



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:41 AM UTC

PDB ID : 6EQ1 / pdb_00006eq1
Title : Structure of the periplasmic binding protein (PBP) MelB (Atu4661) in complex with stachyose from agrobacterium fabrum C58
Authors : Vigouroux, A.; Morera, S.
Deposited on : 2017-10-12
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

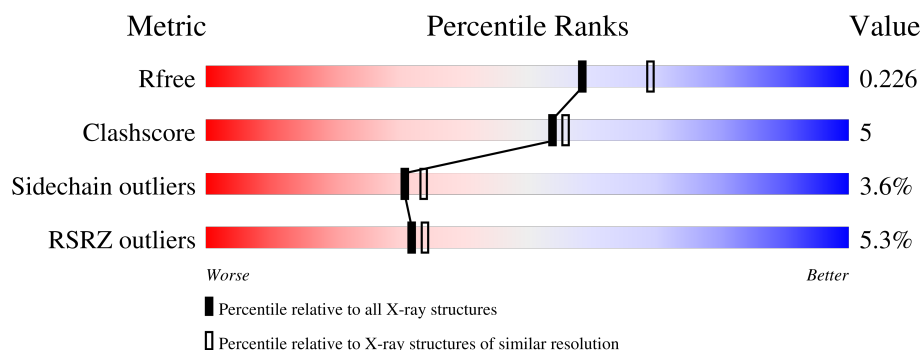
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	683	6% 84% 13% ..
1	B	683	4% 83% 14% ..
2	C	4	25% 25% 50%
2	D	4	75% 25%

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	FRU	C	1	X	-	-	-
2	GAL	C	3	X	-	-	-
2	GAL	C	4	X	-	-	-
2	FRU	D	1	X	-	-	-
2	GAL	D	3	X	-	-	-
2	GAL	D	4	X	-	-	-
4	PEG	B	708	-	-	X	-
5	EDO	B	716	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11000 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.

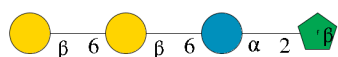
- Molecule 1 is a protein called Periplasmic alpha-galactoside-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	671	Total	C	N	O	S	0	0	0
			5295	3380	899	1000	16			
1	A	669	Total	C	N	O	S	0	0	0
			5277	3370	894	997	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	-	expression tag	UNP A0A083ZM57
B	679	HIS	-	expression tag	UNP A0A083ZM57
B	680	HIS	-	expression tag	UNP A0A083ZM57
B	681	HIS	-	expression tag	UNP A0A083ZM57
B	682	HIS	-	expression tag	UNP A0A083ZM57
B	683	HIS	-	expression tag	UNP A0A083ZM57
A	678	HIS	-	expression tag	UNP A0A083ZM57
A	679	HIS	-	expression tag	UNP A0A083ZM57
A	680	HIS	-	expression tag	UNP A0A083ZM57
A	681	HIS	-	expression tag	UNP A0A083ZM57
A	682	HIS	-	expression tag	UNP A0A083ZM57
A	683	HIS	-	expression tag	UNP A0A083ZM57

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-6)-beta-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose.



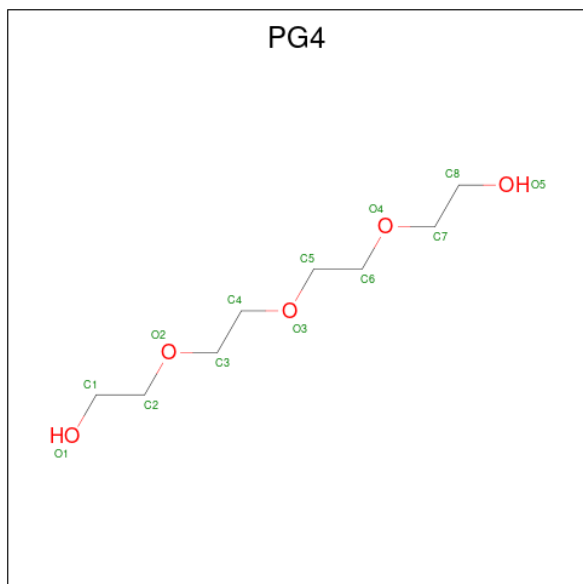
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			

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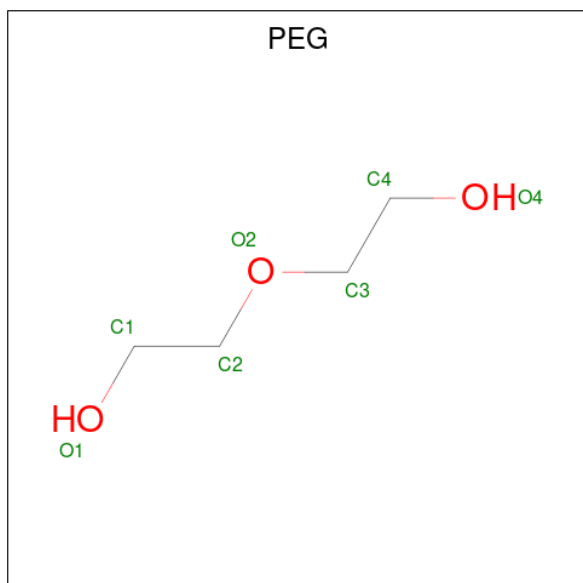
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



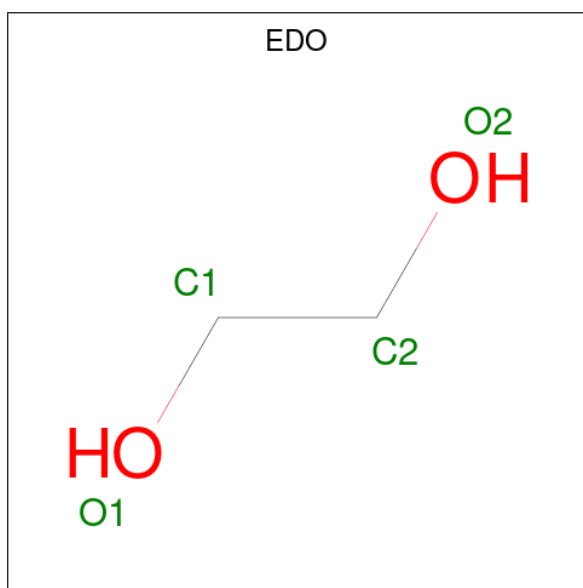
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	8	5		

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



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total Ca 5 5	0	0
6	A	4	Total Ca 4 4	0	0

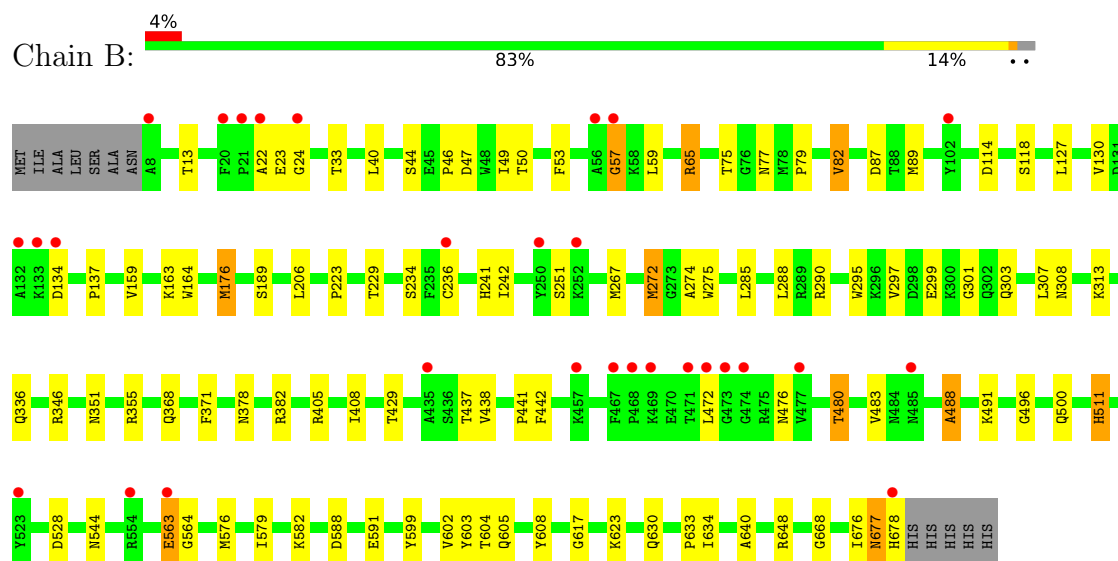
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	145	Total O 145 145	0	0
7	A	63	Total O 63 63	0	0

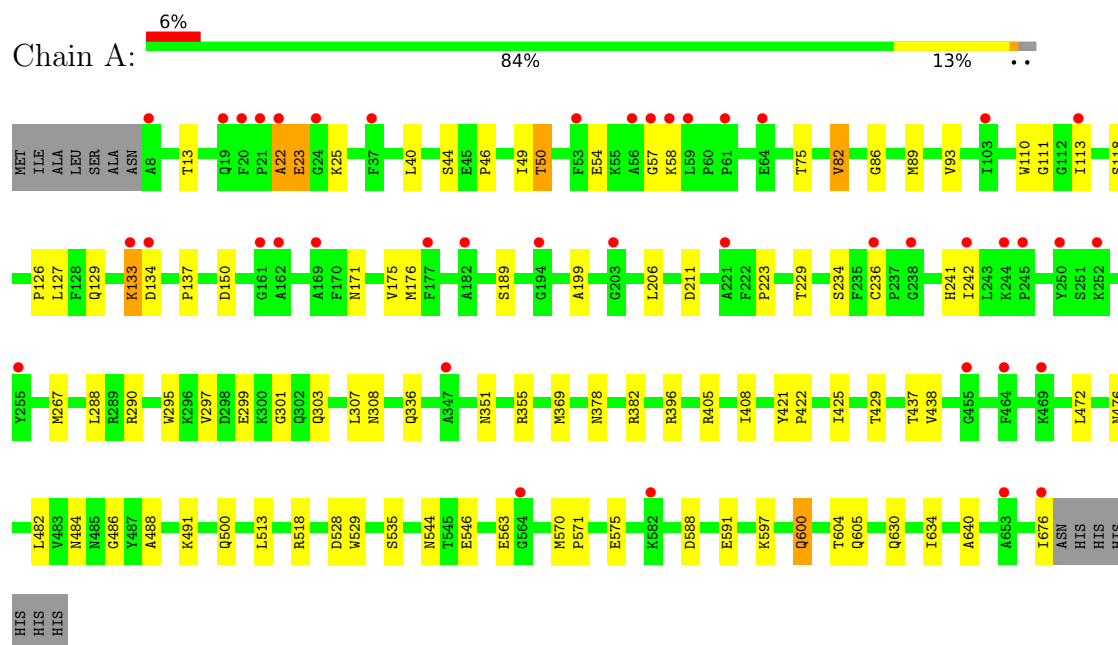
3 Residue-property plots [i](#)

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: Periplasmic alpha-galactoside-binding protein



- Molecule 1: Periplasmic alpha-galactoside-binding protein



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain C:  25% 25% 50%



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-galactopyranose-(1-6)-alpha-D-glucopyranose-(1-2)-beta-D-fructofuranose

Chain D:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.18Å 73.98Å 171.45Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	46.61 – 2.10 46.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	73.4 (46.61-2.10) 73.3 (46.61-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.191 , 0.225 (Not available) , 0.226	Depositor DCC
R_{free} test set	2849 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11000	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, PEG, FRU, PG4, GLC, EDO, CA

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	0.81	0/5429	1.29	29/7387 (0.4%)
1	B	0.91	3/5448 (0.1%)	1.33	31/7413 (0.4%)
All	All	0.86	3/10877 (0.0%)	1.31	60/14800 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	MET	SD-CE	-15.15	1.41	1.79
1	B	176	MET	SD-CE	-6.14	1.64	1.79
1	B	159	VAL	CA-C	5.57	1.58	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	VAL	CA-C-N	9.46	135.01	120.82
1	B	130	VAL	C-N-CA	9.46	135.01	120.82
1	A	22	ALA	CA-C-N	8.43	136.87	121.70
1	A	22	ALA	C-N-CA	8.43	136.87	121.70
1	A	134	ASP	CA-CB-CG	7.95	120.55	112.60
1	B	134	ASP	CA-C-N	7.58	131.51	120.82
1	B	134	ASP	C-N-CA	7.58	131.51	120.82
1	A	476	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	588	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	588	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	87	ASP	CA-C-N	6.43	132.58	122.94
1	B	87	ASP	C-N-CA	6.43	132.58	122.94
1	B	57	GLY	CA-C-N	6.08	133.16	121.54
1	B	57	GLY	C-N-CA	6.08	133.16	121.54
1	B	371	PHE	CA-CB-CG	6.04	119.84	113.80
1	B	591	GLU	CA-C-N	6.03	128.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	GLU	C-N-CA	6.03	128.37	120.28
1	B	677	ASN	CA-C-N	5.89	132.30	121.70
1	B	677	ASN	C-N-CA	5.89	132.30	121.70
1	A	13	THR	CB-CA-C	5.88	117.69	108.63
1	B	491	LYS	CA-C-N	5.82	128.00	120.44
1	B	491	LYS	C-N-CA	5.82	128.00	120.44
1	A	57	GLY	CA-C-N	5.80	132.62	121.54
1	A	57	GLY	C-N-CA	5.80	132.62	121.54
1	A	484	ASN	CA-C-N	5.79	128.04	120.28
1	A	484	ASN	C-N-CA	5.79	128.04	120.28
1	B	544	ASN	CA-C-N	5.74	128.24	120.38
1	B	544	ASN	C-N-CA	5.74	128.24	120.38
1	B	476	ASN	CA-CB-CG	5.73	118.33	112.60
1	B	251	SER	N-CA-C	5.58	115.48	108.45
1	A	544	ASN	CA-C-N	5.58	128.02	120.38
1	A	544	ASN	C-N-CA	5.58	128.02	120.38
1	B	528	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	528	ASP	N-CA-C	-5.55	105.30	112.68
1	A	491	LYS	CA-C-N	5.48	127.57	120.44
1	A	491	LYS	C-N-CA	5.48	127.57	120.44
1	A	528	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	486	GLY	N-CA-C	5.43	120.43	114.40
1	A	597	LYS	CA-C-N	5.40	127.46	120.44
1	A	597	LYS	C-N-CA	5.40	127.46	120.44
1	A	223	PRO	CA-C-N	5.38	129.30	120.63
1	A	223	PRO	C-N-CA	5.38	129.30	120.63
1	B	528	ASP	N-CA-C	-5.36	104.40	111.96
1	A	241	HIS	CA-C-N	5.29	127.79	122.66
1	A	241	HIS	C-N-CA	5.29	127.79	122.66
1	A	591	GLU	CA-C-N	5.27	127.60	120.38
1	A	591	GLU	C-N-CA	5.27	127.60	120.38
1	A	86	GLY	N-CA-C	5.19	117.33	112.08
1	B	241	HIS	CA-C-N	5.19	127.69	122.66
1	B	241	HIS	C-N-CA	5.19	127.69	122.66
1	B	223	PRO	CA-C-N	5.14	128.91	120.63
1	B	223	PRO	C-N-CA	5.14	128.91	120.63
1	B	488	ALA	CA-C-N	5.04	126.99	120.44
1	B	488	ALA	C-N-CA	5.04	126.99	120.44
1	B	496	GLY	CA-C-N	5.04	126.99	120.44
1	B	496	GLY	C-N-CA	5.04	126.99	120.44
1	B	13	THR	CB-CA-C	5.03	116.38	108.63
1	A	175	VAL	CA-C-N	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	C-N-CA	5.03	127.02	120.28
1	A	575	GLU	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5277	0	5100	40	0
1	B	5295	0	5114	63	1
2	C	45	0	39	1	0
2	D	45	0	39	0	0
3	B	13	0	18	1	0
4	A	7	0	10	1	0
4	B	49	0	70	10	0
5	A	4	0	6	0	0
5	B	48	0	72	5	0
6	A	4	0	0	0	0
6	B	5	0	0	0	0
7	A	63	0	0	1	0
7	B	145	0	0	0	0
All	All	11000	0	10468	103	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (103) 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:B:633:PRO:HA	4:B:707:PEG:H11	1.50	0.93
1:B:164:TRP:HA	1:B:272:MET:HE1	1.56	0.86
1:B:405:ARG:H	5:B:716:EDO:H21	1.45	0.81
1:B:164:TRP:HA	1:B:272:MET:CE	2.11	0.81
1:B:164:TRP:CD2	1:B:272:MET:HE3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:HA	4:B:708:PEG:H32	1.68	0.75
1:B:668:GLY:HA2	1:B:676:ILE:HD12	1.69	0.74
1:B:285:LEU:HD13	1:B:313:LYS:HD3	1.72	0.71
1:B:442:PHE:HB2	5:B:716:EDO:H22	1.70	0.71
1:B:382:ARG:HA	1:B:472:LEU:HD11	1.72	0.70
1:A:176:MET:HE1	1:A:206:LEU:HG	1.75	0.68
1:A:382:ARG:HA	1:A:472:LEU:HD11	1.75	0.68
1:B:47:ASP:H	5:B:714:EDO:H22	1.60	0.67
1:B:272:MET:HE2	1:B:272:MET:HA	1.78	0.65
1:B:33:THR:HA	4:B:708:PEG:C3	2.26	0.64
1:A:336:GLN:NE2	1:A:488:ALA:H	1.96	0.64
1:B:79:PRO:HG3	3:B:701:PG4:H12	1.79	0.63
1:B:576:MET:HE2	1:B:603:TYR:HA	1.81	0.62
1:B:176:MET:HE1	1:B:206:LEU:HG	1.82	0.62
1:B:164:TRP:CA	1:B:272:MET:HE1	2.28	0.62
1:B:677:ASN:HB3	1:B:678:HIS:HA	1.83	0.61
1:A:600:GLN:HA	1:A:600:GLN:HE21	1.66	0.60
1:B:290:ARG:HH11	1:B:308:ASN:HD22	1.49	0.60
1:B:33:THR:HG22	4:B:708:PEG:H32	1.83	0.60
1:B:355:ARG:HG3	1:B:623:LYS:HG2	1.84	0.60
1:A:290:ARG:HH11	1:A:308:ASN:HD22	1.49	0.59
1:B:336:GLN:HE22	1:B:488:ALA:H	1.50	0.59
1:B:164:TRP:CE3	1:B:272:MET:HE3	2.36	0.59
1:B:285:LEU:HD13	1:B:313:LYS:CD	2.33	0.58
1:A:46:PRO:HD2	1:A:49:ILE:HD12	1.85	0.58
1:B:677:ASN:CB	1:B:678:HIS:HA	2.33	0.58
1:B:617:GLY:O	4:B:707:PEG:H21	2.04	0.57
1:A:369:MET:HG2	1:A:529:TRP:CD1	2.39	0.57
1:A:50:THR:HA	1:A:54:GLU:HB2	1.85	0.57
1:A:229:THR:O	1:A:234:SER:HB2	2.06	0.55
1:B:267:MET:HA	1:B:267:MET:HE2	1.89	0.54
1:A:171:ASN:HB2	1:A:211:ASP:O	2.08	0.54
1:B:634:ILE:HG23	4:B:707:PEG:H22	1.90	0.54
1:B:579:ILE:HG21	1:B:599:TYR:HB2	1.89	0.53
1:B:438:VAL:HG21	1:B:605:GLN:HB2	1.91	0.53
1:A:425:ILE:H	1:A:600:GLN:HE22	1.55	0.53
1:B:77:ASN:HD22	1:B:648:ARG:HH12	1.57	0.52
1:A:118:SER:HB3	1:A:236:CYS:HB3	1.91	0.52
1:B:346:ARG:HD3	4:B:702:PEG:H42	1.92	0.51
1:A:429:THR:HG23	4:A:701:PEG:H32	1.92	0.51
1:A:438:VAL:HG21	1:A:605:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:THR:O	1:B:234:SER:HB2	2.12	0.50
1:A:336:GLN:HE22	1:A:488:ALA:H	1.58	0.50
1:B:290:ARG:HD2	1:B:308:ASN:HD22	1.76	0.49
1:B:46:PRO:HD2	1:B:49:ILE:HD12	1.93	0.49
1:B:118:SER:HB3	1:B:236:CYS:HB3	1.94	0.49
1:A:290:ARG:HD2	1:A:308:ASN:HD22	1.78	0.49
1:A:295:TRP:H	1:A:295:TRP:CD1	2.30	0.49
1:A:297:VAL:HG12	1:A:303:GLN:HA	1.96	0.48
1:B:40:LEU:HD12	1:B:301:GLY:HA2	1.95	0.48
1:A:89:MET:HB2	1:A:307:LEU:HD13	1.94	0.48
1:B:295:TRP:H	1:B:295:TRP:CD1	2.32	0.48
1:B:75:THR:HG22	1:B:82:VAL:HG23	1.96	0.48
1:B:33:THR:CA	4:B:708:PEG:H32	2.42	0.47
1:B:441:PRO:HA	5:B:716:EDO:H11	1.96	0.47
1:A:369:MET:HG2	1:A:529:TRP:NE1	2.30	0.47
1:A:40:LEU:HD12	1:A:301:GLY:HA2	1.96	0.47
1:A:127:LEU:HD11	1:A:137:PRO:HA	1.97	0.47
1:A:75:THR:HG22	1:A:82:VAL:HG23	1.96	0.47
1:B:22:ALA:HB1	4:B:706:PEG:H12	1.98	0.46
1:B:77:ASN:ND2	1:B:648:ARG:HH12	2.14	0.46
1:A:22:ALA:HA	1:A:23:GLU:O	2.16	0.46
1:B:297:VAL:HG12	1:B:303:GLN:HA	1.99	0.45
1:A:133:LYS:HE3	1:A:133:LYS:H	1.81	0.45
1:B:576:MET:HE3	1:B:602:VAL:HG12	1.98	0.45
1:A:58:LYS:HA	7:A:829:HOH:O	2.16	0.45
1:B:480:THR:HG23	1:B:511:HIS:ND1	2.32	0.44
1:A:110:TRP:O	1:A:113:ILE:HG22	2.18	0.44
1:A:482:LEU:HD11	1:A:513:LEU:HD12	1.99	0.44
1:A:535:SER:HB2	2:C:1:FRU:H12	1.99	0.44
1:B:274:ALA:HB3	1:B:275:TRP:CE3	2.53	0.43
1:B:576:MET:HE1	1:B:608:TYR:HB2	2.00	0.43
1:B:89:MET:HB2	1:B:307:LEU:HD13	2.00	0.43
1:B:59:LEU:HD13	1:B:65:ARG:NH1	2.34	0.43
1:A:290:ARG:HH11	1:A:308:ASN:ND2	2.14	0.43
1:A:634:ILE:HA	1:A:640:ALA:HB2	2.01	0.42
1:A:126:PRO:O	1:A:129:GLN:HG2	2.19	0.42
1:A:396:ARG:HH12	1:A:570:MET:HE1	1.85	0.42
1:B:127:LEU:HD11	1:B:137:PRO:HA	2.00	0.42
1:B:290:ARG:HH11	1:B:308:ASN:ND2	2.14	0.42
1:B:582:LYS:HG3	1:A:571:PRO:HG2	2.00	0.42
1:B:677:ASN:HB3	1:B:678:HIS:CA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HA	1:A:408:ILE:HD12	2.01	0.42
1:A:437:THR:HG23	1:A:604:THR:HG21	2.02	0.42
1:B:437:THR:HG23	1:B:604:THR:HG21	2.02	0.41
1:B:634:ILE:HA	1:B:640:ALA:HB2	2.02	0.41
4:B:708:PEG:H11	4:B:708:PEG:H31	1.84	0.41
1:B:53:PHE:HE2	1:B:676:ILE:HG22	1.85	0.41
1:B:563:GLU:HA	1:B:564:GLY:HA2	1.73	0.41
1:B:23:GLU:HB3	1:B:24:GLY:H	1.36	0.41
1:B:405:ARG:HD2	5:B:716:EDO:H12	2.03	0.41
1:B:405:ARG:HA	1:B:408:ILE:HD12	2.01	0.41
1:A:93:VAL:HG12	1:A:111:GLY:HA3	2.03	0.41
1:A:199:ALA:HA	1:A:546:GLU:HG3	2.03	0.40
1:A:421:TYR:HA	1:A:422:PRO:HD3	1.91	0.40
1:B:677:ASN:CG	1:B:678:HIS:HA	2.47	0.40
1:B:59:LEU:HD13	1:B:65:ARG:HH12	1.85	0.40
1:A:267:MET:HE2	1:A:267:MET:HA	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLY:O	1:B:57:GLY:O[2_556]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	556/568 (98%)	536 (96%)	20 (4%)	31	34
1	B	558/568 (98%)	538 (96%)	20 (4%)	31	34
All	All	1114/1136 (98%)	1074 (96%)	40 (4%)	31	34

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	SER
1	B	50	THR
1	B	65	ARG
1	B	82	VAL
1	B	114	ASP
1	B	163	LYS
1	B	189	SER
1	B	242	ILE
1	B	288	LEU
1	B	299	GLU
1	B	351	ASN
1	B	368	GLN
1	B	378	ASN
1	B	429	THR
1	B	480	THR
1	B	483	VAL
1	B	500	GLN
1	B	511	HIS
1	B	563	GLU
1	B	630	GLN
1	A	23	GLU
1	A	25	LYS
1	A	44	SER
1	A	50	THR
1	A	82	VAL
1	A	133	LYS
1	A	150	ASP
1	A	189	SER
1	A	242	ILE
1	A	288	LEU
1	A	299	GLU
1	A	351	ASN
1	A	355	ARG
1	A	378	ASN
1	A	500	GLN

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Mol	Chain	Res	Type
1	A	518	ARG
1	A	563	GLU
1	A	600	GLN
1	A	630	GLN
1	A	676	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	77	ASN
1	B	152	HIS
1	B	302	GLN
1	B	303	GLN
1	B	308	ASN
1	B	323	GLN
1	B	336	GLN
1	B	339	ASN
1	B	368	GLN
1	B	466	ASN
1	B	517	GLN
1	B	605	GLN
1	A	77	ASN
1	A	152	HIS
1	A	302	GLN
1	A	303	GLN
1	A	308	ASN
1	A	323	GLN
1	A	336	GLN
1	A	374	ASN
1	A	511	HIS
1	A	517	GLN
1	A	600	GLN
1	A	605	GLN
1	A	622	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 ⓘ

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	FRU	C	1	2	11,12,12	2.00	2 (18%)	10,18,18	1.79	2 (20%)
2	GLC	C	2	2	11,11,12	0.98	0	15,15,17	1.00	0
2	GAL	C	3	2	11,11,12	1.32	1 (9%)	15,15,17	1.42	2 (13%)
2	GAL	C	4	2	11,11,12	1.06	0	15,15,17	1.13	1 (6%)
2	FRU	D	1	2	11,12,12	2.56	4 (36%)	10,18,18	1.14	0
2	GLC	D	2	2	11,11,12	1.37	2 (18%)	15,15,17	1.75	3 (20%)
2	GAL	D	3	2	11,11,12	1.47	3 (27%)	15,15,17	1.72	3 (20%)
2	GAL	D	4	2	11,11,12	1.49	1 (9%)	15,15,17	1.04	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	FRU	C	1	2	1/1/4/4	1/5/24/24	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GAL	C	3	2	3/3/4/5	1/2/19/22	0/1/1/1
2	GAL	C	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	FRU	D	1	2	1/1/4/4	3/5/24/24	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GAL	D	3	2	3/3/4/5	1/2/19/22	0/1/1/1
2	GAL	D	4	2	1/1/4/5	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	FRU	O2-C2	6.30	1.51	1.40
2	C	1	FRU	O2-C2	4.50	1.48	1.40
2	C	1	FRU	O5-C2	3.94	1.49	1.43
2	D	4	GAL	O5-C1	3.80	1.50	1.43
2	D	1	FRU	O5-C2	3.65	1.49	1.43
2	C	3	GAL	C2-C3	3.24	1.57	1.52
2	D	1	FRU	O3-C3	2.91	1.48	1.42
2	D	3	GAL	C2-C3	2.68	1.56	1.52
2	D	3	GAL	C1-C2	2.62	1.58	1.52
2	D	2	GLC	C4-C5	2.55	1.58	1.53
2	D	3	GAL	O5-C1	2.31	1.47	1.43
2	D	1	FRU	C1-C2	2.21	1.57	1.52
2	D	2	GLC	C2-C3	2.20	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GAL	C1-C2-C3	4.66	116.42	109.64
2	D	2	GLC	O5-C5-C6	-4.36	99.17	107.66
2	C	1	FRU	O2-C2-O5	3.95	116.91	109.33
2	C	3	GAL	C1-C2-C3	3.89	115.31	109.64
2	C	1	FRU	C6-C5-C4	-3.71	106.33	115.10
2	D	2	GLC	C1-C2-C3	3.26	114.39	109.64
2	C	4	GAL	C1-O5-C5	3.09	116.33	112.19
2	D	3	GAL	C2-C3-C4	2.84	115.86	110.86
2	D	4	GAL	O5-C5-C6	2.58	112.69	107.66
2	D	2	GLC	O6-C6-C5	-2.31	103.48	111.33
2	D	4	GAL	C1-C2-C3	2.26	112.94	109.64
2	D	3	GAL	O4-C4-C3	-2.19	105.22	110.38
2	C	3	GAL	C2-C3-C4	2.09	114.54	110.86

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	FRU	C3
2	C	3	GAL	C3
2	C	3	GAL	C1
2	C	3	GAL	C2
2	C	4	GAL	C1
2	D	1	FRU	C3
2	D	3	GAL	C3

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Mol	Chain	Res	Type	Atom
2	D	3	GAL	C1
2	D	3	GAL	C2
2	D	4	GAL	C1

All (10) torsion outliers are listed below:

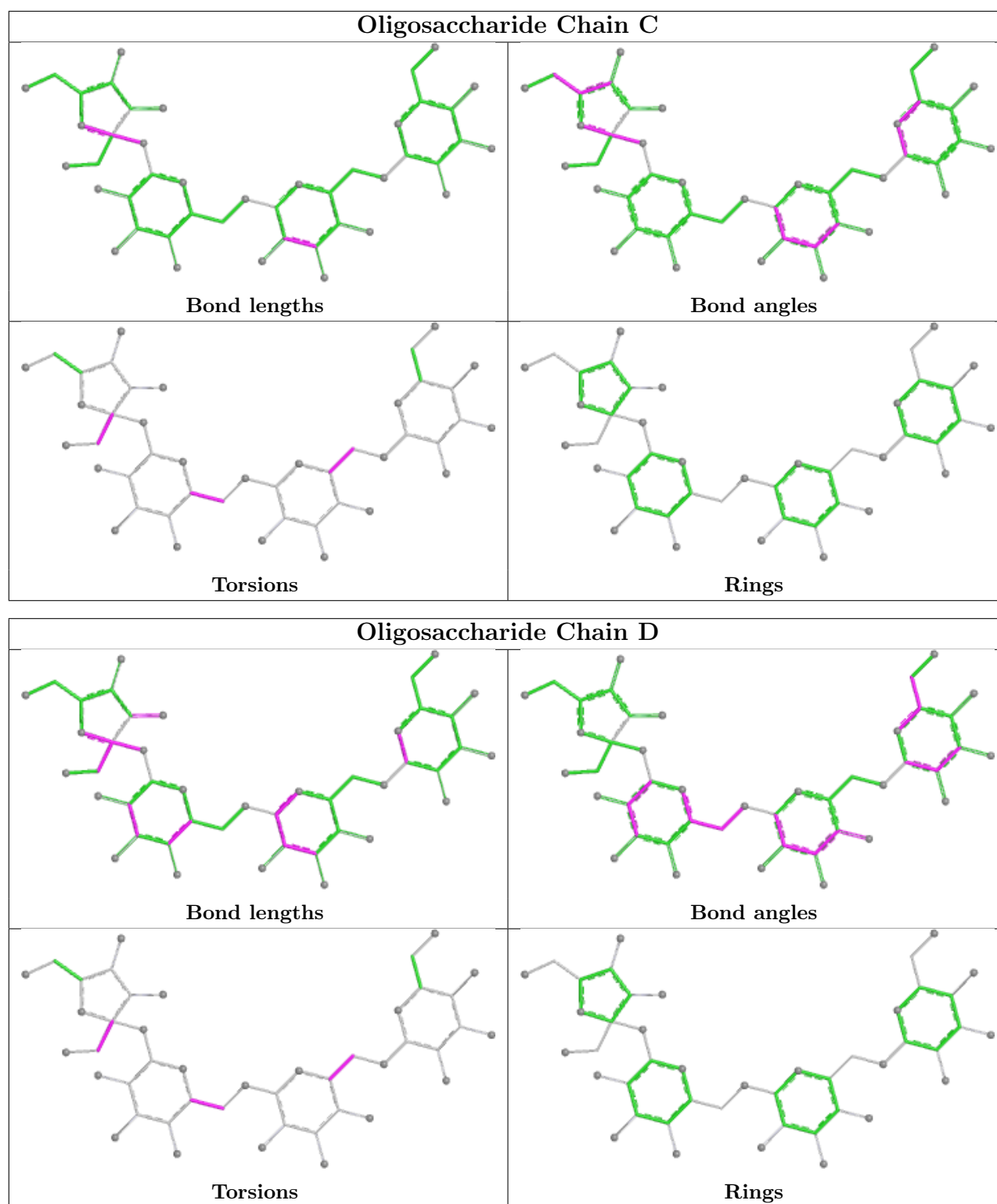
Mol	Chain	Res	Type	Atoms
2	D	1	FRU	O1-C1-C2-C3
2	D	1	FRU	O1-C1-C2-O2
2	C	2	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6
2	D	1	FRU	O1-C1-C2-O5
2	D	3	GAL	O5-C5-C6-O6
2	C	3	GAL	O5-C5-C6-O6
2	C	1	FRU	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	FRU	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.



5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	711	-	3,3,3	0.50	0	2,2,2	0.44	0
4	PEG	B	706	-	6,6,6	0.17	0	5,5,5	0.10	0
5	EDO	B	718	-	3,3,3	0.65	0	2,2,2	0.10	0
4	PEG	B	707	-	6,6,6	0.42	0	5,5,5	0.50	0
3	PG4	B	701	-	12,12,12	0.91	0	11,11,11	0.61	0
4	PEG	B	702	-	6,6,6	0.17	0	5,5,5	0.13	0
5	EDO	B	717	-	3,3,3	0.48	0	2,2,2	0.43	0
4	PEG	A	701	-	6,6,6	0.09	0	5,5,5	0.10	0
5	EDO	B	710	-	3,3,3	0.72	0	2,2,2	0.17	0
5	EDO	B	713	-	3,3,3	0.54	0	2,2,2	0.29	0
5	EDO	B	709	-	3,3,3	0.61	0	2,2,2	0.19	0
5	EDO	B	712	-	3,3,3	0.78	0	2,2,2	0.21	0
4	PEG	B	708	6	6,6,6	0.32	0	5,5,5	0.37	0
4	PEG	B	704	-	6,6,6	0.12	0	5,5,5	0.09	0
5	EDO	B	716	-	3,3,3	0.46	0	2,2,2	0.18	0
5	EDO	B	714	6	3,3,3	0.50	0	2,2,2	0.30	0
5	EDO	B	715	-	3,3,3	0.62	0	2,2,2	0.32	0
4	PEG	B	703	-	6,6,6	0.20	0	5,5,5	0.13	0
5	EDO	B	720	-	3,3,3	0.60	0	2,2,2	0.43	0
5	EDO	A	702	-	3,3,3	0.58	0	2,2,2	0.25	0
5	EDO	B	719	-	3,3,3	0.46	0	2,2,2	0.22	0
4	PEG	B	705	-	6,6,6	0.32	0	5,5,5	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	711	-	-	1/1/1/1	-
4	PEG	B	706	-	-	0/4/4/4	-
5	EDO	B	718	-	-	0/1/1/1	-
4	PEG	B	707	-	-	4/4/4/4	-
3	PG4	B	701	-	-	7/10/10/10	-
4	PEG	B	702	-	-	0/4/4/4	-
5	EDO	B	717	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	701	-	-	1/4/4/4	-
5	EDO	B	710	-	-	0/1/1/1	-
5	EDO	B	713	-	-	1/1/1/1	-
5	EDO	B	709	-	-	0/1/1/1	-
5	EDO	B	712	-	-	1/1/1/1	-
4	PEG	B	708	6	-	3/4/4/4	-
4	PEG	B	704	-	-	0/4/4/4	-
5	EDO	B	716	-	-	0/1/1/1	-
5	EDO	B	714	6	-	0/1/1/1	-
5	EDO	B	715	-	-	1/1/1/1	-
4	PEG	B	703	-	-	1/4/4/4	-
5	EDO	B	720	-	-	1/1/1/1	-
5	EDO	A	702	-	-	1/1/1/1	-
5	EDO	B	719	-	-	0/1/1/1	-
4	PEG	B	705	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	708	PEG	O1-C1-C2-O2
3	B	701	PG4	O3-C5-C6-O4
3	B	701	PG4	C4-C3-O2-C2
3	B	701	PG4	O2-C3-C4-O3
3	B	701	PG4	O1-C1-C2-O2
4	B	707	PEG	O1-C1-C2-O2
4	B	703	PEG	C4-C3-O2-C2
3	B	701	PG4	C5-C6-O4-C7
4	B	707	PEG	C1-C2-O2-C3
4	B	707	PEG	O2-C3-C4-O4
4	B	708	PEG	O2-C3-C4-O4
5	B	713	EDO	O1-C1-C2-O2
3	B	701	PG4	C6-C5-O3-C4
3	B	701	PG4	C1-C2-O2-C3
4	B	708	PEG	C1-C2-O2-C3
4	A	701	PEG	C1-C2-O2-C3
4	B	707	PEG	C4-C3-O2-C2
5	A	702	EDO	O1-C1-C2-O2
5	B	711	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	712	EDO	O1-C1-C2-O2
4	B	705	PEG	C1-C2-O2-C3
5	B	715	EDO	O1-C1-C2-O2
5	B	720	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	PEG	1	0
4	B	707	PEG	3	0
3	B	701	PG4	1	0
4	B	702	PEG	1	0
4	A	701	PEG	1	0
4	B	708	PEG	5	0
5	B	716	EDO	4	0
5	B	714	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	669/683 (97%)	0.64	42 (6%) 26 27	31, 64, 107, 145	0
1	B	671/683 (98%)	0.23	29 (4%) 40 41	15, 56, 104, 150	0
All	All	1340/1366 (98%)	0.43	71 (5%) 32 34	15, 61, 107, 150	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	5.2
1	B	22	ALA	4.5
1	B	132	ALA	4.1
1	A	57	GLY	4.1
1	B	133	LYS	4.1
1	A	56	ALA	4.0
1	A	59	LEU	3.6
1	B	8	ALA	3.4
1	A	676	ILE	3.4
1	A	455	GLY	3.3
1	B	57	GLY	3.2
1	A	8	ALA	3.1
1	B	477	VAL	3.1
1	A	61	PRO	3.0
1	B	236	CYS	3.0
1	A	21	PRO	3.0
1	A	250	TYR	3.0
1	B	678	HIS	2.9
1	A	564	GLY	2.8
1	B	485	ASN	2.7
1	A	347	ALA	2.7
1	B	472	LEU	2.7
1	A	182	ALA	2.7
1	A	242	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	252	LYS	2.7
1	A	53	PHE	2.6
1	A	58	LYS	2.6
1	B	473	GLY	2.6
1	B	20	PHE	2.6
1	A	162	ALA	2.6
1	A	20	PHE	2.6
1	A	203	GLY	2.5
1	A	469	LYS	2.5
1	B	21	PRO	2.5
1	B	56	ALA	2.5
1	B	467	PHE	2.5
1	B	474	GLY	2.4
1	A	113	ILE	2.4
1	B	250	TYR	2.4
1	B	102	TYR	2.4
1	A	134	ASP	2.4
1	A	236	CYS	2.3
1	A	24	GLY	2.3
1	B	468	PRO	2.3
1	A	37	PHE	2.2
1	A	161	GLY	2.2
1	A	238	GLY	2.2
1	B	469	LYS	2.2
1	A	133	LYS	2.2
1	B	554	ARG	2.2
1	A	582	LYS	2.2
1	A	103	ILE	2.2
1	A	221	ALA	2.2
1	A	653	ALA	2.2
1	A	244	LYS	2.2
1	B	435	ALA	2.1
1	A	169	ALA	2.1
1	B	134	ASP	2.1
1	A	64	GLU	2.1
1	B	471	THR	2.1
1	A	19	GLN	2.1
1	A	177	PHE	2.1
1	A	252	LYS	2.1
1	B	523	TYR	2.1
1	A	194	GLY	2.1
1	A	464	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	PRO	2.0
1	B	563	GLU	2.0
1	B	457	LYS	2.0
1	B	24	GLY	2.0
1	A	255	TYR	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](#)

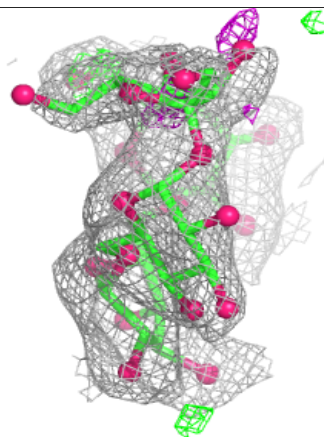
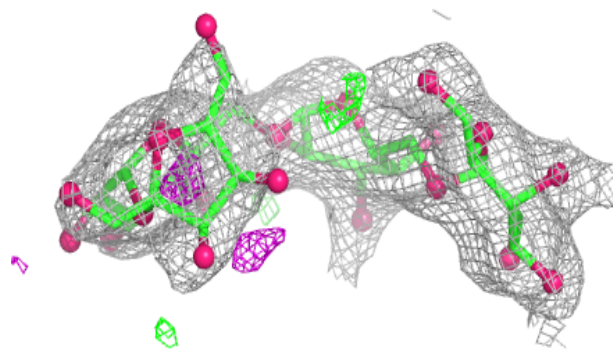
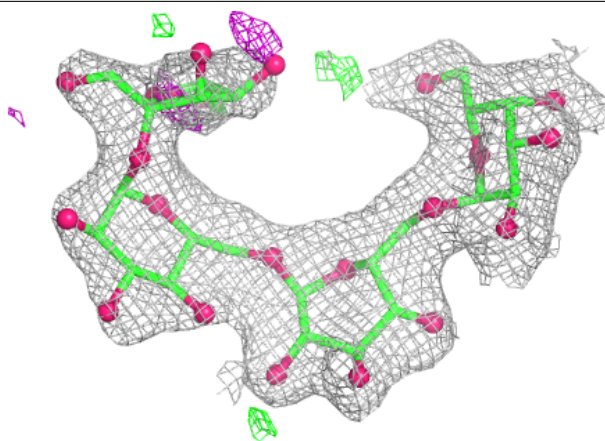
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

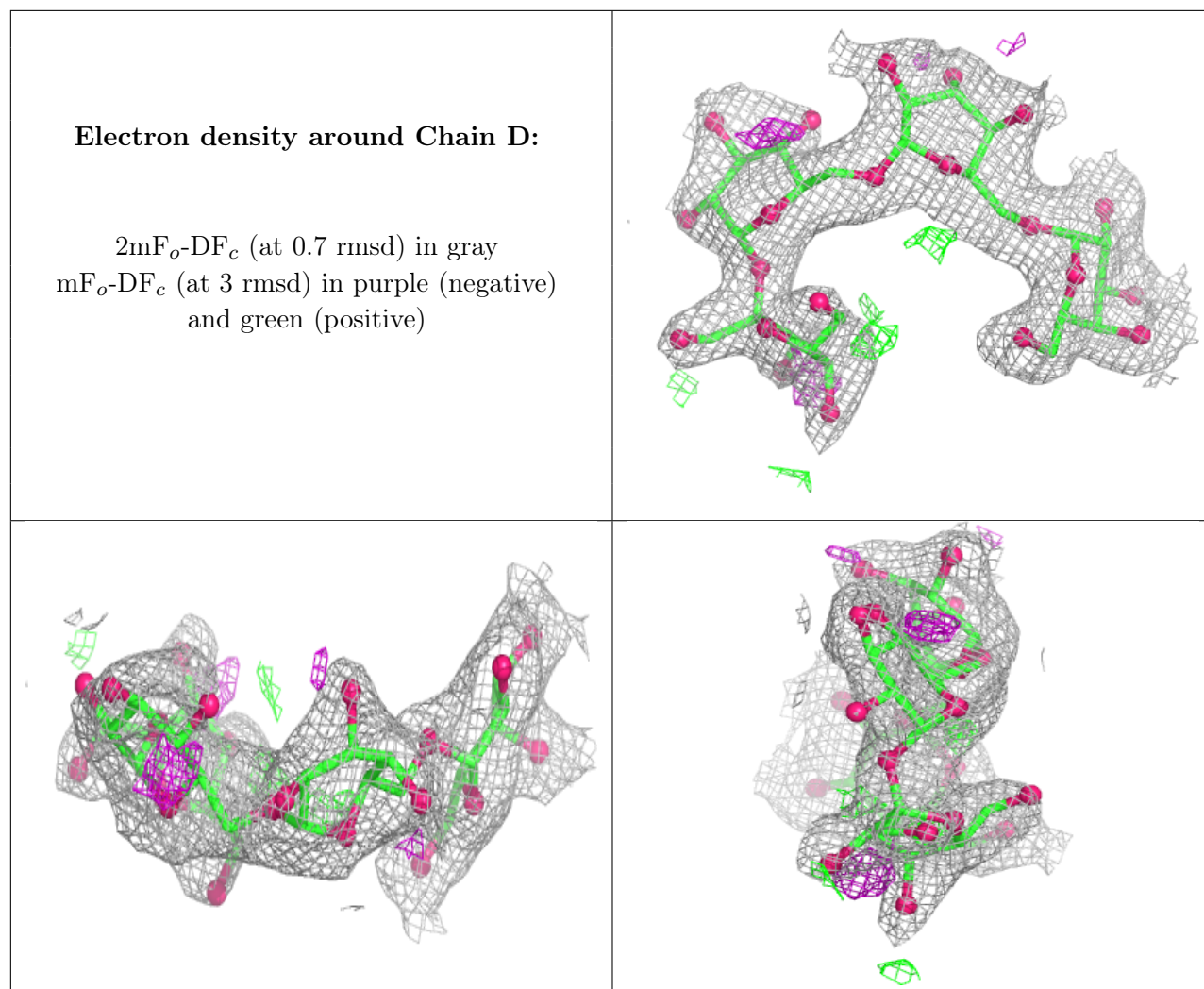
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	C	1	12/12	0.83	0.18	75,78,80,81	0
2	GLC	D	2	11/12	0.83	0.14	45,62,65,66	0
2	FRU	D	1	12/12	0.84	0.16	59,64,65,65	0
2	GAL	D	3	11/12	0.90	0.09	29,41,47,52	0
2	GLC	C	2	11/12	0.91	0.12	63,70,72,73	0
2	GAL	C	3	11/12	0.94	0.07	39,47,53,55	0
2	GAL	C	4	11/12	0.96	0.07	34,37,39,39	0
2	GAL	D	4	11/12	0.97	0.05	19,21,23,25	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 C:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	702	4/4	0.69	0.12	73,74,75,76	0
5	EDO	B	720	4/4	0.74	0.14	53,54,54,55	0
4	PEG	B	703	7/7	0.76	0.15	61,62,64,64	0
5	EDO	B	713	4/4	0.76	0.14	67,68,68,69	0
5	EDO	B	709	4/4	0.77	0.13	60,61,61,61	0
5	EDO	B	717	4/4	0.78	0.11	57,58,59,59	0
4	PEG	B	705	7/7	0.78	0.15	50,59,64,66	0
4	PEG	B	707	7/7	0.78	0.17	40,45,49,49	0
5	EDO	B	712	4/4	0.82	0.15	51,52,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	718	4/4	0.82	0.12	73,76,77,77	0
6	CA	A	704	1/1	0.85	0.11	87,87,87,87	0
5	EDO	B	716	4/4	0.86	0.21	36,37,43,50	0
5	EDO	B	711	4/4	0.86	0.12	54,54,55,56	0
4	PEG	B	706	7/7	0.87	0.12	60,63,72,74	0
6	CA	A	706	1/1	0.87	0.11	93,93,93,93	0
4	PEG	B	708	7/7	0.88	0.23	26,33,42,48	0
6	CA	B	725	1/1	0.88	0.15	84,84,84,84	0
5	EDO	B	715	4/4	0.88	0.10	41,41,42,42	0
5	EDO	B	710	4/4	0.88	0.12	40,41,42,43	0
6	CA	A	705	1/1	0.89	0.09	81,81,81,81	0
3	PG4	B	701	13/13	0.89	0.12	40,44,47,52	0
4	PEG	B	704	7/7	0.90	0.10	51,53,56,56	0
5	EDO	B	714	4/4	0.90	0.09	45,46,46,46	0
4	PEG	A	701	7/7	0.90	0.11	66,69,72,74	0
5	EDO	B	719	4/4	0.91	0.11	33,33,35,38	0
6	CA	B	724	1/1	0.91	0.10	83,83,83,83	0
4	PEG	B	702	7/7	0.94	0.08	29,33,42,48	0
6	CA	B	721	1/1	0.95	0.06	92,92,92,92	0
6	CA	B	722	1/1	0.97	0.05	49,49,49,49	0
6	CA	B	723	1/1	0.97	0.07	32,32,32,32	0
6	CA	A	703	1/1	0.97	0.04	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.