Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2025 – 10:28 PM JST

PDB ID	:	9KYR / pdb_00009kyr
Title	:	GH57 family amylopullulanase from Aquifex aeolicus D352N mutant complex with gama-cyclodextrin
Authors	:	Zhu, Z.M.; Wang, W.W.; Yu, F.; Li, M.J.; Xu, Q.; Zhou, H.; Huang, L.Q.; Wang, Q.S.
Deposited on	:	2024-12-09
Resolution	:	1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

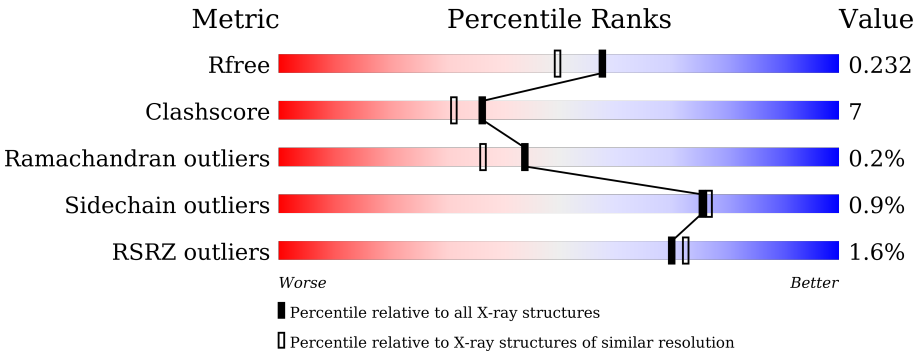
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.89 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	477	83% 14%
1	B	477	81% 18%
1	C	477	3% 82% 15%
1	D	477	2% 90% 9%
2	E	8	38% 62%
2	F	8	25% 25% 50%

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Mol	Chain	Length	Quality of chain
2	G	8	25% 62% 12%
2	H	8	12% 38% 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
2	GLC	E	2	-	-	X	-
5	EDO	B	504	-	-	X	-
5	EDO	B	505	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17203 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.

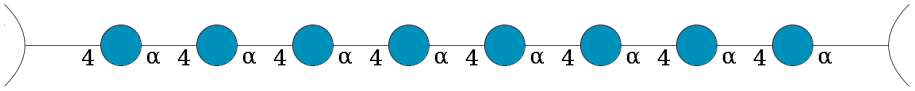
- Molecule 1 is a protein called Glycoside hydrolase family 57 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	2	0
			4034	2639	647	738	10			
1	B	476	Total	C	N	O	S	0	0	0
			4020	2631	645	735	9			
1	C	476	Total	C	N	O	S	0	1	0
			4026	2634	646	737	9			
1	D	477	Total	C	N	O	S	0	1	0
			4034	2639	647	738	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	ASN	ASP	engineered mutation	UNP O66934
B	352	ASN	ASP	engineered mutation	UNP O66934
C	352	ASN	ASP	engineered mutation	UNP O66934
D	352	ASN	ASP	engineered mutation	UNP O66934

- Molecule 2 is an oligosaccharide called Cyclooctakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	8	Total	C	O	0	0	0
			88	48	40			
2	F	8	Total	C	O	0	0	0
			88	48	40			
2	G	8	Total	C	O	0	0	0
			88	48	40			

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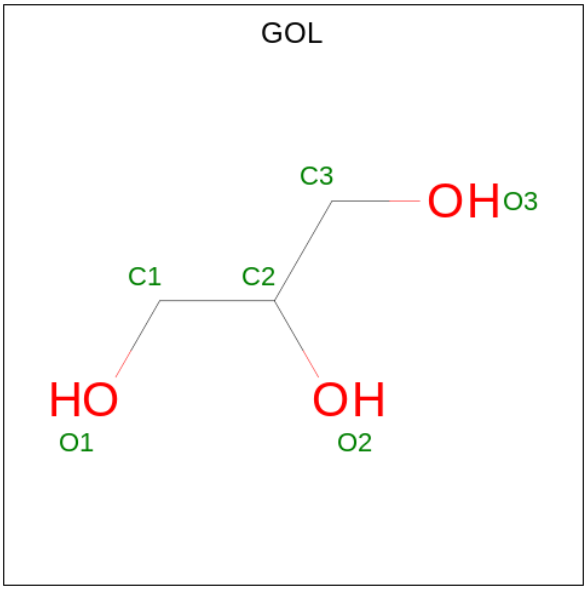
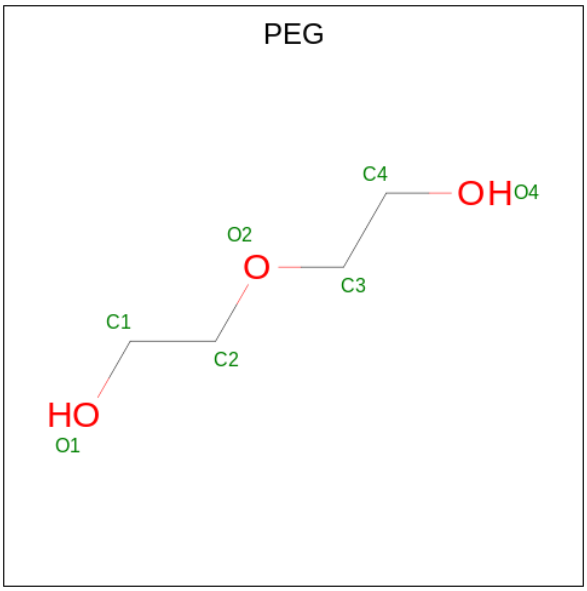
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	8	Total C O 88 48 40	0	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



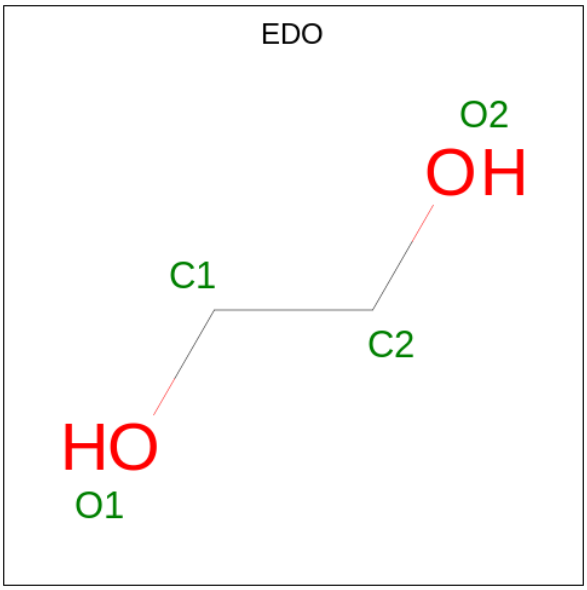
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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



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

- Molecule 6 is water.

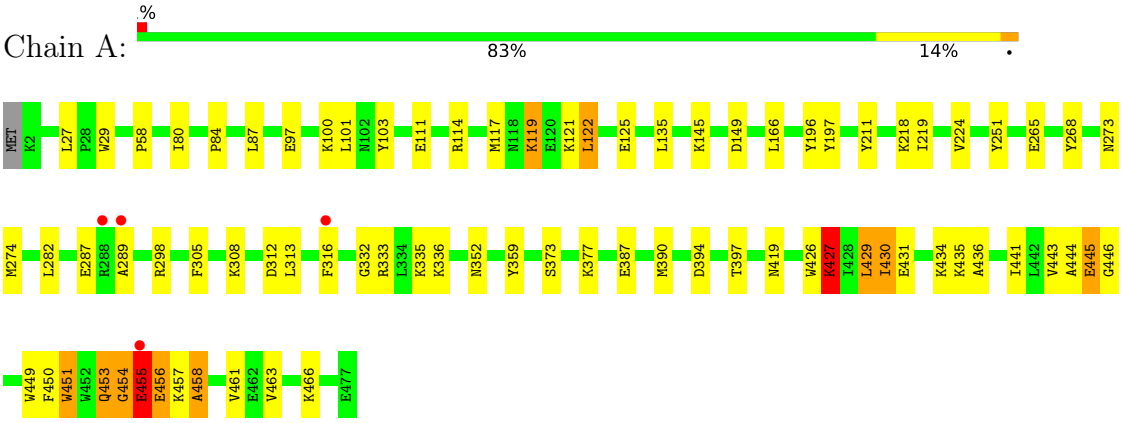
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	193	Total O 193 193	0	0
6	B	170	Total O 170 170	0	0
6	C	107	Total O 107 107	0	0
6	D	175	Total O 175 175	0	0

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.

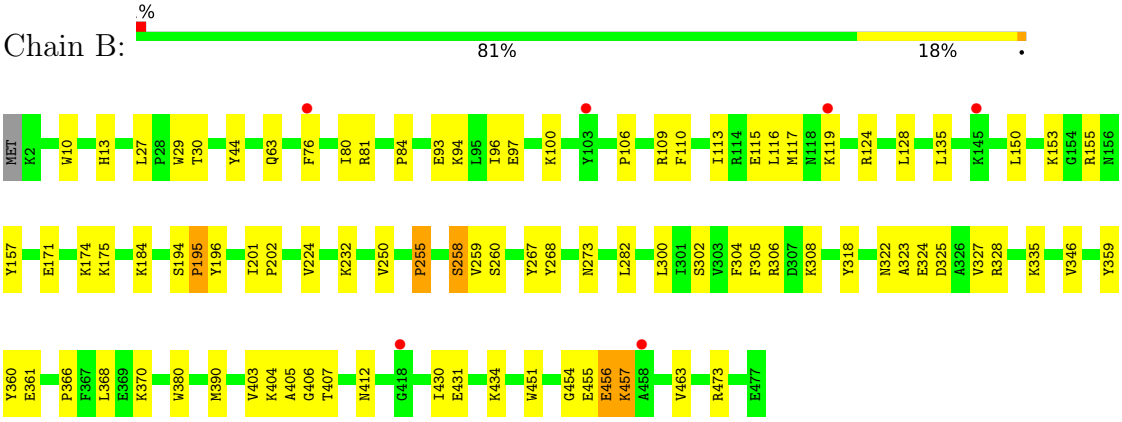
• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain A:



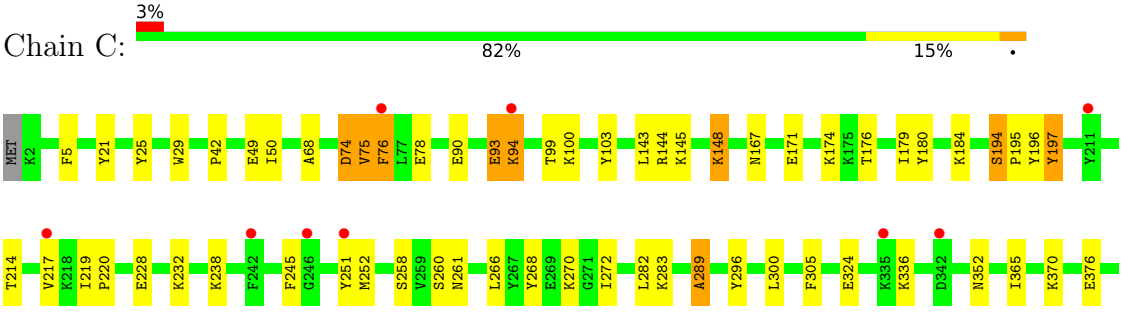
• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

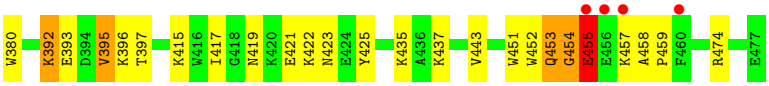
Chain B:



• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

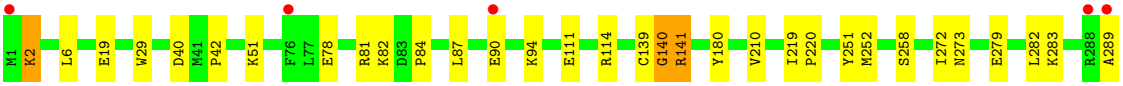
Chain C:





• Molecule 1: Glycoside hydrolase family 57 N-terminal domain-containing protein

Chain D:



• Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

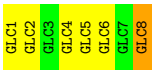
Chain E:

• Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

Chain F:

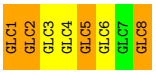
• Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

Chain G:



• Molecule 2: Cyclooctakis-(1-4)-(alpha-D-glucopyranose)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.83Å 61.53Å 195.40Å 83.94° 88.85° 89.09°	Depositor
Resolution (Å)	24.33 – 1.89 24.33 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.33-1.89) 94.6 (24.33-1.89)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.193 , 0.235 0.194 , 0.232	Depositor DCC
R_{free} test set	7682 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17203	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GLC, EDO, 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	0.80	22/4147 (0.5%)	0.67	3/5614 (0.1%)
1	B	0.66	18/4133 (0.4%)	0.60	5/5596 (0.1%)
1	C	0.71	14/4139 (0.3%)	0.60	7/5604 (0.1%)
1	D	0.54	4/4147 (0.1%)	0.58	5/5614 (0.1%)
All	All	0.68	58/16566 (0.4%)	0.61	20/22428 (0.1%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	PHE	C-O	-8.50	1.14	1.24
1	B	456	GLU	CA-C	-7.47	1.43	1.52
1	A	458	ALA	CA-C	-7.20	1.45	1.52
1	A	455	GLU	CA-C	-7.19	1.43	1.52
1	A	427	LYS	C-O	-7.05	1.15	1.24
1	B	403	VAL	C-O	-6.95	1.17	1.24
1	C	455	GLU	CA-C	-6.82	1.44	1.52
1	D	2	LYS	N-CA	-6.81	1.37	1.46
1	C	454	GLY	CA-C	-6.79	1.43	1.51
1	A	430	ILE	C-O	-6.75	1.16	1.24
1	B	405	ALA	C-O	-6.66	1.16	1.23
1	D	139	CYS	C-O	-6.54	1.16	1.23
1	A	426	TRP	C-O	-6.48	1.16	1.24
1	C	453	GLN	CA-C	-6.42	1.44	1.52
1	D	141	ARG	C-O	-6.41	1.16	1.24
1	B	195	PRO	C-O	-6.30	1.16	1.23
1	A	454	GLY	CA-C	-6.26	1.42	1.51
1	A	441	ILE	C-O	-6.13	1.17	1.24
1	B	258	SER	C-O	-6.12	1.16	1.24
1	C	194	SER	C-O	-6.04	1.18	1.24
1	A	451	TRP	C-O	-6.01	1.17	1.24
1	C	76	PHE	C-O	-6.01	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	SER	CA-C	-5.97	1.45	1.52
1	A	445	GLU	C-O	-5.92	1.16	1.24
1	A	446	GLY	C-O	-5.88	1.17	1.23
1	A	122	LEU	CA-C	-5.85	1.45	1.52
1	C	93	GLU	C-O	-5.81	1.16	1.24
1	A	453	GLN	C-O	-5.74	1.16	1.23
1	A	122	LEU	N-CA	-5.73	1.39	1.46
1	C	99	THR	N-CA	-5.73	1.39	1.46
1	B	455	GLU	N-CA	-5.71	1.39	1.46
1	A	429	LEU	C-O	-5.68	1.17	1.24
1	C	74	ASP	CA-C	-5.66	1.45	1.52
1	B	255	PRO	C-O	-5.65	1.16	1.23
1	B	407	THR	C-O	-5.62	1.16	1.24
1	B	196	TYR	C-O	-5.59	1.17	1.24
1	A	449	TRP	C-O	-5.59	1.17	1.24
1	A	352	ASN	C-O	-5.53	1.17	1.23
1	B	76	PHE	CA-CB	-5.53	1.44	1.53
1	D	457	LYS	CA-C	-5.46	1.45	1.52
1	A	453	GLN	CA-C	-5.43	1.45	1.52
1	C	451	TRP	C-O	-5.43	1.17	1.24
1	A	431	GLU	C-O	-5.35	1.18	1.24
1	B	454	GLY	CA-C	-5.32	1.44	1.51
1	A	121	LYS	N-CA	-5.31	1.39	1.45
1	A	436	ALA	C-O	-5.25	1.17	1.23
1	C	197	TYR	C-O	-5.24	1.17	1.24
1	B	456	GLU	N-CA	-5.20	1.39	1.46
1	C	352	ASN	C-O	-5.19	1.17	1.23
1	C	148	LYS	C-N	-5.19	1.27	1.33
1	B	194	SER	C-O	-5.17	1.18	1.24
1	B	10	TRP	C-O	-5.17	1.17	1.24
1	B	406	GLY	C-O	-5.15	1.17	1.23
1	C	395	VAL	C-O	-5.15	1.18	1.23
1	A	444	ALA	C-O	-5.12	1.17	1.24
1	B	259	VAL	N-CA	-5.12	1.39	1.46
1	C	75	VAL	N-CA	-5.09	1.40	1.46
1	A	450	PHE	C-O	-5.04	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	455	GLU	N-CA-C	-10.14	100.66	113.43
1	D	2	LYS	N-CA-C	-9.67	95.37	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	LYS	N-CA-C	-7.97	97.79	110.14
1	C	289	ALA	N-CA-C	7.91	122.29	108.52
1	B	455	GLU	N-CA-C	-7.46	94.84	108.65
1	D	456	GLU	N-CA-C	7.30	126.35	110.80
1	A	119	LYS	N-CA-C	6.88	120.72	109.85
1	C	196	TYR	N-CA-C	6.81	122.54	111.37
1	A	455	GLU	N-CA-C	-6.21	97.58	110.80
1	D	456	GLU	CA-C-N	-6.05	113.51	122.83
1	D	456	GLU	C-N-CA	-6.05	113.51	122.83
1	C	459	PRO	N-CA-C	6.01	120.51	111.14
1	B	405	ALA	N-CA-C	5.98	118.68	110.24
1	C	458	ALA	N-CA-C	5.93	122.92	109.81
1	B	13	HIS	N-CA-C	5.83	118.00	108.55
1	C	457	LYS	N-CA-C	5.60	120.82	113.20
1	C	75	VAL	N-CA-C	5.49	115.69	110.53
1	B	456	GLU	N-CA-C	5.28	118.09	109.59
1	D	140	GLY	N-CA-C	5.08	120.91	112.89
1	B	196	TYR	N-CA-C	5.05	121.56	110.80

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	4034	0	3944	53	0
1	B	4020	0	3932	69	0
1	C	4026	0	3936	63	0
1	D	4034	0	3948	41	0
2	E	88	0	65	10	0
2	F	88	0	72	4	0
2	G	88	0	72	1	0
2	H	88	0	72	6	0
3	A	18	0	23	0	0
3	B	12	0	16	1	0
3	D	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	20	0	0
4	B	7	0	10	1	0
4	C	7	0	10	3	0
5	A	12	0	18	1	0
5	B	12	0	18	12	0
5	C	4	0	6	0	0
6	A	193	0	0	12	0
6	B	170	0	0	9	0
6	C	107	0	0	7	0
6	D	175	0	0	13	0
All	All	17203	0	16170	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:GLU:HG3	1:C:454:GLY:HA3	1.40	1.04
2:E:1:GLC:O6	2:E:2:GLC:H61	1.68	0.93
1:D:141:ARG:N	6:D:601:HOH:O	2.05	0.89
1:B:232:LYS:NZ	6:B:602:HOH:O	2.10	0.85
1:B:473:ARG:NH2	6:B:601:HOH:O	2.08	0.85
1:B:201:ILE:H	5:B:505:EDO:H21	1.42	0.82
1:A:466:LYS:NZ	6:A:604:HOH:O	2.15	0.79
1:C:68:ALA:HB1	1:C:174:LYS:HD2	1.65	0.79
1:B:255:PRO:HD2	5:B:505:EDO:H22	1.65	0.78
1:D:40:ASP:CG	6:D:601:HOH:O	2.26	0.77
1:C:145:LYS:NZ	6:C:604:HOH:O	2.16	0.73
1:C:421:GLU:HG3	1:C:454:GLY:CA	2.17	0.73
1:C:103:TYR:OH	6:C:601:HOH:O	2.06	0.72
1:D:273:ASN:HB3	1:D:390:MET:HE1	1.72	0.72
1:A:149:ASP:OD1	6:A:602:HOH:O	2.09	0.70
1:A:287:GLU:O	6:A:601:HOH:O	2.08	0.70
1:A:335:LYS:NZ	6:A:608:HOH:O	2.22	0.70
1:D:299:GLU:OE1	6:D:602:HOH:O	2.09	0.70
1:C:228:GLU:OE1	1:C:232:LYS:HE3	1.92	0.69
1:A:298:ARG:NH2	6:A:609:HOH:O	2.25	0.69
1:B:267:TYR:OH	5:B:505:EDO:H11	1.94	0.68
1:C:49:GLU:OE2	6:C:603:HOH:O	2.11	0.67
1:B:260:SER:HB2	4:B:503:PEG:H31	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:OH	1:A:387:GLU:HA	1.95	0.67
1:A:251:TYR:CE1	1:A:390:MET:HE3	2.30	0.66
1:D:370:LYS:NZ	6:D:608:HOH:O	2.26	0.66
1:A:27:LEU:HG	1:A:463:VAL:HG11	1.77	0.66
1:C:184:LYS:HE2	1:C:245:PHE:HB3	1.78	0.66
1:A:458:ALA:HB3	1:A:461:VAL:CG1	2.26	0.65
1:C:251:TYR:OH	6:C:602:HOH:O	2.11	0.65
1:A:268:TYR:OH	6:A:603:HOH:O	2.14	0.65
1:D:258[A]:SER:OG	6:D:604:HOH:O	2.15	0.64
1:C:76:PHE:HA	1:C:94:LYS:HE2	1.80	0.63
1:B:100:LYS:HG3	1:B:117:MET:HE3	1.79	0.63
1:C:392:LYS:HG2	1:C:395:VAL:HG13	1.81	0.63
1:B:115:GLU:CD	1:B:155:ARG:HH12	2.07	0.63
1:B:29:TRP:CD2	2:F:8:GLC:H2	2.33	0.62
1:A:135:LEU:HD11	1:A:166:LEU:HG	1.81	0.62
1:C:296:TYR:CE2	1:C:397:THR:HG23	2.36	0.60
1:C:324:GLU:HG3	6:C:637:HOH:O	2.00	0.60
1:C:29:TRP:CD2	2:G:8:GLC:H2	2.36	0.60
1:B:81:ARG:HD3	6:B:717:HOH:O	2.02	0.59
1:A:100:LYS:HD2	1:A:101:LEU:N	2.17	0.59
1:A:29:TRP:CD2	2:E:8:GLC:H2	2.37	0.58
1:D:111:GLU:OE1	1:D:114:ARG:HD3	2.03	0.58
1:C:50:ILE:HG23	1:C:376:GLU:HG3	1.84	0.58
1:B:451:TRP:CZ3	2:F:5:GLC:H62	2.39	0.58
1:D:29:TRP:CD2	2:H:8:GLC:H2	2.39	0.58
1:C:324:GLU:HG2	1:C:370:LYS:HE3	1.87	0.57
1:A:282:LEU:HB2	1:A:305:PHE:CD2	2.40	0.57
1:C:261:ASN:HD22	4:C:502:PEG:H21	1.70	0.57
1:B:456:GLU:O	1:B:457:LYS:C	2.46	0.56
1:A:111:GLU:OE2	1:A:114:ARG:NH1	2.39	0.56
1:C:296:TYR:CE2	1:C:397:THR:CG2	2.87	0.56
1:B:335:LYS:HD2	1:B:380:TRP:CZ2	2.41	0.56
1:D:90:GLU:O	1:D:94:LYS:HG3	2.06	0.55
1:B:27:LEU:HG	1:B:463:VAL:HG11	1.87	0.55
2:E:1:GLC:O6	2:E:2:GLC:C6	2.49	0.55
1:D:140:GLY:C	6:D:601:HOH:O	2.46	0.55
1:D:140:GLY:HA3	6:D:601:HOH:O	2.06	0.55
1:B:110:PHE:HB2	1:B:113:ILE:HD12	1.89	0.55
1:B:473:ARG:CZ	6:B:601:HOH:O	2.50	0.55
1:A:224:VAL:HG11	1:A:434:LYS:HG2	1.88	0.54
1:D:84:PRO:HA	1:D:87:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LEU:HG	1:D:289:ALA:HB1	1.89	0.54
1:C:296:TYR:HE2	1:C:397:THR:HG21	1.71	0.54
1:B:115:GLU:OE1	1:B:155:ARG:NH1	2.40	0.54
1:C:260:SER:HB2	4:C:502:PEG:H41	1.89	0.54
2:E:1:GLC:HO6	2:E:2:GLC:H61	1.70	0.54
1:B:255:PRO:HD2	5:B:505:EDO:C2	2.36	0.53
1:B:308:LYS:HG3	5:B:504:EDO:H12	1.90	0.53
1:A:282:LEU:HG	1:A:289:ALA:HB1	1.90	0.53
1:A:332:GLY:O	1:A:336:LYS:HG2	2.09	0.53
1:C:453:GLN:NE2	1:C:454:GLY:H	2.07	0.53
1:B:124:ARG:HD3	6:B:657:HOH:O	2.09	0.53
1:B:302:SER:OG	1:B:390:MET:HE1	2.09	0.52
1:B:171:GLU:O	1:B:175:LYS:HG2	2.09	0.52
1:A:97:GLU:HA	1:A:100:LYS:HE3	1.92	0.52
1:D:458:ALA:HB3	1:D:461:VAL:CG1	2.38	0.52
1:A:224:VAL:HG22	1:A:430:ILE:HG23	1.92	0.52
1:D:457:LYS:C	6:D:673:HOH:O	2.52	0.52
1:A:451:TRP:CZ3	2:E:5:GLC:H62	2.45	0.52
1:B:304:PHE:HE1	1:B:346:VAL:HG11	1.75	0.52
1:A:458:ALA:HB3	1:A:461:VAL:HG13	1.92	0.51
1:C:258[A]:SER:OG	6:C:605:HOH:O	2.19	0.51
1:C:435:LYS:NZ	6:C:610:HOH:O	2.34	0.51
1:B:282:LEU:HB2	1:B:305:PHE:CD2	2.46	0.51
1:B:116:LEU:HA	1:B:119:LYS:HZ3	1.76	0.51
1:B:150:LEU:HA	1:B:153:LYS:HD3	1.92	0.50
1:A:373:SER:O	1:A:377:LYS:HG3	2.10	0.50
1:C:214:THR:O	1:C:217:VAL:HG12	2.11	0.50
1:B:201:ILE:H	5:B:505:EDO:C2	2.18	0.50
1:C:42:PRO:HG3	1:C:180:TYR:CZ	2.47	0.50
1:A:80:ILE:HG21	1:A:135:LEU:HG	1.94	0.50
1:B:80:ILE:HG21	1:B:135:LEU:HG	1.94	0.50
1:D:458:ALA:HB1	2:H:1:GLC:C6	2.42	0.49
2:H:1:GLC:H61	2:H:2:GLC:O5	2.11	0.49
1:A:456:GLU:O	1:A:457:LYS:CB	2.61	0.49
1:C:74:ASP:O	1:C:78:GLU:HG3	2.12	0.49
1:B:80:ILE:HG21	1:B:135:LEU:HD21	1.94	0.49
1:B:255:PRO:CD	5:B:505:EDO:H22	2.41	0.49
1:C:419:ASN:ND2	1:C:422:LYS:HD2	2.28	0.49
1:C:21:TYR:HD1	1:C:474:ARG:HH21	1.61	0.49
1:B:30:THR:HG21	1:B:63:GLN:HB3	1.95	0.49
1:C:380:TRP:H	1:C:380:TRP:CD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:TYR:CZ	1:C:453:GLN:OE1	2.66	0.49
1:A:224:VAL:CG1	1:A:434:LYS:HG2	2.43	0.49
1:D:458:ALA:HB1	2:H:1:GLC:O6	2.13	0.48
1:B:306:ARG:HH21	5:B:504:EDO:H12	1.78	0.48
1:B:412:ASN:HB2	6:B:634:HOH:O	2.14	0.48
1:D:380:TRP:H	1:D:380:TRP:CD1	2.32	0.48
5:A:507:EDO:O2	6:A:605:HOH:O	2.19	0.48
1:C:25:TYR:O	1:C:75:VAL:HG12	2.14	0.48
1:C:421:GLU:OE1	1:C:421:GLU:N	2.42	0.48
1:C:296:TYR:HE2	1:C:397:THR:CG2	2.27	0.48
1:D:81:ARG:HD3	6:D:603:HOH:O	2.13	0.48
1:D:90:GLU:OE1	1:D:90:GLU:N	2.44	0.48
1:B:93:GLU:O	1:B:97:GLU:HG3	2.14	0.48
1:B:201:ILE:HG12	5:B:505:EDO:H21	1.96	0.48
1:B:431:GLU:OE1	1:B:434:LYS:HE3	2.14	0.47
1:C:392:LYS:HG2	1:C:395:VAL:CG1	2.43	0.47
1:D:140:GLY:CA	6:D:601:HOH:O	2.61	0.47
1:D:279:GLU:HG2	1:D:283:LYS:HE3	1.95	0.47
1:A:114:ARG:NH2	6:A:625:HOH:O	2.47	0.47
1:B:80:ILE:HG21	1:B:135:LEU:CD2	2.45	0.47
1:C:148:LYS:HB2	1:C:148:LYS:HE2	1.63	0.47
1:C:283:LYS:HD3	1:C:289:ALA:HB1	1.96	0.47
1:D:51:LYS:NZ	6:D:622:HOH:O	2.46	0.47
1:D:293:LEU:HD23	1:D:398:GLU:HB2	1.96	0.47
1:A:313:LEU:HD11	1:A:333:ARG:HD2	1.96	0.47
1:A:265:GLU:HB3	6:A:739:HOH:O	2.15	0.47
1:B:184:LYS:NZ	6:B:612:HOH:O	2.46	0.46
1:C:252:MET:HE3	1:C:272:ILE:HD11	1.96	0.46
2:E:1:GLC:O3	2:E:2:GLC:O2	2.23	0.46
1:C:176:THR:O	1:C:179:ILE:HG22	2.16	0.46
1:C:282:LEU:HB2	1:C:305:PHE:CD2	2.50	0.46
1:B:44:TYR:OH	3:B:502:GOL:H32	2.15	0.46
1:C:419:ASN:HD21	1:C:422:LYS:HD2	1.80	0.46
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.56	0.45
1:B:325:ASP:OD1	1:B:328:ARG:NH2	2.49	0.45
1:D:19:GLU:OE2	6:D:605:HOH:O	2.21	0.45
1:A:100:LYS:HA	1:A:103:TYR:HB2	1.98	0.45
1:A:308:LYS:NZ	1:A:312:ASP:OD2	2.50	0.45
1:B:116:LEU:HD23	1:B:119:LYS:HZ1	1.81	0.45
1:C:453:GLN:HE21	1:C:454:GLY:N	2.14	0.45
1:C:5:PHE:CZ	1:C:392:LYS:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:ALA:HB3	1:D:461:VAL:HG13	1.98	0.45
1:C:415:LYS:O	1:C:422:LYS:HE3	2.16	0.45
1:C:435:LYS:O	1:C:437:LYS:HD2	2.17	0.45
1:B:109:ARG:NH2	1:B:361:GLU:OE2	2.50	0.44
1:C:283:LYS:HD3	1:C:289:ALA:CB	2.48	0.44
1:B:153:LYS:HE3	1:B:157:TYR:CE1	2.53	0.44
1:A:145:LYS:HE3	6:A:619:HOH:O	2.18	0.44
1:B:224:VAL:HG22	1:B:430:ILE:HG23	1.99	0.44
1:B:306:ARG:HH21	5:B:504:EDO:C1	2.31	0.44
1:A:394:ASP:OD1	1:A:394:ASP:N	2.51	0.43
1:B:29:TRP:CG	2:F:8:GLC:H2	2.53	0.43
1:A:251:TYR:OH	1:A:387:GLU:OE1	2.27	0.43
1:B:202:PRO:HG2	1:B:258:SER:OG	2.19	0.43
1:B:328:ARG:NH2	1:C:376:GLU:O	2.52	0.43
1:C:194:SER:O	1:C:195:PRO:C	2.61	0.43
1:B:250:VAL:HB	1:B:273:ASN:OD1	2.19	0.43
1:D:308:LYS:NZ	1:D:312:ASP:OD2	2.49	0.43
1:B:328:ARG:HB2	1:C:49:GLU:OE1	2.18	0.43
1:A:101:LEU:HD11	2:E:1:GLC:H2	2.00	0.43
1:A:211:TYR:OH	1:A:219:ILE:HG12	2.19	0.43
1:D:29:TRP:CG	2:H:8:GLC:H2	2.54	0.43
2:E:2:GLC:O4	2:E:2:GLC:O6	2.36	0.43
1:B:255:PRO:HD2	5:B:505:EDO:C1	2.49	0.43
1:B:268:TYR:CE2	1:B:300:LEU:HD22	2.54	0.43
1:C:197:TYR:CE1	1:C:443:VAL:HG22	2.54	0.43
1:C:167:ASN:O	1:C:171:GLU:HG3	2.19	0.43
1:C:392:LYS:HB2	1:C:392:LYS:HE2	1.30	0.43
1:D:451:TRP:CZ3	2:H:5:GLC:H62	2.53	0.43
1:A:251:TYR:HE1	1:A:390:MET:HE3	1.81	0.43
1:D:42:PRO:HG3	1:D:180:TYR:CZ	2.54	0.43
1:D:141:ARG:NH2	6:D:628:HOH:O	2.51	0.43
1:D:78:GLU:O	1:D:82:LYS:HG3	2.18	0.43
1:A:419:ASN:HB2	6:A:662:HOH:O	2.19	0.42
1:D:2:LYS:HB3	1:D:2:LYS:HE2	1.88	0.42
1:D:251:TYR:OH	1:D:387:GLU:HA	2.19	0.42
1:C:452:TRP:O	1:C:455:GLU:HG3	2.19	0.42
2:F:3:GLC:H61	2:F:4:GLC:H5	2.02	0.42
1:A:251:TYR:CD1	1:A:274[B]:MET:HE2	2.54	0.42
1:B:323:ALA:O	1:B:327:VAL:HG12	2.20	0.42
1:C:268:TYR:CZ	1:C:300:LEU:HD22	2.54	0.42
1:D:210:VAL:HG21	1:D:219:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLN:HG3	1:A:454:GLY:N	2.34	0.42
1:A:458:ALA:HB3	1:A:461:VAL:HG11	2.00	0.42
1:B:366:PRO:O	1:B:370:LYS:HG3	2.18	0.42
1:C:261:ASN:HB2	4:C:502:PEG:H11	2.02	0.42
1:C:266:LEU:O	1:C:270:LYS:HG2	2.19	0.42
1:D:220:PRO:HD3	1:D:423:ASN:CG	2.43	0.42
1:D:252:MET:HE3	1:D:272:ILE:HD11	2.01	0.42
1:B:84:PRO:HG2	1:B:128:LEU:HG	2.02	0.42
1:C:219:ILE:HG22	1:C:417:ILE:HG12	2.02	0.42
1:A:359:TYR:OH	2:E:2:GLC:O2	2.25	0.41
1:B:306:ARG:NH2	5:B:504:EDO:C1	2.83	0.41
1:A:197:TYR:CZ	1:A:443:VAL:HG22	2.54	0.41
1:A:125:GLU:CD	1:A:125:GLU:H	2.28	0.41
1:C:143:LEU:HA	1:C:143:LEU:HD23	1.79	0.41
1:A:251:TYR:HD1	1:A:274[B]:MET:HE2	1.84	0.41
1:D:283:LYS:HA	1:D:283:LYS:HD3	1.89	0.41
1:B:96:ILE:HG23	1:B:117:MET:HE1	2.02	0.41
1:B:94:LYS:NZ	6:B:619:HOH:O	2.53	0.41
1:B:380:TRP:CD1	1:B:380:TRP:H	2.38	0.41
1:A:58:PRO:HG2	1:A:196:TYR:HA	2.02	0.41
1:B:322:ASN:OD1	1:B:324:GLU:N	2.54	0.41
1:B:390:MET:O	1:B:390:MET:HE3	2.21	0.41
1:A:273:ASN:HB2	1:A:390:MET:HE1	2.02	0.41
1:A:316:PHE:CE1	2:E:4:GLC:H2	2.56	0.41
1:A:218:LYS:HD3	6:A:617:HOH:O	2.21	0.41
1:B:174:LYS:HB2	1:B:175:LYS:HE3	2.02	0.41
1:B:195:PRO:HD2	1:B:255:PRO:HD3	2.03	0.41
1:B:431:GLU:HG2	6:B:668:HOH:O	2.20	0.41
1:C:144:ARG:NH1	1:C:365:ILE:HG21	2.36	0.41
1:A:84:PRO:HA	1:A:87:LEU:HG	2.03	0.41
1:A:429:LEU:HD21	1:A:445:GLU:HG2	2.03	0.41
1:B:80:ILE:HG21	1:B:135:LEU:CG	2.51	0.41
1:B:106:PRO:HD2	1:B:359:TYR:HA	2.02	0.41
1:D:363:ASN:ND2	3:D:501:GOL:H2	2.35	0.41
1:B:318:TYR:HB2	1:B:360:TYR:OH	2.21	0.40
1:C:100:LYS:HA	1:C:103:TYR:HB2	2.02	0.40
1:A:456:GLU:CB	1:A:461:VAL:HG21	2.51	0.40
1:B:224:VAL:CG1	1:B:434:LYS:HG2	2.51	0.40
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.86	0.40
1:C:336:LYS:HB3	1:C:336:LYS:HE2	1.56	0.40
1:D:6:LEU:O	1:D:383:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASP:HB3	3:D:501:GOL:H12	2.04	0.40
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.95	0.40
1:C:220:PRO:HD3	1:C:423:ASN:CG	2.46	0.40
1:C:238:LYS:HE2	1:C:238:LYS:HB3	1.89	0.40

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	476/477 (100%)	466 (98%)	8 (2%)	2 (0%)	30	22
1	B	474/477 (99%)	460 (97%)	13 (3%)	1 (0%)	44	36
1	C	475/477 (100%)	463 (98%)	12 (2%)	0	100	100
1	D	476/477 (100%)	467 (98%)	8 (2%)	1 (0%)	44	36
All	All	1901/1908 (100%)	1856 (98%)	41 (2%)	4 (0%)	44	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	GLU
1	B	457	LYS
1	D	456	GLU
1	A	456	GLU

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	432/437 (99%)	425 (98%)	7 (2%)	58 56
1	B	430/437 (98%)	429 (100%)	1 (0%)	92 93
1	C	431/437 (99%)	424 (98%)	7 (2%)	58 56
1	D	432/437 (99%)	432 (100%)	0	100 100
All	All	1725/1748 (99%)	1710 (99%)	15 (1%)	75 77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	MET
1	A	119	LYS
1	A	122	LEU
1	A	397	THR
1	A	427	LYS
1	A	435	LYS
1	A	455	GLU
1	B	404	LYS
1	C	90	GLU
1	C	93	GLU
1	C	94	LYS
1	C	392	LYS
1	C	393	GLU
1	C	396	LYS
1	C	455	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	156	ASN
1	B	319	HIS
1	B	352	ASN
1	C	208	ASN
1	C	216	ASN
1	C	322	ASN
1	C	453	GLN
1	D	69	GLN
1	D	156	ASN

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Mol	Chain	Res	Type
1	D	216	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

32 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	GLC	E	1	2	11,11,12	2.00	4 (36%)	15,15,17	2.62	7 (46%)
2	GLC	E	2	2	11,11,12	1.71	2 (18%)	15,15,17	2.42	8 (53%)
2	GLC	E	3	2	11,11,12	1.14	2 (18%)	15,15,17	2.75	10 (66%)
2	GLC	E	4	2	11,11,12	0.70	0	15,15,17	1.55	2 (13%)
2	GLC	E	5	2	11,11,12	0.56	0	15,15,17	1.70	3 (20%)
2	GLC	E	6	2	11,11,12	2.48	5 (45%)	15,15,17	2.29	4 (26%)
2	GLC	E	7	2	11,11,12	2.79	4 (36%)	15,15,17	2.25	3 (20%)
2	GLC	E	8	2	11,11,12	0.59	0	15,15,17	1.02	1 (6%)
2	GLC	F	1	2	11,11,12	0.74	0	15,15,17	1.06	0
2	GLC	F	2	2	11,11,12	0.54	0	15,15,17	1.48	1 (6%)
2	GLC	F	3	2	11,11,12	0.51	0	15,15,17	1.42	3 (20%)
2	GLC	F	4	2	11,11,12	0.65	0	15,15,17	1.14	3 (20%)
2	GLC	F	5	2	11,11,12	0.52	0	15,15,17	2.11	4 (26%)
2	GLC	F	6	2	11,11,12	0.76	0	15,15,17	1.25	1 (6%)
2	GLC	F	7	2	11,11,12	0.51	0	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	F	8	2	11,11,12	0.70	0	15,15,17	1.03	1 (6%)
2	GLC	G	1	2	11,11,12	0.66	0	15,15,17	0.81	1 (6%)
2	GLC	G	2	2	11,11,12	0.69	0	15,15,17	1.37	4 (26%)
2	GLC	G	3	2	11,11,12	0.71	0	15,15,17	0.90	0
2	GLC	G	4	2	11,11,12	0.58	0	15,15,17	1.42	3 (20%)
2	GLC	G	5	2	11,11,12	0.54	0	15,15,17	1.86	4 (26%)
2	GLC	G	6	2	11,11,12	0.51	0	15,15,17	1.22	2 (13%)
2	GLC	G	7	2	11,11,12	0.64	0	15,15,17	0.77	0
2	GLC	G	8	2	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
2	GLC	H	1	2	11,11,12	0.55	0	15,15,17	1.54	1 (6%)
2	GLC	H	2	2	11,11,12	0.74	0	15,15,17	1.63	3 (20%)
2	GLC	H	3	2	11,11,12	0.54	0	15,15,17	1.44	3 (20%)
2	GLC	H	4	2	11,11,12	0.57	0	15,15,17	1.71	2 (13%)
2	GLC	H	5	2	11,11,12	0.50	0	15,15,17	1.87	4 (26%)
2	GLC	H	6	2	11,11,12	0.55	0	15,15,17	1.06	1 (6%)
2	GLC	H	7	2	11,11,12	0.68	0	15,15,17	0.65	0
2	GLC	H	8	2	11,11,12	0.64	0	15,15,17	1.09	2 (13%)

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	GLC	E	1	2	-	1/2/19/22	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	7	2	-	0/2/19/22	0/1/1/1
2	GLC	E	8	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/19/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	2/2/19/22	0/1/1/1
2	GLC	F	6	2	-	0/2/19/22	0/1/1/1
2	GLC	F	7	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	F	8	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	2/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	1/2/19/22	0/1/1/1
2	GLC	G	7	2	-	0/2/19/22	0/1/1/1
2	GLC	G	8	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/19/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	1/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	6	2	-	0/2/19/22	0/1/1/1
2	GLC	H	7	2	-	0/2/19/22	0/1/1/1
2	GLC	H	8	2	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	GLC	O5-C1	-5.00	1.35	1.43
2	E	7	GLC	O3-C3	-4.82	1.31	1.43
2	E	7	GLC	O5-C5	-4.44	1.34	1.43
2	E	6	GLC	O4-C4	-4.07	1.33	1.43
2	E	6	GLC	O2-C2	-3.78	1.35	1.43
2	E	2	GLC	O2-C2	-3.68	1.35	1.43
2	E	1	GLC	O5-C1	-3.59	1.38	1.43
2	E	1	GLC	O2-C2	-3.32	1.36	1.43
2	E	6	GLC	O5-C5	-3.28	1.36	1.43
2	E	6	GLC	O3-C3	-3.20	1.35	1.43
2	E	6	GLC	O6-C6	-3.10	1.29	1.42
2	E	2	GLC	O5-C1	-2.99	1.38	1.43
2	E	1	GLC	O4-C4	-2.83	1.36	1.43
2	E	7	GLC	O4-C4	-2.60	1.36	1.43
2	E	1	GLC	C2-C3	-2.46	1.48	1.52
2	E	3	GLC	C4-C3	-2.14	1.46	1.52
2	E	3	GLC	C1-C2	2.03	1.56	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	7	GLC	C1-O5-C5	6.38	120.84	112.19
2	E	6	GLC	O5-C1-C2	-6.01	101.49	110.77
2	E	3	GLC	O3-C3-C4	-5.66	97.26	110.35
2	F	5	GLC	C1-O5-C5	5.41	119.53	112.19
2	H	4	GLC	C1-O5-C5	5.07	119.06	112.19
2	E	1	GLC	O5-C1-C2	-4.94	103.15	110.77
2	E	2	GLC	O5-C5-C6	4.91	114.90	107.20
2	H	1	GLC	C1-O5-C5	4.80	118.70	112.19
2	E	1	GLC	O5-C5-C6	4.67	114.52	107.20
2	H	5	GLC	C1-O5-C5	4.50	118.30	112.19
2	E	7	GLC	O2-C2-C3	4.50	119.15	110.14
2	E	4	GLC	C1-C2-C3	4.41	115.08	109.67
2	F	2	GLC	O5-C1-C2	-4.40	103.98	110.77
2	E	2	GLC	C1-O5-C5	-4.17	106.55	112.19
2	G	5	GLC	C1-O5-C5	4.11	117.77	112.19
2	E	3	GLC	O5-C5-C6	3.72	113.04	107.20
2	H	2	GLC	C1-C2-C3	3.71	114.23	109.67
2	E	1	GLC	C1-O5-C5	3.57	117.03	112.19
2	G	5	GLC	O4-C4-C3	-3.55	102.15	110.35
2	E	5	GLC	O4-C4-C3	-3.53	102.18	110.35
2	F	3	GLC	O5-C1-C2	-3.52	105.33	110.77
2	H	2	GLC	C2-C3-C4	3.52	116.98	110.89
2	E	6	GLC	O5-C5-C6	3.51	112.70	107.20
2	F	5	GLC	O4-C4-C5	3.42	117.79	109.30
2	E	6	GLC	O2-C2-C1	3.23	115.76	109.15
2	E	1	GLC	O6-C6-C5	3.22	122.35	111.29
2	F	6	GLC	C1-C2-C3	-3.22	105.70	109.67
2	E	3	GLC	O2-C2-C1	3.17	115.64	109.15
2	H	3	GLC	O5-C1-C2	-3.06	106.05	110.77
2	E	3	GLC	O3-C3-C2	3.04	115.82	109.99
2	H	5	GLC	O4-C4-C3	-3.04	103.33	110.35
2	H	4	GLC	O5-C5-C6	-2.98	102.53	107.20
2	F	3	GLC	O4-C4-C3	-2.95	103.52	110.35
2	G	4	GLC	C1-O5-C5	2.95	116.19	112.19
2	E	5	GLC	C1-O5-C5	2.91	116.14	112.19
2	E	3	GLC	O4-C4-C3	-2.90	103.64	110.35
2	E	1	GLC	C1-C2-C3	2.86	113.18	109.67
2	E	3	GLC	C6-C5-C4	-2.85	106.33	113.00
2	E	3	GLC	C1-C2-C3	2.85	113.17	109.67
2	E	3	GLC	O5-C5-C4	2.84	117.74	110.83
2	E	6	GLC	C1-O5-C5	2.78	115.96	112.19
2	G	5	GLC	O4-C4-C5	2.77	116.17	109.30
2	E	5	GLC	O4-C4-C5	2.74	116.09	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	GLC	O5-C1-C2	-2.73	106.55	110.77
2	E	3	GLC	C1-O5-C5	2.71	115.87	112.19
2	G	6	GLC	O5-C5-C6	2.71	111.45	107.20
2	E	3	GLC	C3-C4-C5	2.69	115.05	110.24
2	G	4	GLC	C3-C4-C5	-2.69	105.43	110.24
2	E	2	GLC	O4-C4-C3	-2.69	104.12	110.35
2	H	8	GLC	C1-O5-C5	2.66	115.80	112.19
2	G	2	GLC	C1-C2-C3	2.63	112.90	109.67
2	E	1	GLC	O5-C5-C4	-2.61	104.48	110.83
2	E	1	GLC	O2-C2-C1	2.59	114.46	109.15
2	G	4	GLC	C1-C2-C3	2.58	112.84	109.67
2	G	2	GLC	O4-C4-C3	-2.57	104.41	110.35
2	F	8	GLC	O5-C1-C2	-2.53	106.87	110.77
2	G	5	GLC	O5-C1-C2	-2.50	106.92	110.77
2	H	3	GLC	C1-O5-C5	2.48	115.56	112.19
2	G	8	GLC	C1-O5-C5	2.47	115.53	112.19
2	E	2	GLC	O5-C1-C2	-2.45	106.99	110.77
2	H	5	GLC	O4-C4-C5	2.45	115.39	109.30
2	H	6	GLC	O5-C1-C2	-2.41	107.06	110.77
2	H	2	GLC	O5-C5-C6	2.38	110.93	107.20
2	E	7	GLC	O2-C2-C1	2.36	113.98	109.15
2	E	2	GLC	O2-C2-C1	-2.31	104.42	109.15
2	H	3	GLC	C3-C4-C5	2.29	114.33	110.24
2	E	2	GLC	C1-C2-C3	2.29	112.48	109.67
2	E	8	GLC	C2-C3-C4	-2.29	106.94	110.89
2	G	2	GLC	O5-C5-C6	2.25	110.72	107.20
2	E	2	GLC	C6-C5-C4	2.22	118.20	113.00
2	G	1	GLC	O5-C1-C2	-2.21	107.35	110.77
2	H	5	GLC	C1-C2-C3	2.18	112.35	109.67
2	F	4	GLC	O4-C4-C5	2.16	114.65	109.30
2	E	4	GLC	C3-C4-C5	-2.14	106.41	110.24
2	E	2	GLC	O6-C6-C5	-2.14	103.95	111.29
2	F	4	GLC	C3-C4-C5	-2.10	106.49	110.24
2	H	8	GLC	O5-C1-C2	-2.08	107.56	110.77
2	F	5	GLC	O4-C4-C3	-2.08	105.54	110.35
2	G	6	GLC	O5-C1-C2	-2.06	107.59	110.77
2	G	2	GLC	O5-C1-C2	-2.03	107.63	110.77
2	F	4	GLC	C6-C5-C4	2.03	117.75	113.00
2	F	3	GLC	O5-C5-C6	2.02	110.38	107.20

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	F	5	GLC	C4-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	G	6	GLC	C4-C5-C6-O6
2	F	5	GLC	O5-C5-C6-O6
2	H	3	GLC	O5-C5-C6-O6

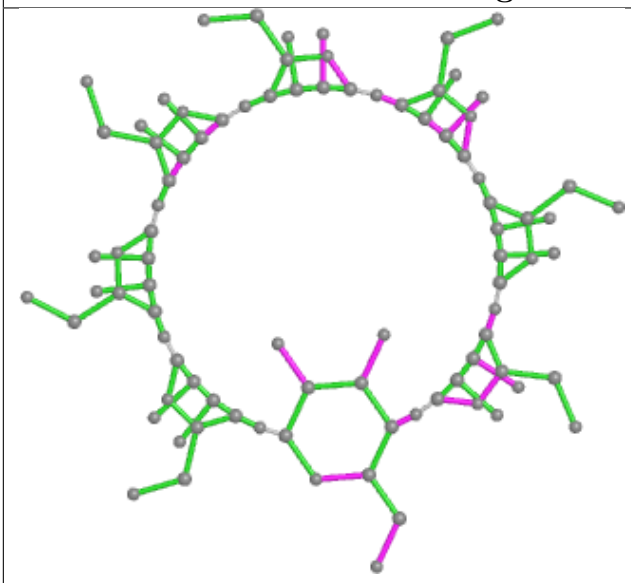
There are no ring outliers.

14 monomers are involved in 21 short contacts:

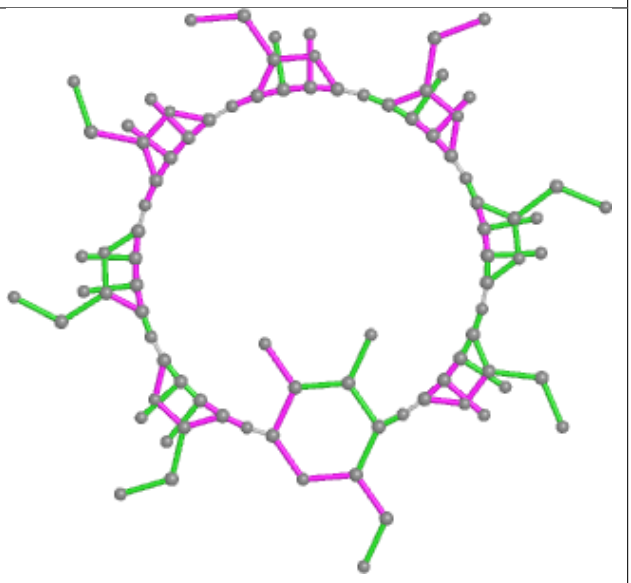
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	8	GLC	1	0
2	E	4	GLC	1	0
2	H	8	GLC	2	0
2	E	5	GLC	1	0
2	E	2	GLC	6	0
2	F	5	GLC	1	0
2	H	2	GLC	1	0
2	E	1	GLC	5	0
2	H	5	GLC	1	0
2	G	8	GLC	1	0
2	F	4	GLC	1	0
2	F	8	GLC	2	0
2	H	1	GLC	3	0
2	F	3	GLC	1	0

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

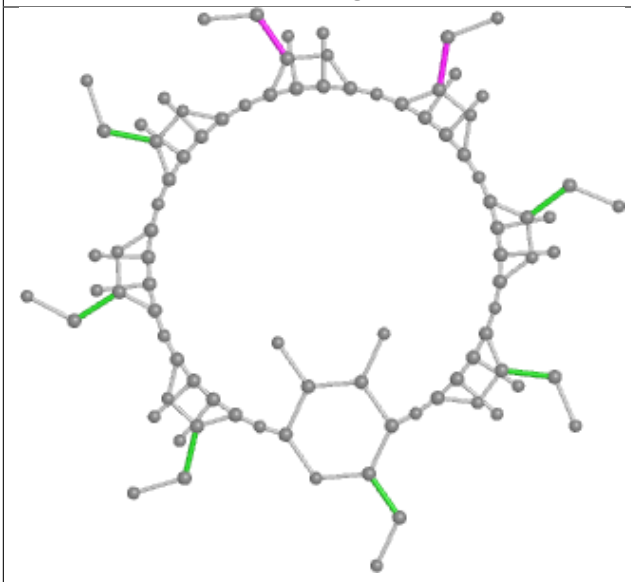
Oligosaccharide Chain E



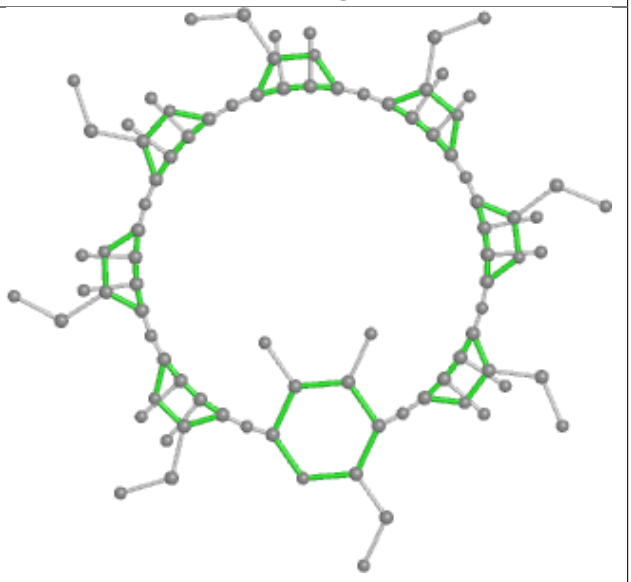
Bond lengths



Bond angles

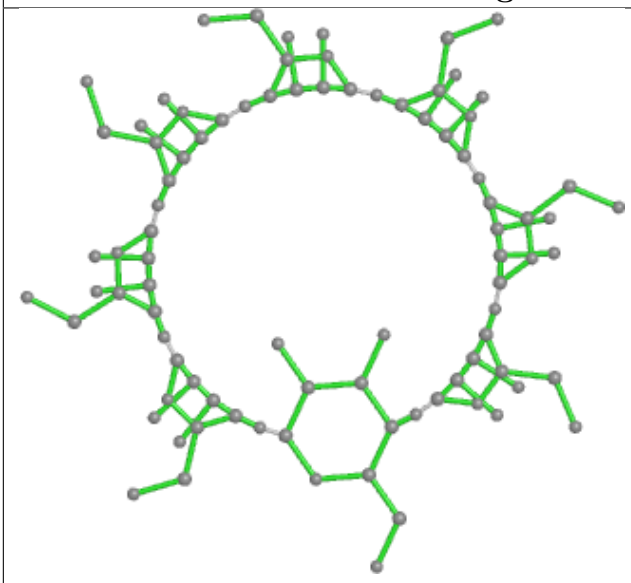


Torsions

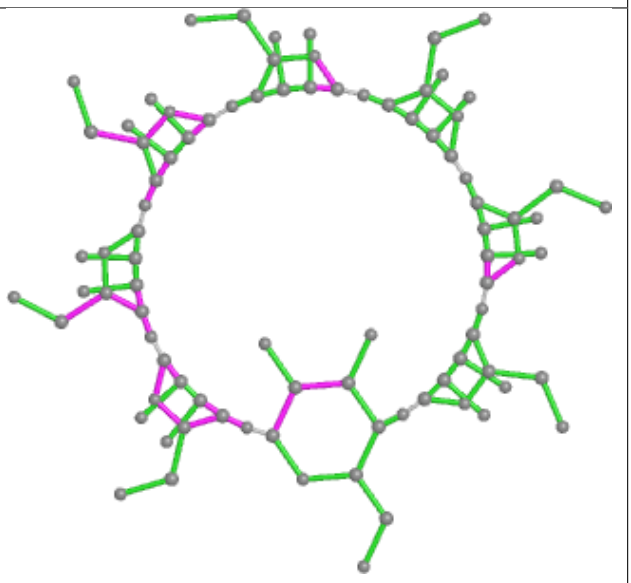


Rings

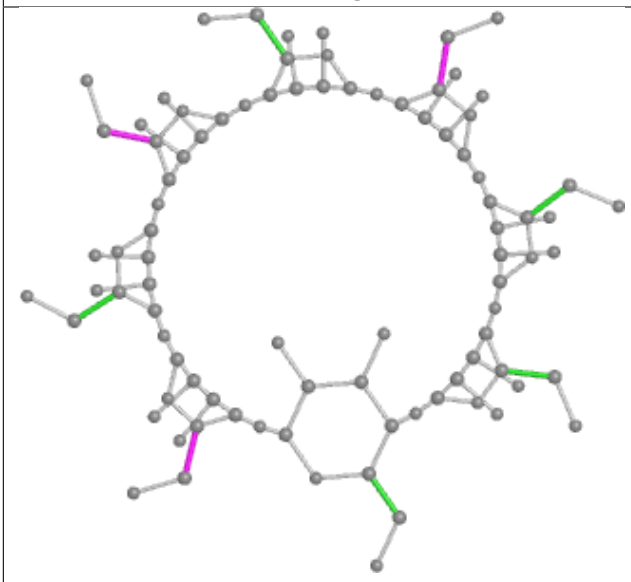
Oligosaccharide Chain F



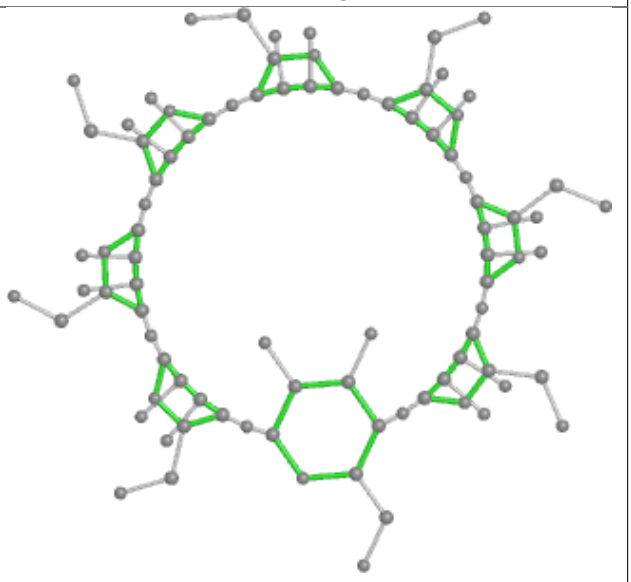
Bond lengths



Bond angles

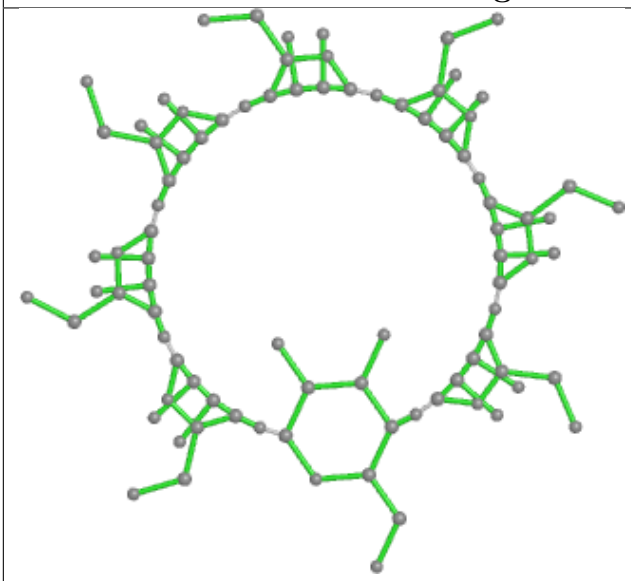


Torsions

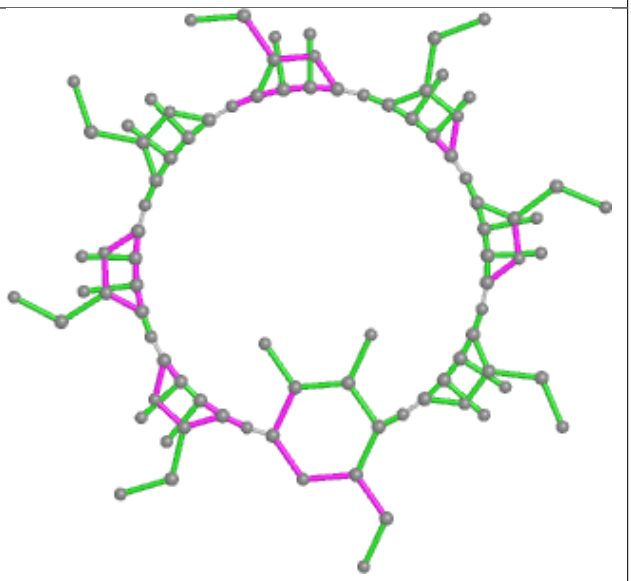


Rings

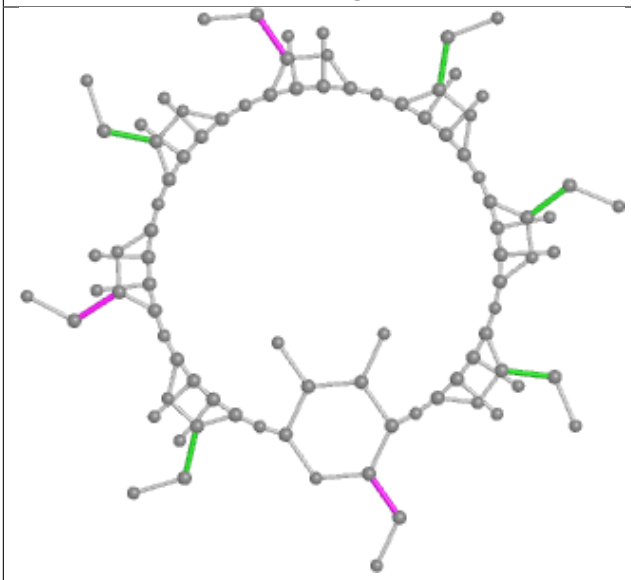
Oligosaccharide Chain G



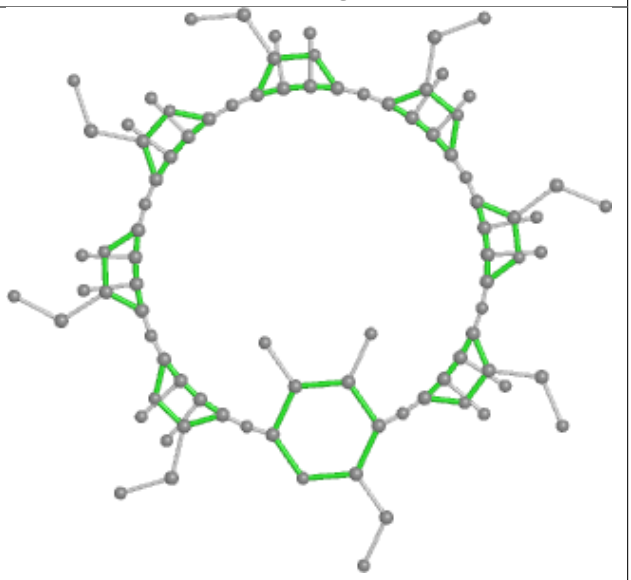
Bond lengths



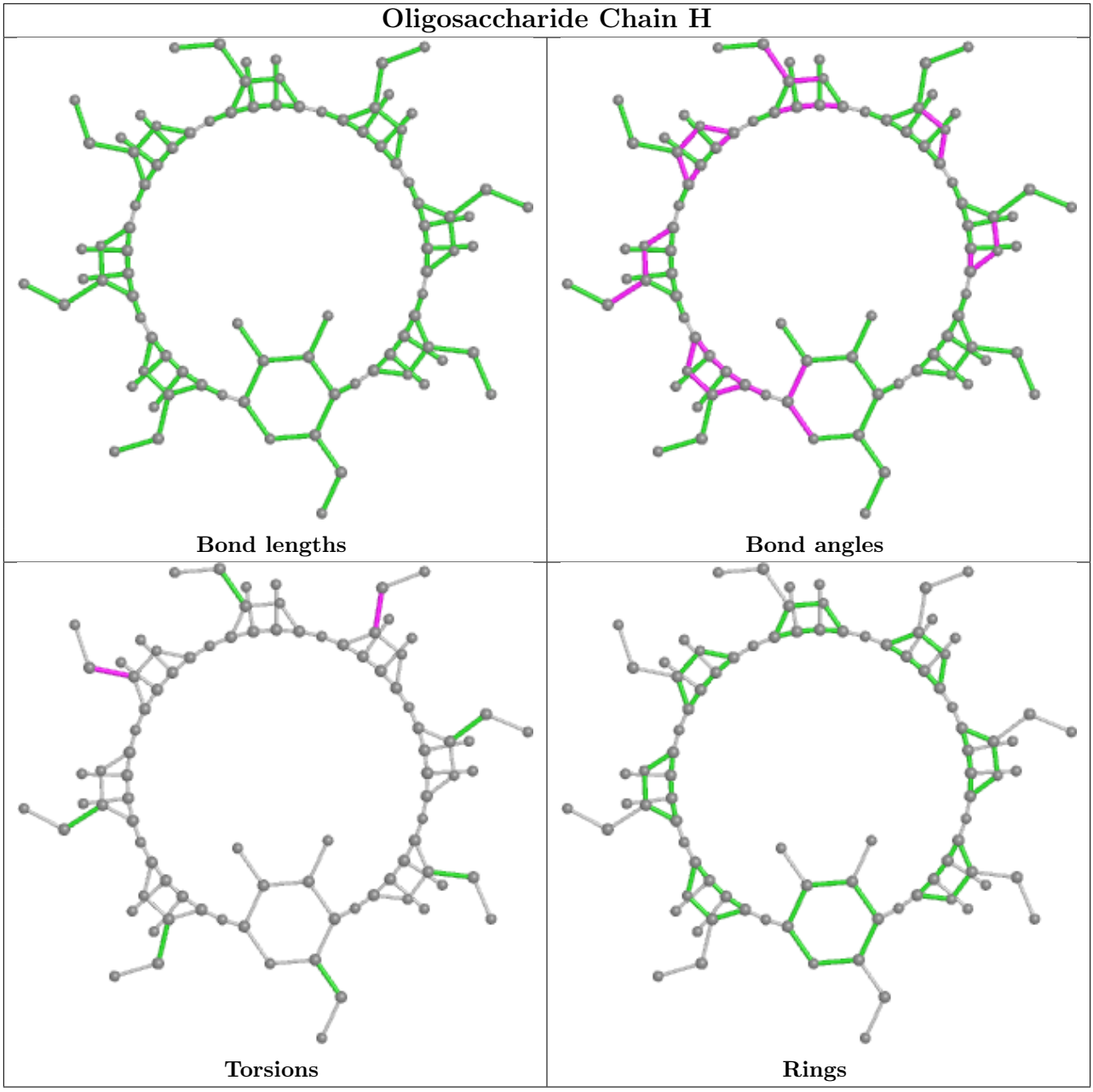
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

17 ligands 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	$\#\|Z\|>2$
5	EDO	A	506	-	3,3,3	0.55	0	2,2,2	0.29	0
3	GOL	D	501	-	5,5,5	1.06	0	5,5,5	1.34	1 (20%)
3	GOL	B	502	-	5,5,5	0.82	0	5,5,5	1.18	0
5	EDO	A	507	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	B	505	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	C	501	-	3,3,3	0.68	0	2,2,2	0.16	0
4	PEG	A	505	-	6,6,6	0.44	0	5,5,5	0.44	0
4	PEG	C	502	-	6,6,6	0.45	0	5,5,5	0.32	0
5	EDO	B	504	-	3,3,3	0.55	0	2,2,2	0.32	0
3	GOL	B	501	-	5,5,5	0.90	0	5,5,5	0.96	0
4	PEG	B	503	-	6,6,6	0.48	0	5,5,5	0.31	0
4	PEG	A	504	-	6,6,6	0.46	0	5,5,5	0.49	0
5	EDO	B	506	-	3,3,3	0.47	0	2,2,2	0.24	0
3	GOL	A	501	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	A	503	-	5,5,5	0.99	0	5,5,5	0.90	0
5	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.29	0
3	GOL	A	502	-	5,5,5	0.95	0	5,5,5	1.59	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	506	-	-	1/1/1/1	-
3	GOL	D	501	-	-	4/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	C	501	-	-	0/1/1/1	-
4	PEG	A	505	-	-	2/4/4/4	-
4	PEG	C	502	-	-	2/4/4/4	-
5	EDO	B	504	-	-	1/1/1/1	-
3	GOL	B	501	-	-	1/4/4/4	-
4	PEG	B	503	-	-	1/4/4/4	-
4	PEG	A	504	-	-	1/4/4/4	-
5	EDO	B	506	-	-	1/1/1/1	-
3	GOL	A	501	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
5	EDO	A	508	-	-	0/1/1/1	-
3	GOL	A	502	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	GOL	C3-C2-C1	-2.77	100.93	111.70
3	D	501	GOL	C3-C2-C1	-2.23	103.03	111.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-O2
3	B	502	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-C3
3	D	501	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	B	501	GOL	C1-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
3	D	501	GOL	O2-C2-C3-O3
4	A	504	PEG	O2-C3-C4-O4
4	A	505	PEG	O1-C1-C2-O2
4	B	503	PEG	C1-C2-O2-C3
3	A	502	GOL	O2-C2-C3-O3
4	A	505	PEG	O2-C3-C4-O4
5	A	506	EDO	O1-C1-C2-O2
5	B	506	EDO	O1-C1-C2-O2
4	C	502	PEG	O1-C1-C2-O2
3	A	502	GOL	C1-C2-C3-O3
5	B	504	EDO	O1-C1-C2-O2
4	C	502	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GOL	2	0
3	B	502	GOL	1	0
5	A	507	EDO	1	0
5	B	505	EDO	8	0
4	C	502	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	EDO	4	0
4	B	503	PEG	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, 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	476/477 (99%)	-0.15	4 (0%)	82	84	11, 29, 49, 76	2 (0%)
1	B	476/477 (99%)	0.03	6 (1%)	74	76	22, 35, 56, 74	0
1	C	476/477 (99%)	0.27	13 (2%)	56	58	17, 44, 71, 89	1 (0%)
1	D	477/477 (100%)	-0.04	8 (1%)	69	71	13, 32, 60, 84	1 (0%)
All	All	1905/1908 (99%)	0.03	31 (1%)	70	72	11, 35, 62, 89	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	289	ALA	4.1
1	C	457	LYS	3.4
1	D	288	ARG	3.2
1	C	246	GLY	3.0
1	A	288	ARG	2.9
1	C	456	GLU	2.8
1	C	455	GLU	2.8
1	A	289	ALA	2.7
1	C	251	TYR	2.7
1	C	217	VAL	2.7
1	D	456	GLU	2.7
1	C	76	PHE	2.6
1	C	342	ASP	2.6
1	D	90	GLU	2.5
1	B	418	GLY	2.5
1	A	316	PHE	2.4
1	B	458	ALA	2.3
1	C	242	PHE	2.3
1	C	460	PHE	2.3
1	D	76	PHE	2.3
1	B	76	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	94	LYS	2.2
1	D	397	THR	2.2
1	D	409	PHE	2.2
1	B	103	TYR	2.2
1	C	211	TYR	2.1
1	B	119	LYS	2.1
1	A	455	GLU	2.1
1	B	145	LYS	2.1
1	C	335	LYS	2.1
1	D	1	MET	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, 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	GLC	G	3	11/12	0.55	0.14	70,72,73,74	0
2	GLC	E	3	11/12	0.63	0.14	72,79,80,81	0
2	GLC	H	2	11/12	0.63	0.15	64,69,74,75	0
2	GLC	F	2	11/12	0.70	0.15	76,80,84,85	0
2	GLC	G	2	11/12	0.72	0.13	63,65,67,69	0
2	GLC	H	3	11/12	0.73	0.13	73,78,80,81	0
2	GLC	E	2	11/12	0.79	0.11	64,67,73,79	0
2	GLC	F	3	11/12	0.80	0.13	75,77,78,78	0
2	GLC	E	4	11/12	0.82	0.13	45,60,66,68	0
2	GLC	F	4	11/12	0.85	0.12	54,71,75,76	0
2	GLC	G	4	11/12	0.85	0.11	45,60,66,69	0
2	GLC	H	1	11/12	0.86	0.11	38,43,49,57	0
2	GLC	H	4	11/12	0.86	0.12	48,60,66,69	0
2	GLC	G	1	11/12	0.87	0.10	45,52,61,62	0
2	GLC	E	1	11/12	0.91	0.08	34,40,55,58	0
2	GLC	F	5	11/12	0.92	0.10	27,42,48,49	0
2	GLC	G	7	11/12	0.92	0.07	21,23,27,27	0
2	GLC	F	1	11/12	0.93	0.08	40,49,62,70	0

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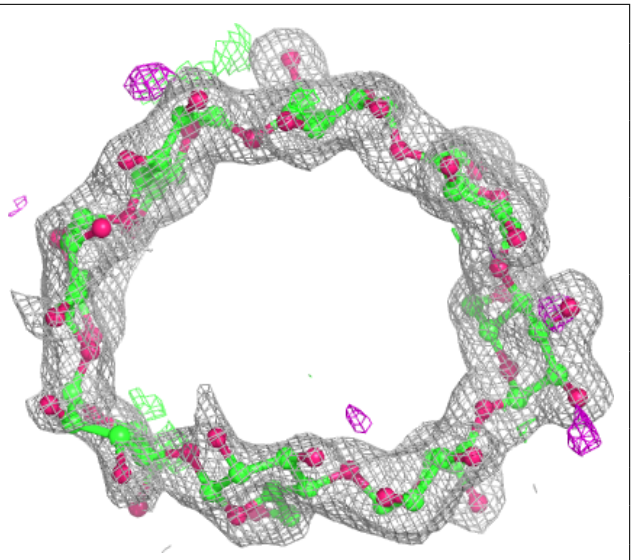
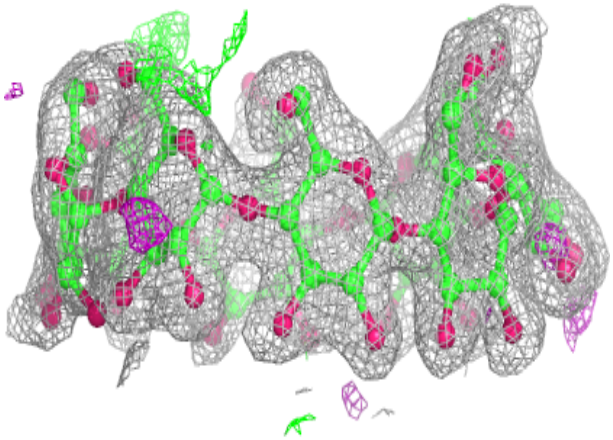
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	G	5	11/12	0.93	0.07	32,38,45,47	0
2	GLC	G	6	11/12	0.94	0.06	22,25,30,32	0
2	GLC	F	7	11/12	0.94	0.06	20,22,27,27	0
2	GLC	G	8	11/12	0.94	0.07	23,28,34,34	0
2	GLC	E	6	11/12	0.94	0.06	20,20,20,20	0
2	GLC	E	7	11/12	0.95	0.06	20,20,20,20	0
2	GLC	E	5	11/12	0.95	0.06	24,31,37,38	0
2	GLC	F	6	11/12	0.95	0.07	16,19,23,24	0
2	GLC	H	5	11/12	0.95	0.07	28,38,42,46	0
2	GLC	F	8	11/12	0.96	0.06	22,27,30,30	0
2	GLC	E	8	11/12	0.96	0.06	17,21,26,27	0
2	GLC	H	6	11/12	0.96	0.06	18,22,24,27	0
2	GLC	H	7	11/12	0.96	0.05	21,23,28,28	0
2	GLC	H	8	11/12	0.96	0.05	20,26,27,31	0

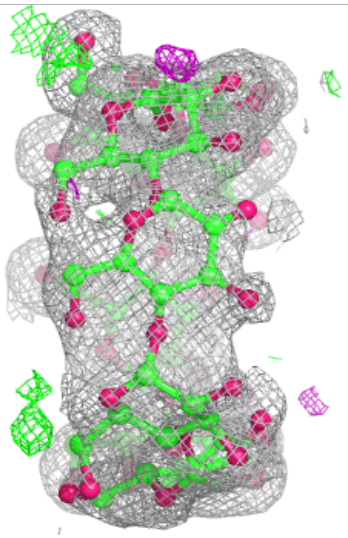
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

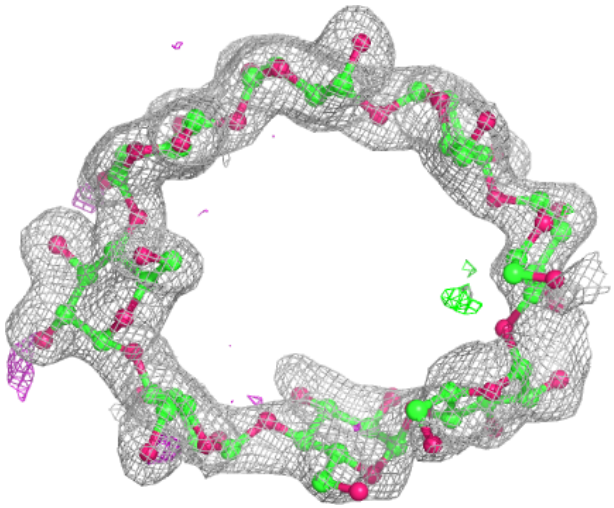


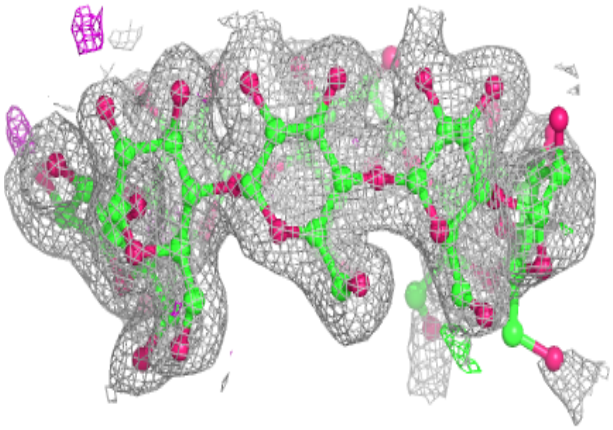


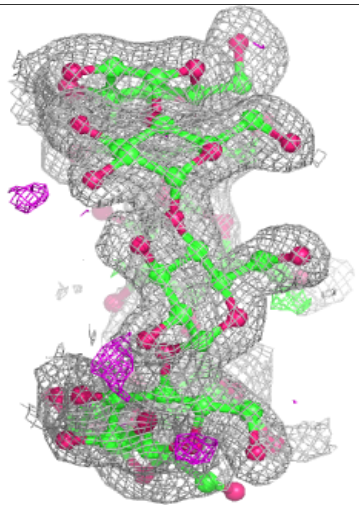


Electron density around Chain F:

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

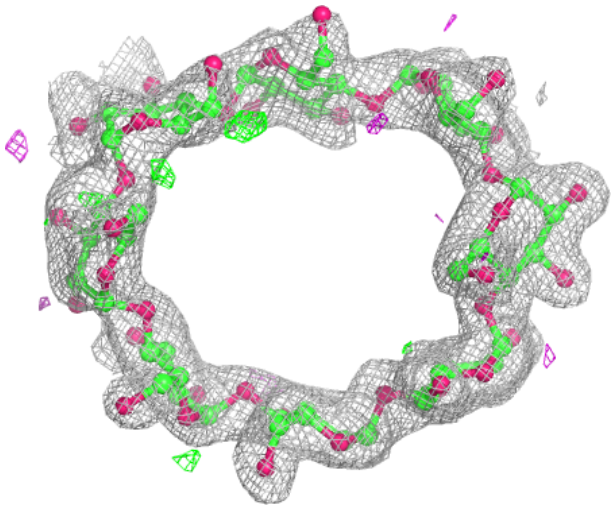


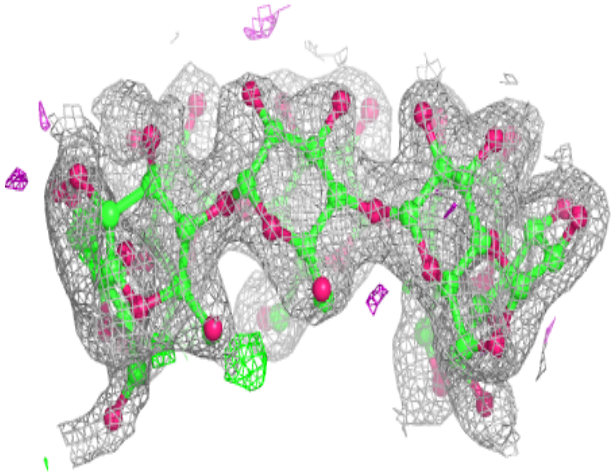


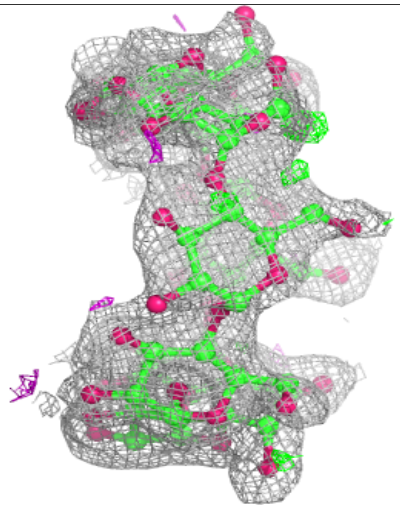


Electron density around Chain G:

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

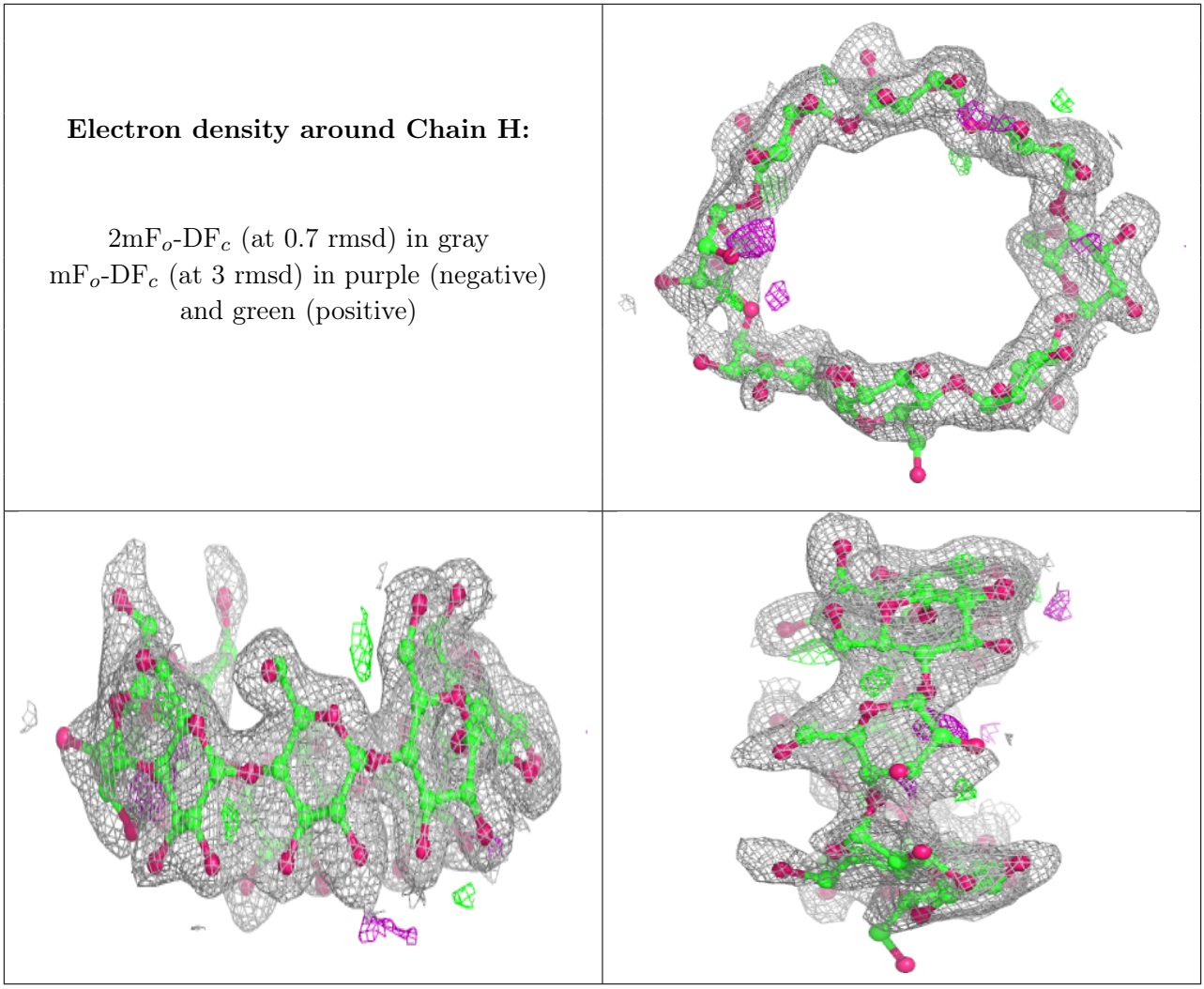






Electron density around Chain H:

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



6.4 Ligands

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
5	EDO	B	504	4/4	0.60	0.26	53,58,59,60	0
5	EDO	B	506	4/4	0.67	0.25	69,70,71,73	0
4	PEG	B	503	7/7	0.68	0.19	66,67,69,70	0
4	PEG	C	502	7/7	0.73	0.15	53,55,58,59	0
4	PEG	A	504	7/7	0.79	0.15	48,53,55,57	0
5	EDO	A	506	4/4	0.79	0.15	43,49,51,51	0
5	EDO	A	507	4/4	0.80	0.15	60,64,65,65	0
5	EDO	A	508	4/4	0.80	0.17	53,53,54,55	0
4	PEG	A	505	7/7	0.81	0.15	57,64,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	502	6/6	0.84	0.14	39,49,52,54	0
3	GOL	B	501	6/6	0.84	0.10	53,55,58,60	0
5	EDO	B	505	4/4	0.85	0.19	36,38,39,41	0
3	GOL	A	503	6/6	0.85	0.12	39,55,57,58	0
5	EDO	C	501	4/4	0.85	0.11	29,33,35,38	0
3	GOL	A	502	6/6	0.89	0.15	27,30,33,36	0
3	GOL	A	501	6/6	0.90	0.10	47,49,53,57	0
3	GOL	D	501	6/6	0.94	0.12	26,34,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.