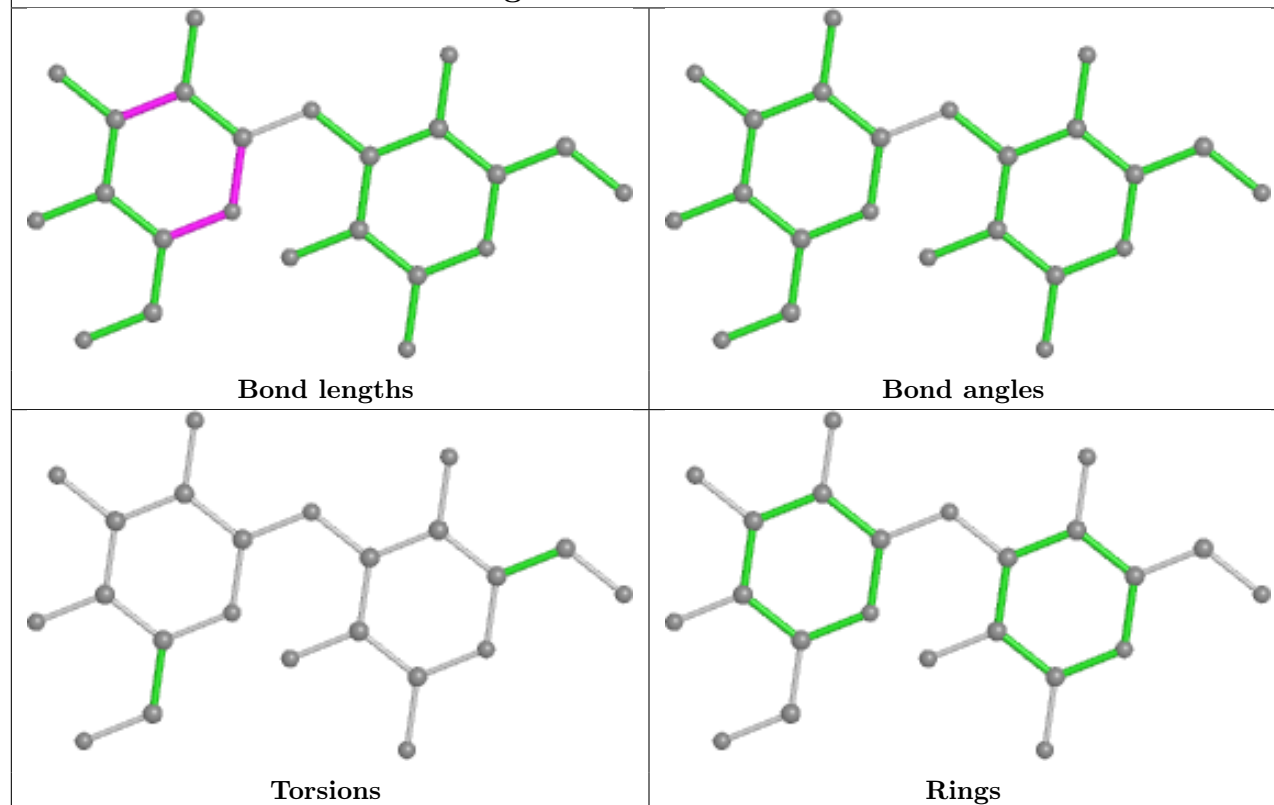
Mol	Chain	Res	Type	Atoms
2	F	2	GLA	O5-C5-C6-O6
2	H	2	GLA	O5-C5-C6-O6

There are no ring outliers.

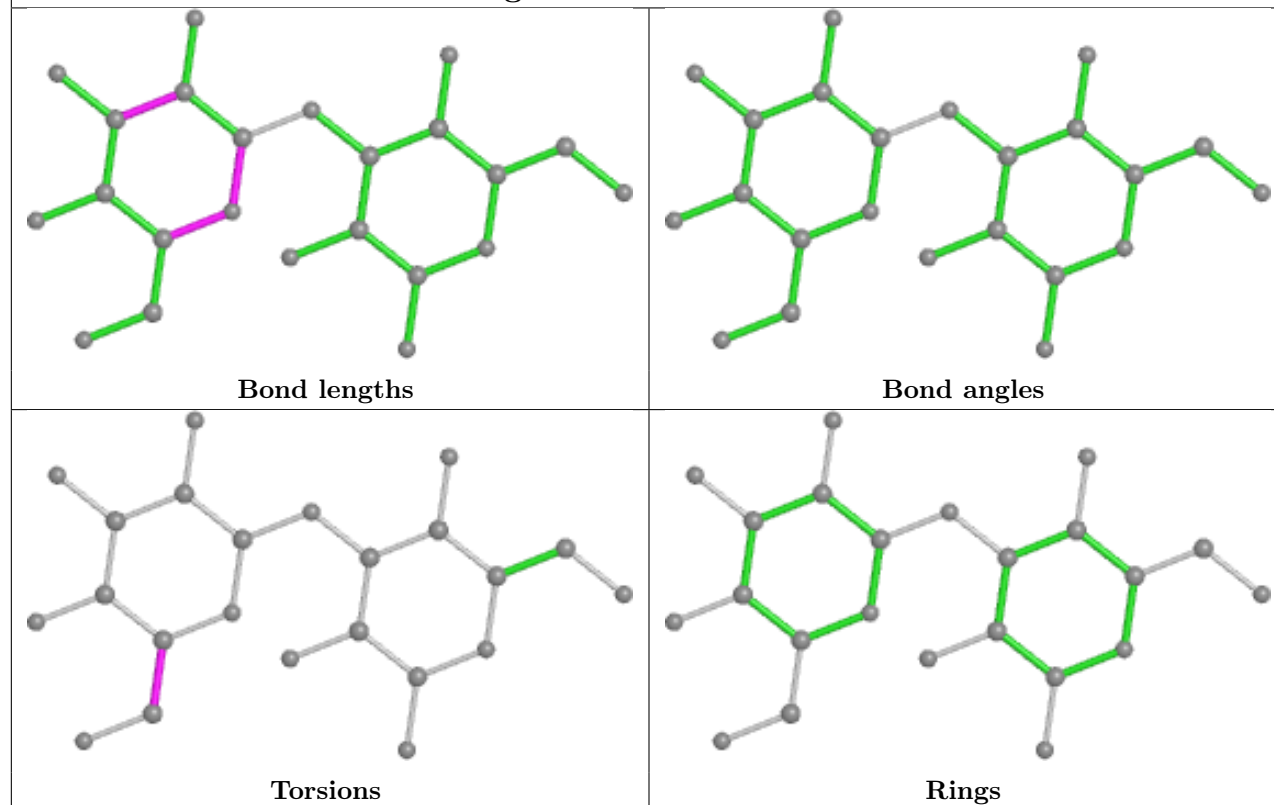
No monomer is involved in short contacts.

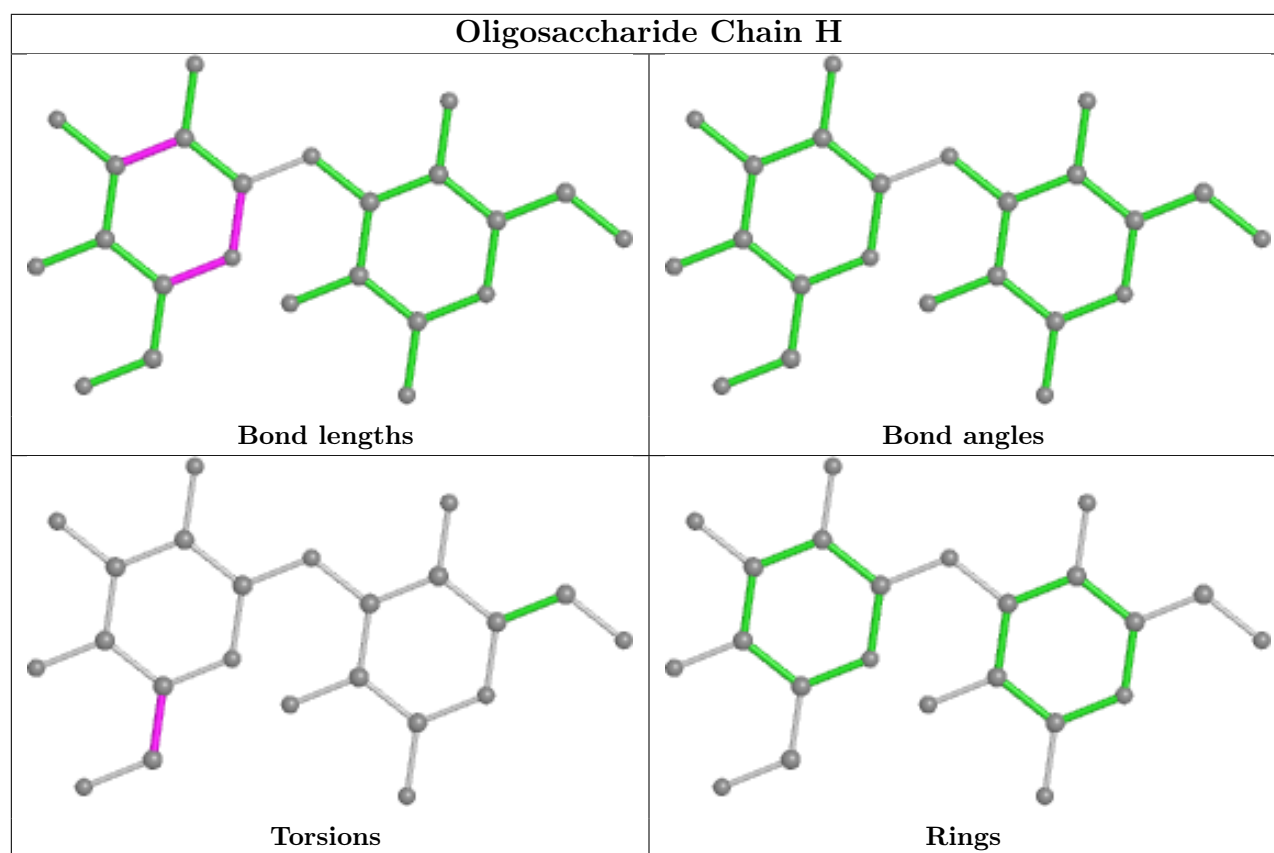
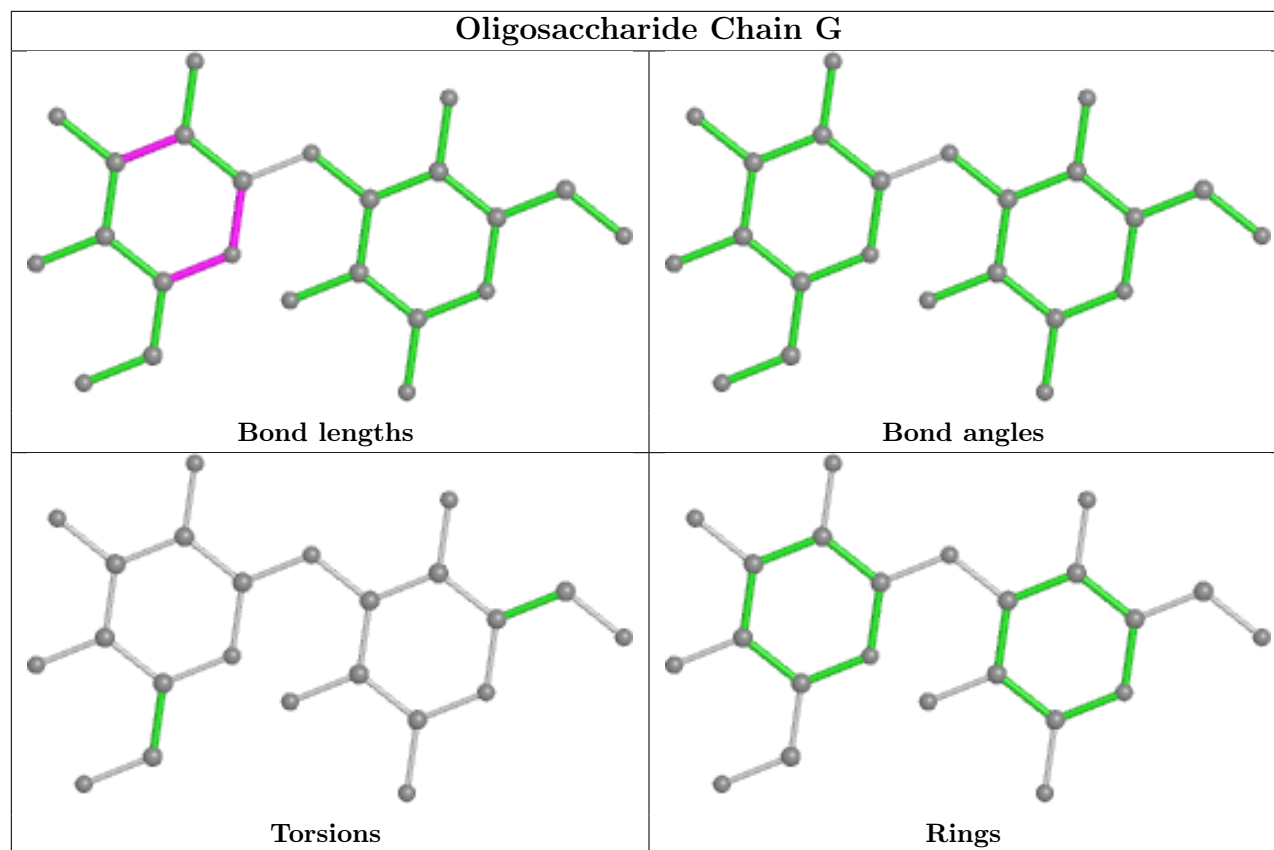
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F





5.6 Ligand geometry

Of 193 ligands modelled in this entry, 131 are monoatomic - leaving 62 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	707	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	712	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	709	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	B	713	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	A	713	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	C	714	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	B	712	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	D	705	-	3,3,3	0.43	0	2,2,2	0.36	0
3	MLT	C	702	-	2,8,8	0.48	0	3,10,10	0.87	0
4	EDO	A	705	-	3,3,3	0.45	0	2,2,2	0.35	0
6	PG4	D	747	-	12,12,12	0.54	0	11,11,11	0.22	0
4	EDO	B	708	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	B	703	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	B	709	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	D	709	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	D	704	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	C	710	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	A	707	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	D	712	-	3,3,3	0.46	0	2,2,2	0.33	0
8	ACT	A	747	-	1,3,3	6.24	1 (100%)	0,3,3	0.00	-
4	EDO	A	703	-	3,3,3	0.46	0	2,2,2	0.32	0
3	MLT	A	701	-	2,8,8	0.52	0	3,10,10	0.72	0
4	EDO	B	706	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	A	711	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	D	711	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	C	706	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	702	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	D	703	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	D	706	-	3,3,3	0.44	0	2,2,2	0.34	0
8	ACT	C	701	-	1,3,3	6.42	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	708	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	A	708	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	B	714	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	C	704	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	B	704	-	3,3,3	0.42	0	2,2,2	0.30	0
6	PG4	A	745	-	12,12,12	0.54	0	11,11,11	0.23	0
8	ACT	B	744	-	1,3,3	6.35	1 (100%)	0,3,3	0.00	-
4	EDO	B	705	-	3,3,3	0.41	0	2,2,2	0.35	0
4	EDO	C	709	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	C	707	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	701	-	3,3,3	0.44	0	2,2,2	0.34	0
4	EDO	C	708	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	C	705	-	3,3,3	0.46	0	2,2,2	0.30	0
3	MLT	D	749	-	2,8,8	0.46	0	3,10,10	0.92	0
10	MLA	D	745	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	C	712	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	B	710	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	C	713	-	3,3,3	0.45	0	2,2,2	0.34	0
12	EPE	D	748	-	15,15,15	0.87	1 (6%)	18,20,20	2.04	7 (38%)
11	MLI	D	746	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	C	703	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	A	710	-	3,3,3	0.46	0	2,2,2	0.31	0
3	MLT	D	701	-	2,8,8	0.49	0	3,10,10	0.51	0
4	EDO	A	702	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	D	702	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	C	715	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	B	711	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	D	710	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	C	711	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	D	707	-	3,3,3	0.46	0	2,2,2	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	707	-	-	0/1/1/1	-
4	EDO	A	712	-	-	0/1/1/1	-
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	A	709	-	-	0/1/1/1	-
4	EDO	B	713	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	713	-	-	0/1/1/1	-
4	EDO	C	714	-	-	0/1/1/1	-
4	EDO	B	712	-	-	0/1/1/1	-
4	EDO	A	706	-	-	0/1/1/1	-
4	EDO	D	705	-	-	0/1/1/1	-
3	MLT	C	702	-	-	0/2/8/8	-
4	EDO	A	705	-	-	0/1/1/1	-
6	PG4	D	747	-	-	5/10/10/10	-
4	EDO	B	708	-	-	0/1/1/1	-
4	EDO	B	703	-	-	1/1/1/1	-
4	EDO	B	709	-	-	0/1/1/1	-
4	EDO	D	709	-	-	0/1/1/1	-
4	EDO	D	704	-	-	0/1/1/1	-
4	EDO	A	707	-	-	1/1/1/1	-
4	EDO	D	712	-	-	0/1/1/1	-
4	EDO	C	710	-	-	0/1/1/1	-
4	EDO	A	703	-	-	0/1/1/1	-
3	MLT	A	701	-	-	2/2/8/8	-
4	EDO	B	706	-	-	0/1/1/1	-
4	EDO	A	711	-	-	0/1/1/1	-
4	EDO	D	711	-	-	0/1/1/1	-
4	EDO	C	706	-	-	0/1/1/1	-
4	EDO	B	702	-	-	0/1/1/1	-
4	EDO	D	703	-	-	0/1/1/1	-
4	EDO	D	706	-	-	0/1/1/1	-
4	EDO	D	708	-	-	0/1/1/1	-
4	EDO	A	708	-	-	0/1/1/1	-
4	EDO	B	714	-	-	0/1/1/1	-
4	EDO	C	704	-	-	0/1/1/1	-
4	EDO	B	704	-	-	0/1/1/1	-
6	PG4	A	745	-	-	6/10/10/10	-
4	EDO	B	705	-	-	0/1/1/1	-
4	EDO	C	709	-	-	0/1/1/1	-
4	EDO	C	707	-	-	0/1/1/1	-
4	EDO	B	701	-	-	0/1/1/1	-
4	EDO	C	708	-	-	0/1/1/1	-
4	EDO	C	705	-	-	0/1/1/1	-
3	MLT	D	749	-	-	0/2/8/8	-
10	MLA	D	745	-	-	0/0/4/4	-
4	EDO	C	712	-	-	0/1/1/1	-
4	EDO	B	710	-	-	0/1/1/1	-
4	EDO	C	713	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EPE	D	748	-	-	1/9/19/19	0/1/1/1
11	MLI	D	746	-	-	0/0/4/4	-
4	EDO	C	703	-	-	0/1/1/1	-
4	EDO	A	710	-	-	0/1/1/1	-
3	MLT	D	701	-	-	2/2/8/8	-
4	EDO	A	702	-	-	1/1/1/1	-
4	EDO	D	702	-	-	0/1/1/1	-
4	EDO	C	715	-	-	0/1/1/1	-
4	EDO	B	711	-	-	0/1/1/1	-
4	EDO	D	710	-	-	0/1/1/1	-
4	EDO	C	711	-	-	0/1/1/1	-
4	EDO	D	707	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	701	ACT	CH3-C	6.42	1.56	1.48
8	B	744	ACT	CH3-C	6.35	1.56	1.48
8	A	747	ACT	CH3-C	6.24	1.56	1.48
12	D	748	EPE	C10-S	2.82	1.81	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	748	EPE	C7-N4-C3	3.63	120.51	111.23
12	D	748	EPE	C7-N4-C5	3.43	120.01	111.23
12	D	748	EPE	C5-N4-C3	3.38	116.43	108.83
12	D	748	EPE	O1S-S-C10	2.79	110.27	106.92
12	D	748	EPE	C9-N1-C6	-2.77	104.16	111.23
12	D	748	EPE	O2S-S-C10	2.23	109.60	106.92
12	D	748	EPE	C6-N1-C2	2.23	113.84	108.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	MLT	C1-C2-C3-C4
3	A	701	MLT	O3-C2-C3-C4
12	D	748	EPE	C8-C7-N4-C5
3	D	701	MLT	C1-C2-C3-C4
6	A	745	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	D	747	PG4	O3-C5-C6-O4
6	D	747	PG4	O2-C3-C4-O3
6	D	747	PG4	O1-C1-C2-O2
6	A	745	PG4	O1-C1-C2-O2
6	A	745	PG4	O4-C7-C8-O5
6	A	745	PG4	O3-C5-C6-O4
6	A	745	PG4	C1-C2-O2-C3
6	D	747	PG4	C5-C6-O4-C7
6	A	745	PG4	C6-C5-O3-C4
6	D	747	PG4	C4-C3-O2-C2
3	D	701	MLT	O3-C2-C3-C4
4	B	703	EDO	O1-C1-C2-O2
4	A	707	EDO	O1-C1-C2-O2
4	A	702	EDO	O1-C1-C2-O2

There are no ring outliers.

23 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	712	EDO	2	0
4	A	704	EDO	1	0
4	B	712	EDO	1	0
4	A	706	EDO	1	0
4	B	703	EDO	1	0
4	B	709	EDO	2	0
4	D	704	EDO	1	0
4	A	707	EDO	1	0
4	A	703	EDO	2	0
4	A	711	EDO	1	0
4	D	711	EDO	1	0
4	D	708	EDO	1	0
4	B	714	EDO	1	0
4	B	704	EDO	1	0
4	B	705	EDO	1	0
4	C	708	EDO	1	0
12	D	748	EPE	3	0
4	C	703	EDO	1	0
4	A	710	EDO	1	0
3	D	701	MLT	2	0
4	A	702	EDO	1	0
4	D	702	EDO	4	0
4	B	711	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	584/620 (94%)	-0.06	15 (2%) 56 56	25, 32, 43, 67	2 (0%)
1	B	582/620 (93%)	0.03	11 (1%) 66 67	25, 33, 48, 70	0
1	C	582/620 (93%)	-0.07	14 (2%) 59 59	26, 33, 48, 68	0
1	D	582/620 (93%)	-0.12	9 (1%) 73 74	24, 32, 45, 62	2 (0%)
All	All	2330/2480 (93%)	-0.06	49 (2%) 63 64	24, 33, 46, 70	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	PHE	6.2
1	B	25	ASP	5.5
1	D	181	PHE	5.1
1	B	181	PHE	5.1
1	D	25	ASP	4.8
1	C	192	LEU	4.8
1	A	181	PHE	4.7
1	C	25	ASP	4.6
1	B	180	LEU	4.4
1	A	617	ARG	3.9
1	C	190	ASP	3.9
1	B	238	ASN	3.8
1	B	190	ASP	3.8
1	A	25	ASP	3.7
1	A	180	LEU	3.6
1	A	192	LEU	3.6
1	C	238	ASN	3.4
1	A	190	ASP	3.3
1	D	190	ASP	3.3
1	B	192	LEU	3.1
1	B	194	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	478	LEU	2.9
1	A	241	ASP	2.8
1	A	515	ILE	2.6
1	C	180	LEU	2.6
1	A	240	GLY	2.5
1	D	516	ALA	2.5
1	D	478	LEU	2.5
1	C	528	THR	2.4
1	C	241	ASP	2.4
1	B	456	LEU	2.4
1	D	241	ASP	2.4
1	C	477	ILE	2.3
1	C	594	ILE	2.3
1	A	478	LEU	2.3
1	B	515	ILE	2.2
1	C	196	GLN	2.2
1	B	595	ASN	2.2
1	D	514	ILE	2.2
1	C	193	LYS	2.2
1	A	477	ILE	2.1
1	D	476	ALA	2.1
1	A	238	ASN	2.0
1	A	456	LEU	2.0
1	C	514	ILE	2.0
1	D	477	ILE	2.0
1	A	602	SER	2.0
1	A	550	ILE	2.0
1	B	590	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

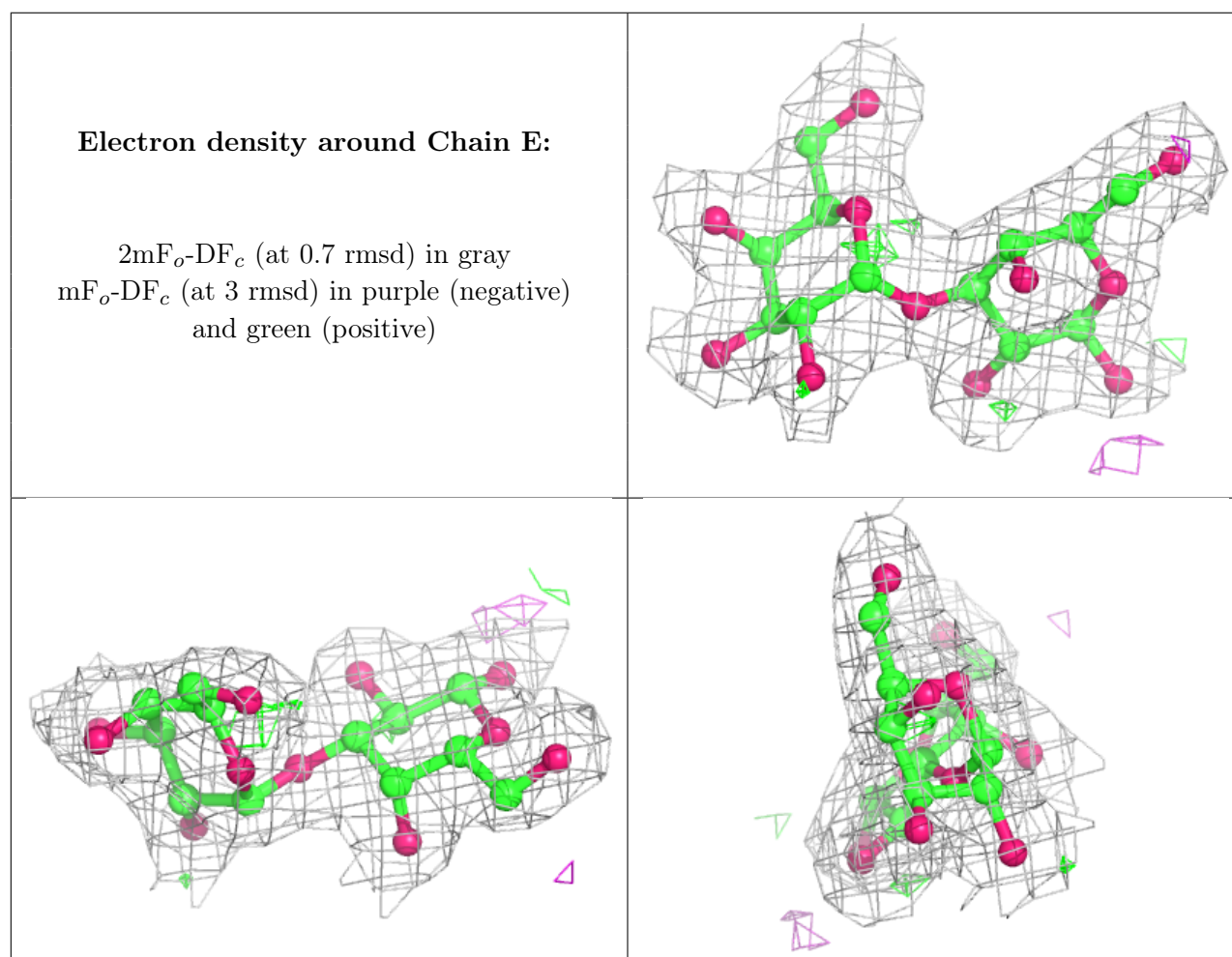
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

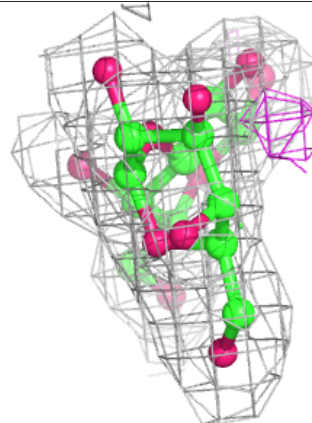
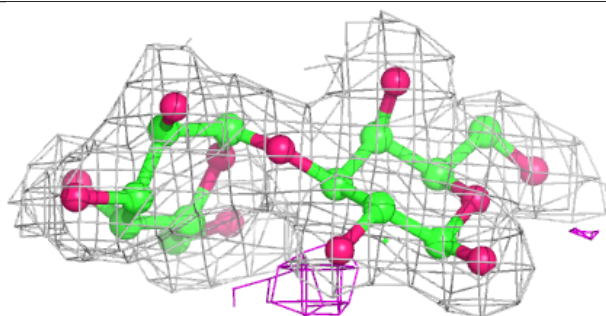
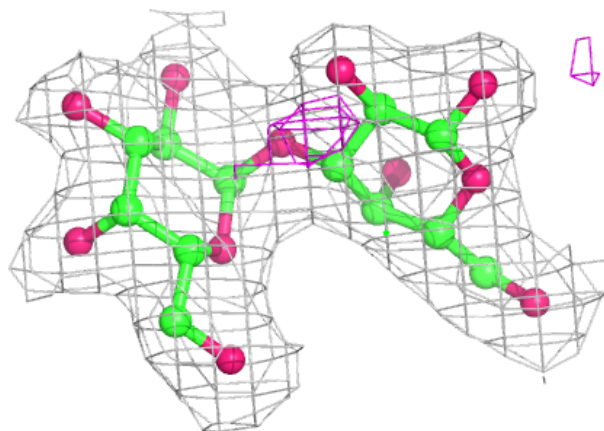
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLA	H	2	11/12	0.94	0.11	23,27,29,31	0
2	GAL	F	1	12/12	0.94	0.09	26,29,32,34	0
2	GLA	E	2	11/12	0.95	0.12	26,29,32,34	0
2	GAL	E	1	12/12	0.95	0.08	28,33,34,34	0
2	GLA	F	2	11/12	0.96	0.12	25,28,29,30	0
2	GAL	H	1	12/12	0.96	0.08	26,30,31,33	0
2	GAL	G	1	12/12	0.96	0.09	26,30,34,36	0
2	GLA	G	2	11/12	0.97	0.11	27,29,31,32	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.



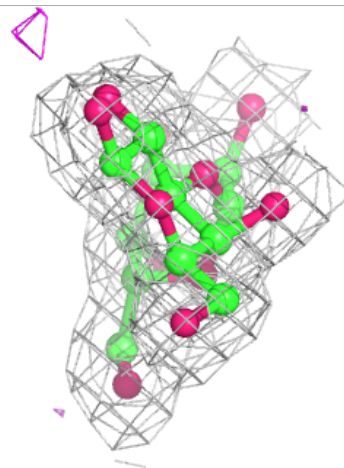
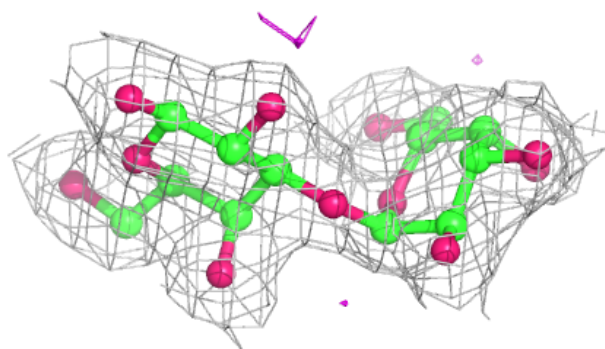
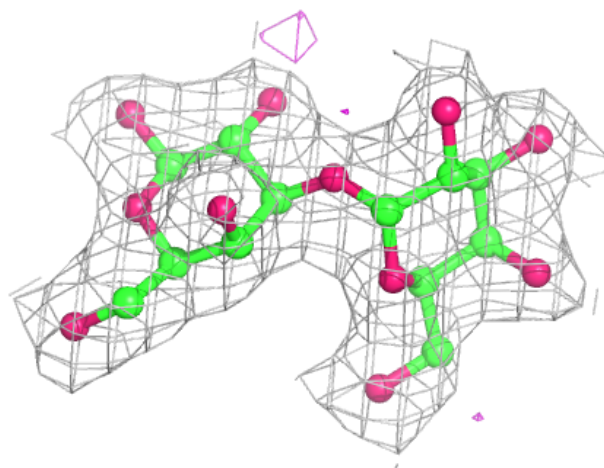
Electron density around Chain F:

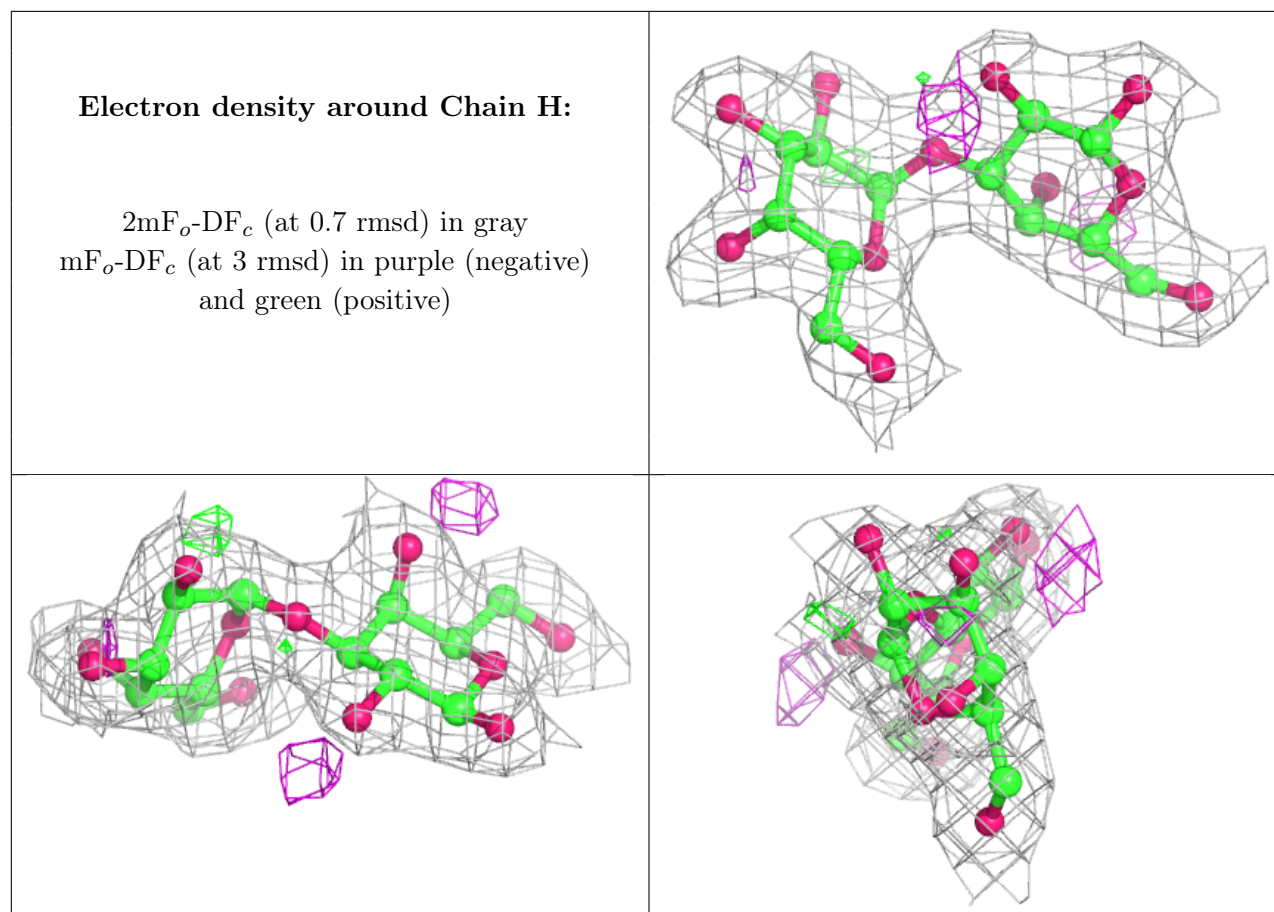
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IOD	D	720	1/1	0.29	0.20	63,63,63,63	1
4	EDO	C	710	4/4	0.54	0.37	66,68,71,72	0
4	EDO	A	703	4/4	0.69	0.20	47,49,51,55	0
5	IOD	D	722	1/1	0.73	0.12	123,123,123,123	0
4	EDO	C	707	4/4	0.73	0.10	46,46,52,54	0
3	MLT	D	749	9/9	0.74	0.26	51,55,62,67	0
4	EDO	B	713	4/4	0.75	0.31	41,47,54,55	0
4	EDO	D	707	4/4	0.76	0.21	34,43,46,48	0
12	EPE	D	748	15/15	0.76	0.47	56,66,69,73	4
9	CL	A	748	1/1	0.76	0.08	62,62,62,62	0
4	EDO	B	709	4/4	0.77	0.15	46,48,49,54	0
11	MLI	D	746	7/7	0.78	0.23	42,47,50,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	A	726	1/1	0.78	0.12	101,101,101,101	0
4	EDO	A	713	4/4	0.79	0.19	46,47,54,56	0
3	MLT	A	701	9/9	0.79	0.22	38,45,50,53	0
4	EDO	D	710	4/4	0.80	0.21	39,45,46,54	0
4	EDO	A	708	4/4	0.81	0.25	51,54,56,58	0
4	EDO	C	711	4/4	0.81	0.29	51,52,54,58	0
4	EDO	D	704	4/4	0.81	0.24	45,47,48,52	0
4	EDO	A	704	4/4	0.81	0.19	35,36,44,50	0
5	IOD	D	744	1/1	0.82	0.10	60,60,60,60	1
4	EDO	C	713	4/4	0.83	0.20	35,39,39,47	0
4	EDO	C	709	4/4	0.84	0.12	49,49,52,57	0
6	PG4	D	747	13/13	0.84	0.26	48,53,56,58	0
5	IOD	C	721	1/1	0.84	0.07	87,87,87,87	1
3	MLT	D	701	9/9	0.84	0.22	39,40,50,52	0
6	PG4	A	745	13/13	0.85	0.20	33,46,54,54	0
3	MLT	C	702	9/9	0.85	0.37	55,59,62,65	0
4	EDO	A	706	4/4	0.85	0.21	31,33,34,44	0
4	EDO	D	711	4/4	0.86	0.15	44,48,49,50	0
4	EDO	B	707	4/4	0.86	0.16	44,45,45,46	0
5	IOD	B	723	1/1	0.86	0.07	66,66,66,66	1
10	MLA	D	745	7/7	0.86	0.34	55,59,60,66	0
5	IOD	C	728	1/1	0.86	0.28	135,135,135,135	0
4	EDO	B	712	4/4	0.86	0.31	48,49,50,55	0
5	IOD	A	744	1/1	0.87	0.07	63,63,63,63	1
4	EDO	A	709	4/4	0.87	0.21	39,46,47,54	0
4	EDO	A	707	4/4	0.88	0.22	36,39,46,49	0
4	EDO	D	702	4/4	0.88	0.27	42,44,45,48	0
4	EDO	B	702	4/4	0.88	0.15	39,40,42,46	0
4	EDO	D	708	4/4	0.89	0.20	40,47,52,52	0
4	EDO	B	710	4/4	0.89	0.26	46,49,49,53	0
5	IOD	D	716	1/1	0.89	0.12	73,73,73,73	1
5	IOD	C	724	1/1	0.89	0.13	76,76,76,76	1
4	EDO	A	710	4/4	0.89	0.34	47,47,47,50	0
4	EDO	C	706	4/4	0.89	0.19	43,48,51,53	0
4	EDO	D	706	4/4	0.90	0.15	34,37,41,41	0
4	EDO	B	714	4/4	0.90	0.16	40,43,44,47	0
9	CL	C	743	1/1	0.90	0.09	45,45,45,45	0
4	EDO	C	712	4/4	0.90	0.15	38,40,42,48	0
5	IOD	B	721	1/1	0.90	0.08	57,57,57,57	1
4	EDO	C	708	4/4	0.91	0.26	35,35,38,39	0
4	EDO	B	708	4/4	0.91	0.18	48,50,54,63	0
4	EDO	A	705	4/4	0.91	0.11	44,46,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	706	4/4	0.91	0.22	33,37,42,49	0
4	EDO	C	704	4/4	0.91	0.11	37,41,47,50	0
7	CA	A	746	1/1	0.91	0.23	54,54,54,54	0
4	EDO	A	711	4/4	0.92	0.12	36,37,44,45	0
5	IOD	B	719	1/1	0.92	0.06	67,67,67,67	1
9	CL	B	748	1/1	0.92	0.17	29,29,29,29	0
9	CL	D	750	1/1	0.92	0.09	50,50,50,50	0
5	IOD	A	732	1/1	0.92	0.04	50,50,50,50	1
4	EDO	B	704	4/4	0.92	0.20	22,26,38,46	0
4	EDO	B	705	4/4	0.92	0.15	33,35,35,40	0
4	EDO	C	714	4/4	0.92	0.25	38,40,43,44	0
4	EDO	D	712	4/4	0.92	0.14	48,50,50,51	0
5	IOD	C	737	1/1	0.92	0.05	58,58,58,58	1
4	EDO	C	705	4/4	0.92	0.13	32,35,36,39	0
5	IOD	B	742	1/1	0.92	0.07	55,55,55,55	1
5	IOD	C	727	1/1	0.92	0.06	56,56,56,56	1
4	EDO	B	703	4/4	0.92	0.14	28,31,34,43	0
9	CL	B	747	1/1	0.93	0.09	43,43,43,43	0
4	EDO	B	711	4/4	0.93	0.24	48,50,52,54	0
5	IOD	B	743	1/1	0.93	0.07	54,54,54,54	1
5	IOD	D	741	1/1	0.93	0.15	91,91,91,91	0
9	CL	A	749	1/1	0.93	0.06	53,53,53,53	0
4	EDO	A	702	4/4	0.93	0.19	27,32,34,35	0
5	IOD	C	741	1/1	0.93	0.07	67,67,67,67	1
4	EDO	A	712	4/4	0.94	0.11	35,42,42,43	0
5	IOD	B	724	1/1	0.94	0.09	45,45,45,45	1
5	IOD	A	725	1/1	0.94	0.14	90,90,90,90	0
8	ACT	A	747	4/4	0.94	0.26	42,42,50,59	0
5	IOD	A	743	1/1	0.94	0.06	56,56,56,56	1
5	IOD	D	719	1/1	0.94	0.05	47,47,47,47	1
5	IOD	D	718	1/1	0.94	0.10	45,45,45,45	1
5	IOD	A	719	1/1	0.94	0.05	63,63,63,63	1
8	ACT	C	701	4/4	0.94	0.23	44,45,52,54	0
4	EDO	D	703	4/4	0.94	0.13	28,32,39,45	0
5	IOD	D	721	1/1	0.94	0.08	48,48,48,48	1
5	IOD	B	734	1/1	0.95	0.04	58,58,58,58	1
5	IOD	D	740	1/1	0.95	0.04	45,45,45,45	1
5	IOD	B	731	1/1	0.95	0.04	48,48,48,48	1
8	ACT	B	744	4/4	0.95	0.17	43,44,45,46	0
5	IOD	C	720	1/1	0.95	0.05	54,54,54,54	1
4	EDO	D	709	4/4	0.95	0.29	37,39,41,45	0
4	EDO	C	715	4/4	0.95	0.11	35,36,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	D	736	1/1	0.95	0.06	55,55,55,55	1
5	IOD	A	738[B]	1/1	0.96	0.05	61,61,61,61	1
5	IOD	C	742	1/1	0.96	0.05	63,63,63,63	1
5	IOD	A	716	1/1	0.96	0.04	51,51,51,51	1
5	IOD	C	723	1/1	0.96	0.04	53,53,53,53	1
5	IOD	A	722	1/1	0.96	0.05	51,51,51,51	1
5	IOD	B	720	1/1	0.96	0.10	67,67,67,67	1
5	IOD	B	741	1/1	0.96	0.05	59,59,59,59	1
5	IOD	A	721	1/1	0.96	0.06	62,62,62,62	1
4	EDO	D	705	4/4	0.96	0.24	24,24,34,35	0
5	IOD	B	717	1/1	0.96	0.07	49,49,49,49	1
5	IOD	C	725	1/1	0.96	0.10	67,67,67,67	1
4	EDO	B	701	4/4	0.96	0.20	24,27,34,37	0
5	IOD	A	724	1/1	0.96	0.03	58,58,58,58	1
4	EDO	C	703	4/4	0.96	0.15	21,24,26,31	0
5	IOD	A	740	1/1	0.96	0.08	53,53,53,53	1
5	IOD	A	723	1/1	0.96	0.07	56,56,56,56	1
5	IOD	A	738[A]	1/1	0.96	0.05	48,48,48,48	1
5	IOD	B	716	1/1	0.96	0.07	50,50,50,50	1
5	IOD	B	740	1/1	0.97	0.03	53,53,53,53	1
5	IOD	B	736	1/1	0.97	0.04	60,60,60,60	1
5	IOD	C	734	1/1	0.97	0.04	51,51,51,51	1
5	IOD	C	735	1/1	0.97	0.04	49,49,49,49	1
5	IOD	C	740	1/1	0.97	0.04	58,58,58,58	1
5	IOD	B	726	1/1	0.97	0.03	56,56,56,56	1
5	IOD	A	741	1/1	0.97	0.03	64,64,64,64	1
5	IOD	C	722	1/1	0.97	0.08	51,51,51,51	1
5	IOD	D	733	1/1	0.97	0.05	59,59,59,59	1
5	IOD	D	738	1/1	0.97	0.03	50,50,50,50	1
5	IOD	B	727	1/1	0.97	0.04	42,42,42,42	1
5	IOD	D	727	1/1	0.97	0.06	44,44,44,44	1
5	IOD	C	732	1/1	0.97	0.06	41,41,41,41	1
5	IOD	D	743	1/1	0.97	0.05	56,56,56,56	1
9	CL	B	746	1/1	0.97	0.06	50,50,50,50	0
5	IOD	A	736	1/1	0.97	0.04	48,48,48,48	1
5	IOD	A	739	1/1	0.97	0.06	53,53,53,53	1
5	IOD	D	728	1/1	0.97	0.07	39,39,39,39	1
9	CL	A	750	1/1	0.98	0.05	36,36,36,36	0
5	IOD	A	720	1/1	0.98	0.05	53,53,53,53	1
5	IOD	A	718	1/1	0.98	0.03	48,48,48,48	1
5	IOD	A	734	1/1	0.98	0.06	45,45,45,45	1
5	IOD	B	733	1/1	0.98	0.03	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	D	726	1/1	0.98	0.05	44,44,44,44	1
5	IOD	A	731	1/1	0.98	0.03	43,43,43,43	1
5	IOD	D	730	1/1	0.98	0.04	53,53,53,53	1
5	IOD	B	725	1/1	0.98	0.07	39,39,39,39	1
5	IOD	D	725	1/1	0.98	0.03	46,46,46,46	1
5	IOD	D	734	1/1	0.98	0.03	46,46,46,46	1
5	IOD	D	739	1/1	0.98	0.07	50,50,50,50	1
5	IOD	B	722	1/1	0.98	0.07	47,47,47,47	1
5	IOD	D	735	1/1	0.98	0.05	48,48,48,48	1
5	IOD	B	735	1/1	0.98	0.03	68,68,68,68	1
5	IOD	B	738	1/1	0.98	0.05	46,46,46,46	1
5	IOD	C	719	1/1	0.98	0.04	52,52,52,52	1
5	IOD	D	717	1/1	0.98	0.03	42,42,42,42	1
9	CL	B	745	1/1	0.98	0.07	51,51,51,51	0
5	IOD	B	718	1/1	0.99	0.03	48,48,48,48	1
5	IOD	C	730	1/1	0.99	0.04	39,39,39,39	1
5	IOD	A	742	1/1	0.99	0.09	37,37,37,37	1
5	IOD	D	737	1/1	0.99	0.03	49,49,49,49	1
5	IOD	C	739	1/1	0.99	0.04	47,47,47,47	1
5	IOD	C	717	1/1	0.99	0.03	55,55,55,55	1
5	IOD	B	739	1/1	0.99	0.07	38,38,38,38	1
5	IOD	B	737	1/1	0.99	0.03	44,44,44,44	1
5	IOD	B	732	1/1	0.99	0.02	50,50,50,50	1
5	IOD	D	714	1/1	0.99	0.04	43,43,43,43	1
5	IOD	B	730	1/1	0.99	0.04	39,39,39,39	1
5	IOD	A	733	1/1	0.99	0.03	48,48,48,48	1
5	IOD	C	718	1/1	0.99	0.04	44,44,44,44	1
5	IOD	A	728	1/1	0.99	0.04	43,43,43,43	1
5	IOD	C	726	1/1	0.99	0.02	54,54,54,54	1
5	IOD	B	729	1/1	0.99	0.03	43,43,43,43	1
5	IOD	D	742	1/1	0.99	0.07	37,37,37,37	1
5	IOD	C	731	1/1	0.99	0.03	49,49,49,49	1
5	IOD	A	735	1/1	0.99	0.04	45,45,45,45	1
9	CL	C	744	1/1	0.99	0.03	40,40,40,40	0
5	IOD	D	729	1/1	0.99	0.03	43,43,43,43	1
5	IOD	D	732	1/1	0.99	0.02	48,48,48,48	1
5	IOD	C	736	1/1	0.99	0.03	47,47,47,47	1
5	IOD	D	724	1/1	0.99	0.06	36,36,36,36	1
5	IOD	D	731	1/1	0.99	0.04	45,45,45,45	1
5	IOD	A	715	1/1	0.99	0.03	47,47,47,47	1
5	IOD	A	737	1/1	0.99	0.03	49,49,49,49	1
5	IOD	C	738	1/1	0.99	0.05	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IOD	C	733	1/1	0.99	0.04	50,50,50,50	1
5	IOD	A	730	1/1	0.99	0.05	36,36,36,36	1
5	IOD	D	715	1/1	0.99	0.02	48,48,48,48	1
5	IOD	B	728	1/1	1.00	0.06	33,33,33,33	1
5	IOD	C	729	1/1	1.00	0.06	39,39,39,39	1
5	IOD	D	723	1/1	1.00	0.02	42,42,42,42	1
5	IOD	D	713	1/1	1.00	0.05	34,34,34,34	0
5	IOD	A	727	1/1	1.00	0.04	36,36,36,36	1
5	IOD	A	714	1/1	1.00	0.04	32,32,32,32	0
5	IOD	A	717	1/1	1.00	0.05	33,33,33,33	0
5	IOD	B	715	1/1	1.00	0.04	34,34,34,34	0
5	IOD	C	716	1/1	1.00	0.06	34,34,34,34	0
5	IOD	A	729	1/1	1.00	0.05	36,36,36,36	1

6.5 Other polymers [i](#)

There are no such residues in this entry.