



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:17 PM UTC

PDB ID : 5KDX / pdb_00005kdx
Title : IMPa metallopeptidase in complex with T-antigen
Authors : Noach, I.; Boraston, A.B.
Deposited on : 2016-06-08
Resolution : 2.40 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

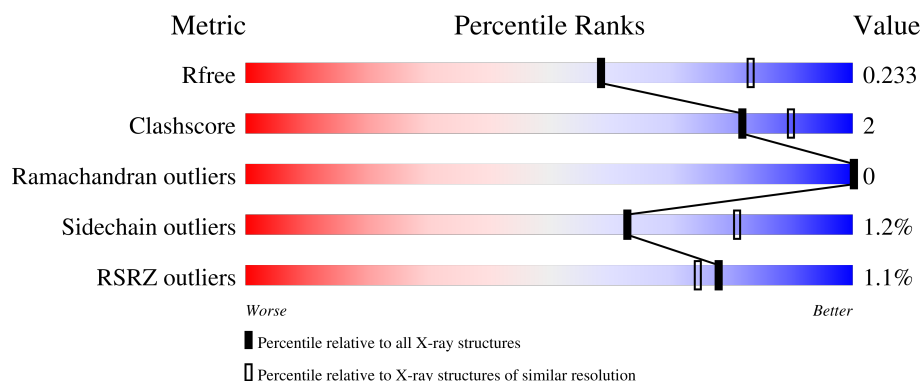
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	885	94% 6%
1	B	885	95% 5%
2	C	2	100%
2	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	1008	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15077 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.

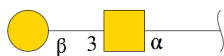
- Molecule 1 is a protein called Metallopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	884	Total	C	N	O	S	0	0	0
			6789	4250	1214	1311	14			
1	B	883	Total	C	N	O	S	0	0	0
			6780	4245	1213	1308	14			

There are 6 discrepancies between the modelled and reference sequences:

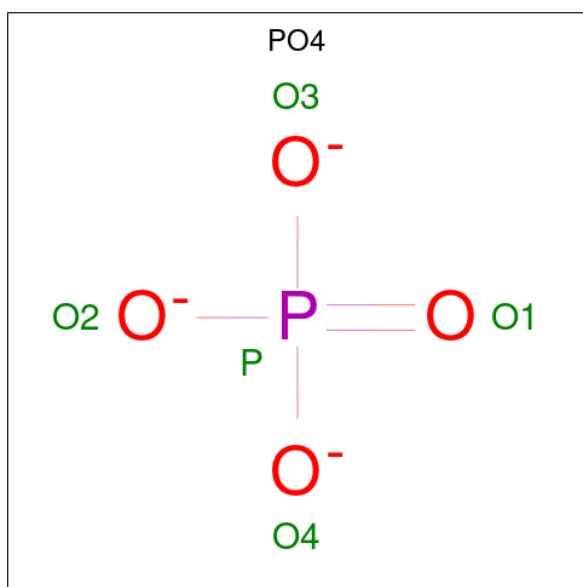
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q9I5W4
A	924	LEU	-	expression tag	UNP Q9I5W4
A	925	GLU	-	expression tag	UNP Q9I5W4
B	41	MET	-	initiating methionine	UNP Q9I5W4
B	924	LEU	-	expression tag	UNP Q9I5W4
B	925	GLU	-	expression tag	UNP Q9I5W4

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			25	14	1	10			
2	D	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

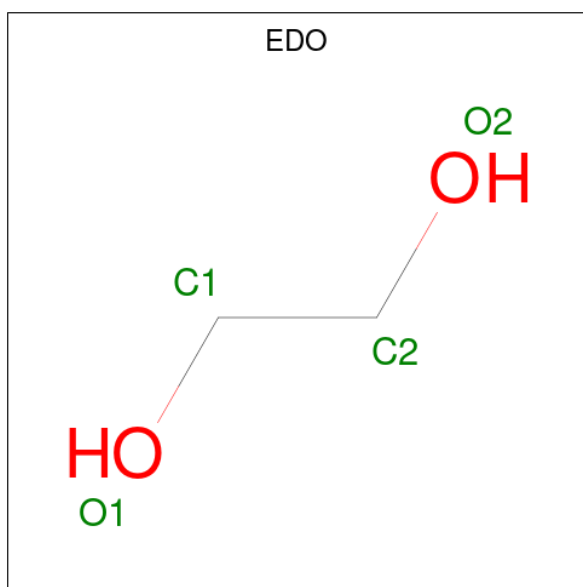


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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

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

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



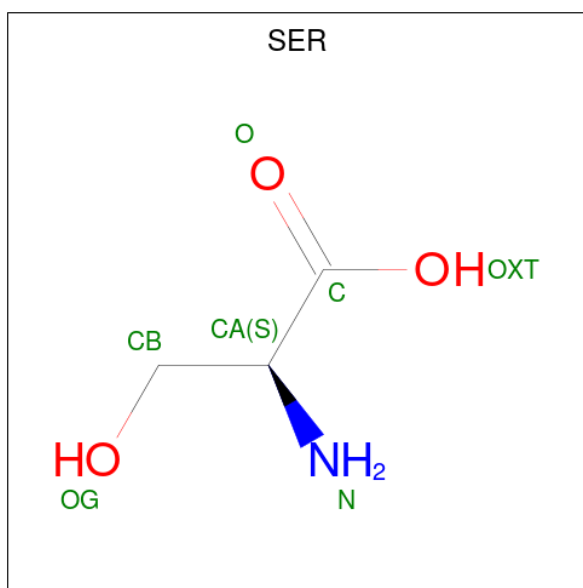
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total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

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

- Molecule 6 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



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

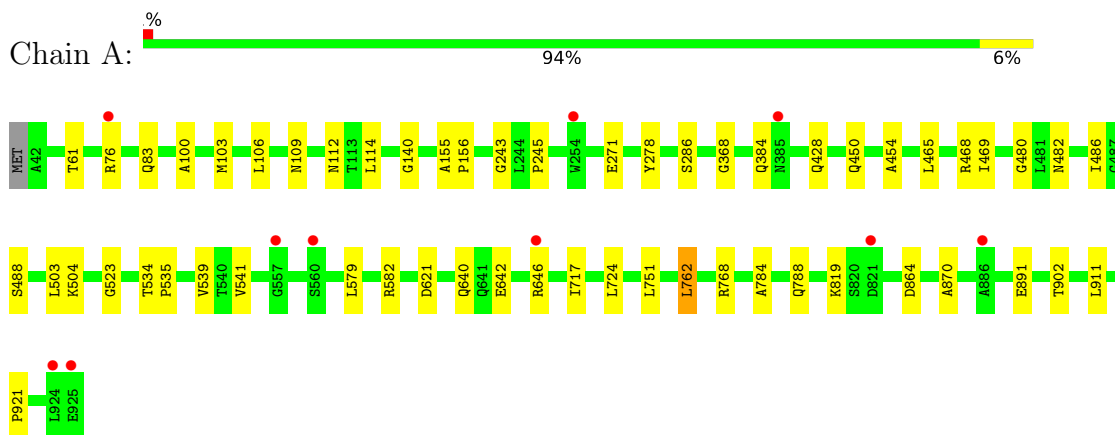
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	657	Total	O	0	0
			657	657		
7	B	656	Total	O	0	0
			656	656		

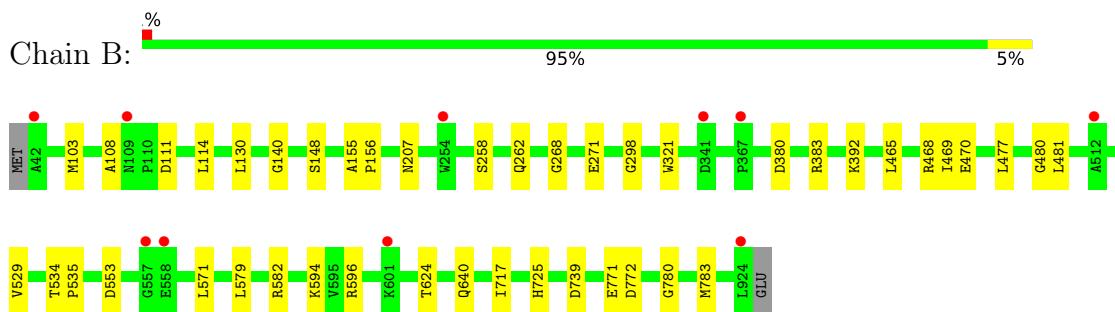
3 Residue-property plots

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.

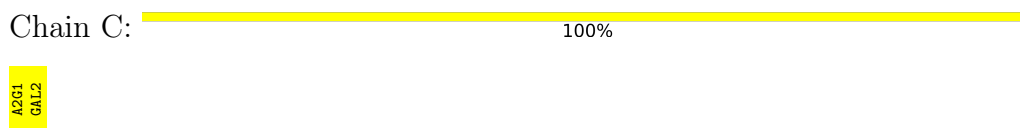
- Molecule 1: Metallopeptidase



- Molecule 1: Metallopeptidase



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



- Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-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	99.41Å 133.10Å 103.78Å 90.00° 103.12° 90.00°	Depositor
Resolution (Å)	48.12 – 2.40 48.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.12-2.40) 99.6 (48.12-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.254 (Not available) , 0.233	Depositor DCC
R_{free} test set	5027 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.090 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15077	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: ZN, EDO, PO4, A2G, GAL

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	0.66	0/6937	0.83	2/9442 (0.0%)
1	B	0.67	0/6928	0.83	1/9430 (0.0%)
All	All	0.66	0/13865	0.83	3/18872 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	717	ILE	CB-CA-C	-6.14	105.58	111.05
1	A	717	ILE	CB-CA-C	-6.07	105.65	111.05
1	A	486	ILE	N-CA-C	5.12	116.45	110.62

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	6789	0	6592	37	0
1	B	6780	0	6586	30	0
2	C	25	0	21	0	0
2	D	25	0	21	0	0
3	A	10	0	0	0	0
3	B	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	60	0	90	9	0
5	B	44	0	66	9	0
6	A	7	0	3	0	0
6	B	7	0	3	0	0
7	A	657	0	0	4	0
7	B	656	0	0	4	0
All	All	15077	0	13382	68	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 2.

All (68) 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:468:ARG:NH2	1:B:470:GLU:OE2	2.11	0.83
1:A:61:THR:HG22	1:A:384:GLN:HG2	1.70	0.74
1:B:298:GLY:O	7:B:1101:HOH:O	2.07	0.72
1:B:469:ILE:CD1	1:B:477:LEU:HD13	2.22	0.70
1:A:454:ALA:O	1:A:582:ARG:NH1	2.25	0.69
1:A:103:MET:HE2	1:A:271:GLU:HG2	1.74	0.69
1:A:428:GLN:H	1:A:428:GLN:CD	2.08	0.61
1:A:480:GLY:HA3	5:A:1011:EDO:C1	2.31	0.61
1:B:469:ILE:HD12	1:B:477:LEU:HD13	1.83	0.60
1:A:468:ARG:HD3	7:A:1177:HOH:O	2.00	0.59
1:B:103:MET:HE2	1:B:271:GLU:HG2	1.86	0.58
1:A:902:THR:HG22	5:A:1006:EDO:H22	1.84	0.57
1:B:480:GLY:HA3	5:B:1009:EDO:H12	1.86	0.57
1:B:380:ASP:OD1	1:B:383:ARG:NH1	2.32	0.57
1:B:579:LEU:C	1:B:579:LEU:HD12	2.31	0.56
1:A:469:ILE:HG22	1:A:541:VAL:HG22	1.88	0.56
1:A:621:ASP:OD2	5:A:1008:EDO:H12	2.07	0.55
1:A:465:LEU:HD12	1:A:465:LEU:C	2.32	0.54
1:A:724:LEU:HB3	5:A:1006:EDO:H11	1.88	0.54
1:B:571:LEU:O	1:B:596:ARG:NH2	2.43	0.52
1:A:103:MET:HE2	1:A:271:GLU:CG	2.39	0.52
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.92	0.52
1:B:321:TRP:CE2	1:B:392:LYS:HG2	2.44	0.52
1:A:100:ALA:HB1	1:A:278:TYR:HA	1.91	0.52
5:B:1009:EDO:H11	7:B:1212:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ILE:HD12	1:A:469:ILE:O	2.11	0.51
1:A:106:LEU:HD12	1:A:106:LEU:N	2.25	0.50
1:A:480:GLY:HA3	5:A:1011:EDO:H12	1.95	0.49
1:A:112:ASN:ND2	7:A:1121:HOH:O	2.46	0.48
1:A:762:LEU:CD2	1:A:870:ALA:HA	2.43	0.48
1:A:534:THR:O	1:A:535:PRO:C	2.57	0.47
1:B:780:GLY:HA2	1:B:783:MET:HE3	1.96	0.47
1:A:523:GLY:O	5:A:1009:EDO:O1	2.28	0.47
1:B:481:LEU:CB	5:B:1008:EDO:H12	2.45	0.47
1:A:482:ASN:O	1:A:504:LYS:HG3	2.14	0.47
1:B:624:THR:HG21	5:B:1010:EDO:H11	1.97	0.47
1:A:428:GLN:CD	1:A:428:GLN:N	2.73	0.47
1:B:108:ALA:HB3	1:B:268:GLY:O	2.15	0.46
1:A:243:GLY:O	1:A:245:PRO:HD3	2.16	0.46
1:B:534:THR:O	1:B:535:PRO:C	2.57	0.46
1:A:109:ASN:ND2	1:A:368:GLY:O	2.47	0.45
1:A:579:LEU:C	1:A:579:LEU:HD12	2.42	0.45
1:A:488:SER:HB2	5:A:1007:EDO:H11	1.99	0.45
1:A:642:GLU:HG2	7:A:1297:HOH:O	2.17	0.44
1:B:624:THR:HG21	5:B:1010:EDO:C1	2.48	0.44
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.99	0.43
1:A:864:ASP:HB3	1:A:891:GLU:HA	2.01	0.43
1:A:103:MET:O	1:A:140:GLY:HA3	2.19	0.43
1:B:258:SER:O	1:B:262:GLN:HG3	2.19	0.42
1:B:321:TRP:CD2	1:B:392:LYS:HG2	2.55	0.42
1:B:111:ASP:OD1	3:B:1003:PO4:O4	2.37	0.41
1:B:207:ASN:OD1	1:B:207:ASN:C	2.63	0.41
1:B:481:LEU:HB3	5:B:1008:EDO:H11	2.02	0.41
1:A:762:LEU:HD22	1:A:870:ALA:HA	2.02	0.41
1:B:772:ASP:OD1	1:B:772:ASP:C	2.64	0.41
1:B:725:HIS:NE2	7:B:1106:HOH:O	2.36	0.41
1:A:621:ASP:OD2	5:A:1008:EDO:C1	2.69	0.41
1:A:784:ALA:O	1:A:788:GLN:HG2	2.20	0.41
1:B:481:LEU:HB2	5:B:1008:EDO:H12	2.02	0.41
1:B:553:ASP:OD1	1:B:582:ARG:HD2	2.21	0.41
1:A:503:LEU:O	5:A:1009:EDO:C2	2.69	0.41
1:A:911:LEU:HD21	1:A:921:PRO:HG3	2.04	0.40
1:B:481:LEU:HB3	5:B:1008:EDO:C1	2.50	0.40
1:B:529:VAL:HG12	5:B:1014:EDO:H11	2.03	0.40
1:A:751:LEU:HD22	1:A:768:ARG:HB3	2.04	0.40
1:B:103:MET:O	1:B:140:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:GLU:CG	7:A:1297:HOH:O	2.69	0.40
1:B:594:LYS:NZ	7:B:1149:HOH:O	2.54	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	882/885 (100%)	864 (98%)	18 (2%)	0	100	100
1	B	881/885 (100%)	860 (98%)	21 (2%)	0	100	100
All	All	1763/1770 (100%)	1724 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	700/701 (100%)	690 (99%)	10 (1%)	59	79
1	B	699/701 (100%)	692 (99%)	7 (1%)	68	84
All	All	1399/1402 (100%)	1382 (99%)	17 (1%)	63	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	83	GLN
1	A	114	LEU
1	A	286	SER
1	A	450	GLN
1	A	539	VAL
1	A	640	GLN
1	A	646	ARG
1	A	762	LEU
1	A	819	LYS
1	B	114	LEU
1	B	130	LEU
1	B	148	SER
1	B	465	LEU
1	B	640	GLN
1	B	739	ASP
1	B	771	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	72	GLN
1	A	90	GLN
1	A	225	ASN
1	A	252	ASN
1	A	308	GLN
1	A	385	ASN
1	B	90	GLN
1	B	109	ASN
1	B	225	ASN
1	B	252	ASN
1	B	270	GLN
1	B	361	GLN
1	B	562	GLN
1	B	633	GLN
1	B	852	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	C	2	2	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
2	GAL	D	2	2	11,11,12	0.67	0	15,15,17	1.03	1 (6%)

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	C	2	2	-	1/2/19/22	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	O3-C3-C2	-2.12	105.72	110.05
2	C	2	GAL	C1-C2-C3	-2.10	106.59	109.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2G	C	1	2,6	14,14,15	0.74	1 (7%)	17,19,21	1.20	1 (5%)
2	GAL	C	2	2	11,11,12	0.71	0	15,15,17	0.89	1 (6%)
2	A2G	D	1	2,6	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
2	GAL	D	2	2	11,11,12	0.67	0	15,15,17	1.03	1 (6%)

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	A2G	C	1	2,6	-	2/6/23/26	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	A2G	D	1	2,6	-	1/6/23/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	A2G	C1-C2	2.05	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	A2G	C1-O5-C5	2.19	115.12	112.19
2	D	2	GAL	O3-C3-C2	-2.12	105.72	110.05
2	C	1	A2G	C2-N2-C7	2.11	125.73	122.90
2	C	2	GAL	C1-C2-C3	-2.10	106.59	109.64

There are no chirality outliers.

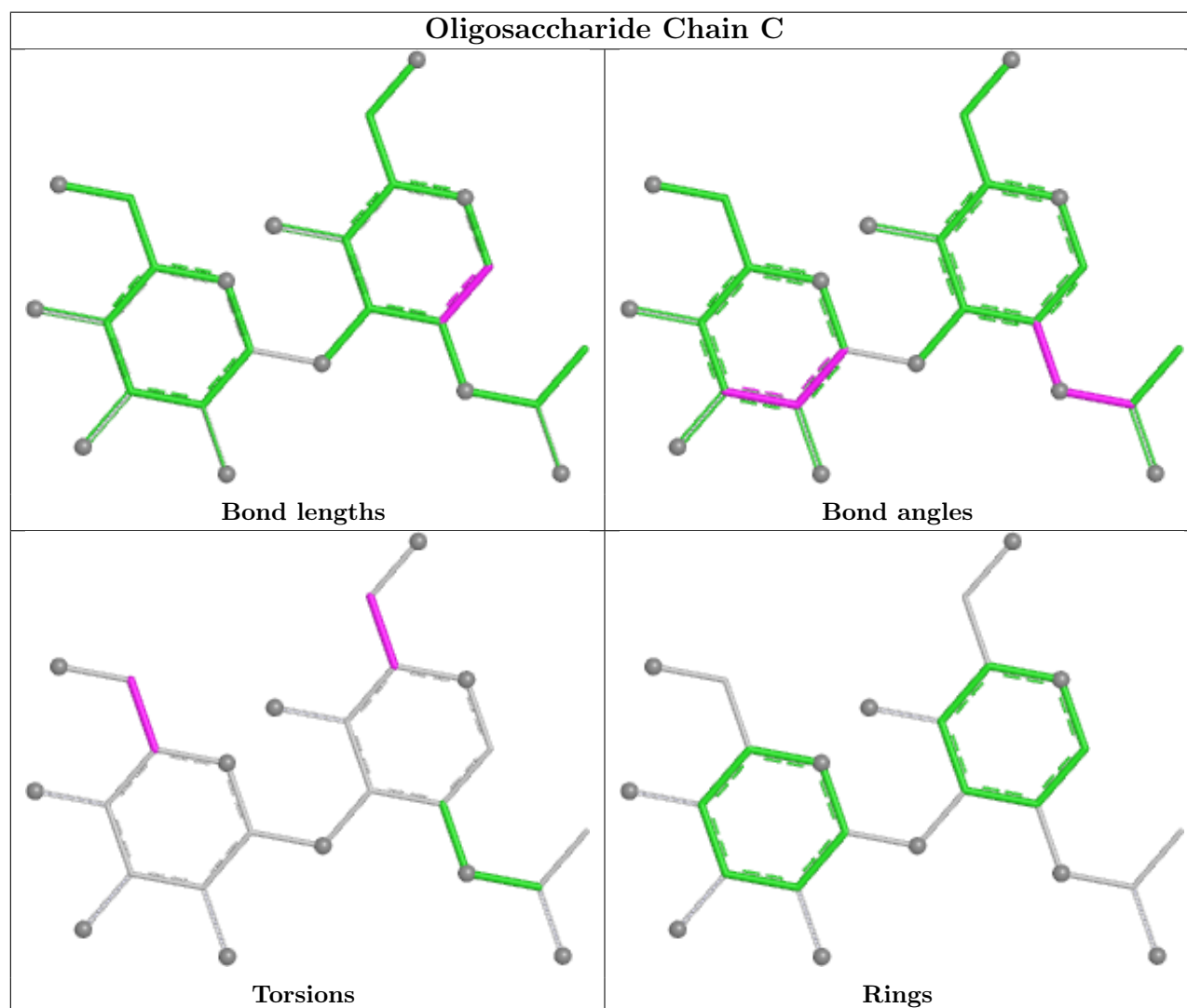
All (6) torsion outliers are listed below:

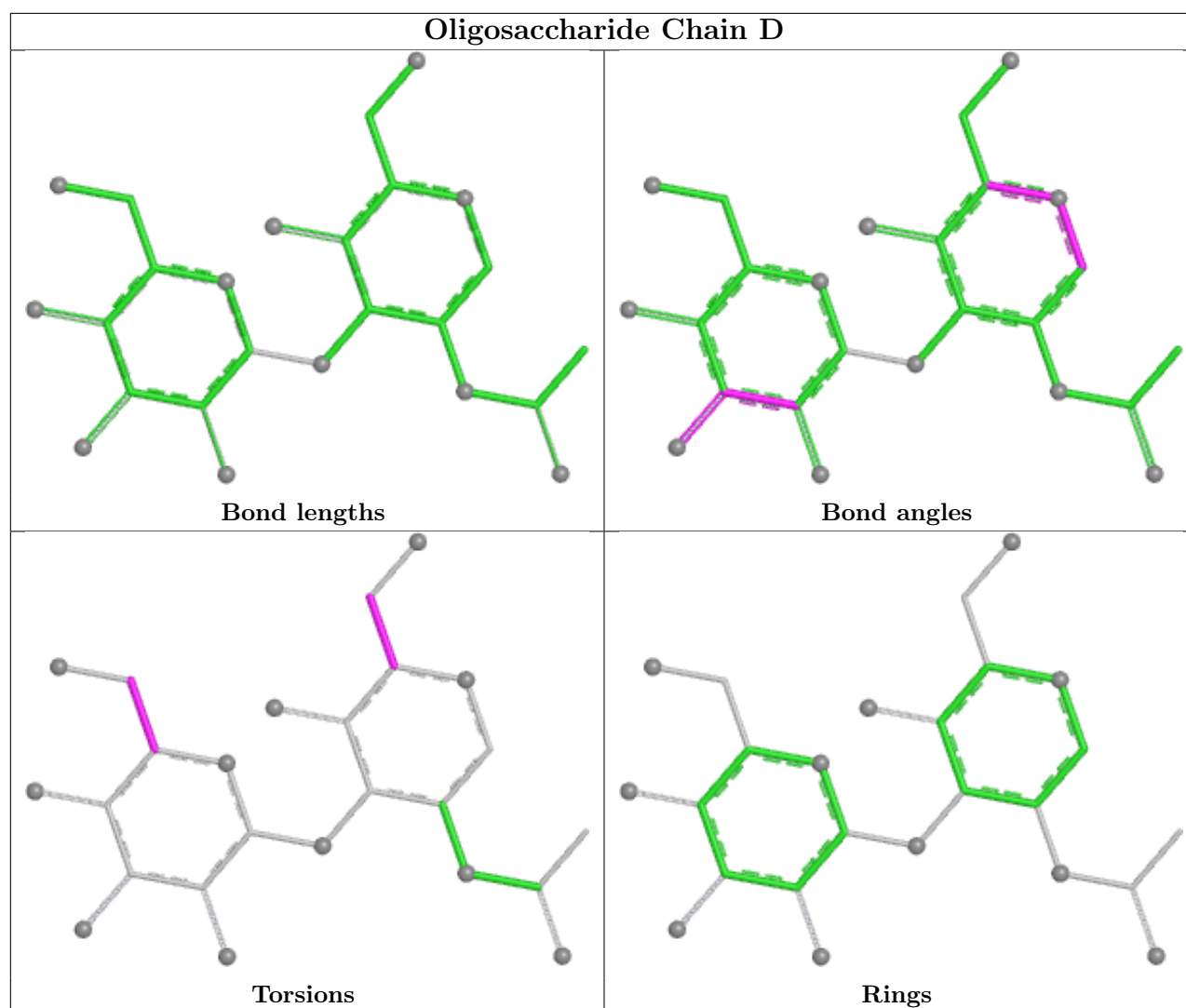
Mol	Chain	Res	Type	Atoms
2	D	2	GAL	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	1	A2G	C4-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6
2	C	1	A2G	O5-C5-C6-O6
2	D	1	A2G	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	A	1010	-	3,3,3	0.66	0	2,2,2	0.26	0
5	EDO	A	1014	-	3,3,3	0.43	0	2,2,2	0.68	0
5	EDO	A	1006	-	3,3,3	0.40	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SER	B	1018	2	4,6,6	1.07	1 (25%)	2,7,7	1.26	0
5	EDO	A	1009	-	3,3,3	0.35	0	2,2,2	0.20	0
5	EDO	B	1008	-	3,3,3	0.24	0	2,2,2	0.41	0
5	EDO	B	1011	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	A	1007	-	3,3,3	0.47	0	2,2,2	0.10	0
5	EDO	B	1010	-	3,3,3	0.43	0	2,2,2	0.29	0
5	EDO	A	1017	-	3,3,3	0.42	0	2,2,2	0.36	0
3	PO4	B	1004	-	4,4,4	1.10	0	6,6,6	0.34	0
5	EDO	A	1013	-	3,3,3	0.40	0	2,2,2	0.44	0
5	EDO	A	1008	-	3,3,3	0.43	0	2,2,2	0.27	0
5	EDO	A	1018	-	3,3,3	0.49	0	2,2,2	0.10	0
5	EDO	B	1016	-	3,3,3	0.49	0	2,2,2	0.14	0
3	PO4	B	1003	-	4,4,4	0.84	0	6,6,6	0.68	0
5	EDO	A	1019	-	3,3,3	0.36	0	2,2,2	0.44	0
3	PO4	A	1003	-	4,4,4	0.83	0	6,6,6	0.50	0
5	EDO	A	1015	-	3,3,3	0.63	0	2,2,2	0.21	0
5	EDO	A	1016	-	3,3,3	0.38	0	2,2,2	0.46	0
5	EDO	B	1015	-	3,3,3	0.51	0	2,2,2	0.17	0
5	EDO	A	1011	-	3,3,3	0.54	0	2,2,2	0.31	0
5	EDO	B	1014	-	3,3,3	0.42	0	2,2,2	0.34	0
5	EDO	B	1012	-	3,3,3	0.36	0	2,2,2	0.48	0
3	PO4	B	1005	-	4,4,4	0.79	0	6,6,6	0.84	0
5	EDO	A	1012	-	3,3,3	0.53	0	2,2,2	0.03	0
5	EDO	B	1007	-	3,3,3	0.41	0	2,2,2	0.37	0
6	SER	A	1021	2	4,6,6	1.15	1 (25%)	2,7,7	2.06	1 (50%)
3	PO4	A	1004	-	4,4,4	0.78	0	6,6,6	0.68	0
5	EDO	A	1020	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	B	1017	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	B	1013	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	B	1009	-	3,3,3	0.43	0	2,2,2	0.27	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	A	1010	-	-	0/1/1/1	-
5	EDO	A	1014	-	-	1/1/1/1	-
5	EDO	A	1006	-	-	1/1/1/1	-
6	SER	B	1018	2	-	0/6/6/6	-
5	EDO	A	1009	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1008	-	-	1/1/1/1	-
5	EDO	B	1011	-	-	0/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	B	1010	-	-	0/1/1/1	-
5	EDO	A	1017	-	-	0/1/1/1	-
5	EDO	A	1008	-	-	1/1/1/1	-
5	EDO	A	1013	-	-	1/1/1/1	-
5	EDO	A	1018	-	-	1/1/1/1	-
5	EDO	B	1016	-	-	0/1/1/1	-
5	EDO	A	1019	-	-	0/1/1/1	-
5	EDO	A	1015	-	-	0/1/1/1	-
5	EDO	A	1016	-	-	1/1/1/1	-
5	EDO	B	1015	-	-	1/1/1/1	-
5	EDO	A	1011	-	-	1/1/1/1	-
5	EDO	B	1014	-	-	1/1/1/1	-
5	EDO	B	1012	-	-	1/1/1/1	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	1/1/1/1	-
6	SER	A	1021	2	-	0/6/6/6	-
5	EDO	A	1020	-	-	1/1/1/1	-
5	EDO	B	1017	-	-	0/1/1/1	-
5	EDO	B	1013	-	-	1/1/1/1	-
5	EDO	B	1009	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1021	SER	OXT-C	-2.21	1.23	1.30
6	B	1018	SER	OXT-C	-2.04	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1021	SER	OXT-C-O	-2.85	117.61	124.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1007	EDO	O1-C1-C2-O2
5	A	1016	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	1014	EDO	O1-C1-C2-O2
5	B	1015	EDO	O1-C1-C2-O2
5	A	1008	EDO	O1-C1-C2-O2
5	B	1012	EDO	O1-C1-C2-O2
5	A	1011	EDO	O1-C1-C2-O2
5	A	1020	EDO	O1-C1-C2-O2
5	B	1007	EDO	O1-C1-C2-O2
5	A	1006	EDO	O1-C1-C2-O2
5	A	1013	EDO	O1-C1-C2-O2
5	A	1018	EDO	O1-C1-C2-O2
5	B	1013	EDO	O1-C1-C2-O2
5	A	1014	EDO	O1-C1-C2-O2
5	B	1008	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	EDO	2	0
5	A	1009	EDO	2	0
5	B	1008	EDO	4	0
5	A	1007	EDO	1	0
5	B	1010	EDO	2	0
5	A	1008	EDO	2	0
3	B	1003	PO4	1	0
5	A	1011	EDO	2	0
5	B	1014	EDO	1	0
5	B	1009	EDO	2	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	884/885 (99%)	0.23	10 (1%) 78 74	16, 26, 40, 73	0
1	B	883/885 (99%)	0.18	10 (1%) 78 74	16, 25, 40, 68	0
All	All	1767/1770 (99%)	0.20	20 (1%) 78 74	16, 26, 40, 73	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	925	GLU	4.1
1	B	924	LEU	4.0
1	B	42	ALA	3.7
1	A	924	LEU	3.6
1	B	601	LYS	3.0
1	B	557	GLY	2.9
1	B	558	GLU	2.7
1	A	646	ARG	2.6
1	A	254	TRP	2.5
1	B	109	ASN	2.3
1	A	557	GLY	2.2
1	A	886	ALA	2.2
1	A	385	ASN	2.2
1	B	512	ALA	2.2
1	A	76	ARG	2.1
1	B	341	ASP	2.1
1	A	560	SER	2.0
1	B	367	PRO	2.0
1	B	254	TRP	2.0
1	A	821	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	GAL	C	2	11/12	0.69	0.21	40,43,45,46	11
2	GAL	D	2	11/12	0.74	0.22	42,45,47,47	11

6.3 Carbohydrates [i](#)

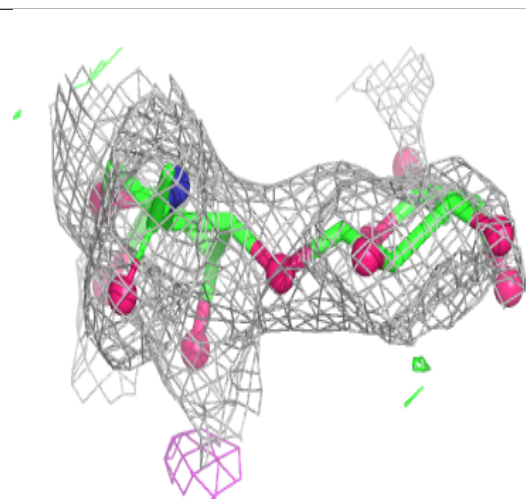
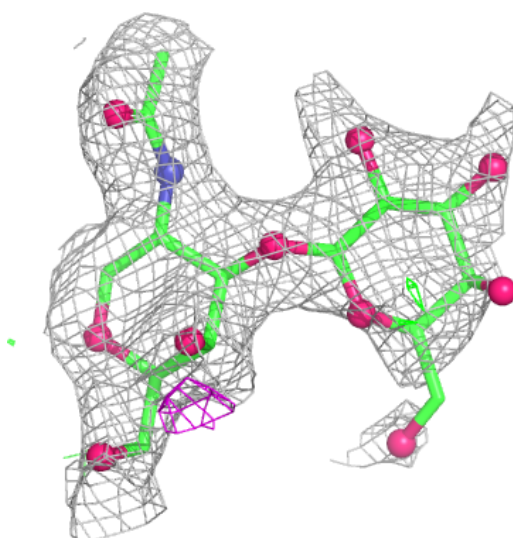
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

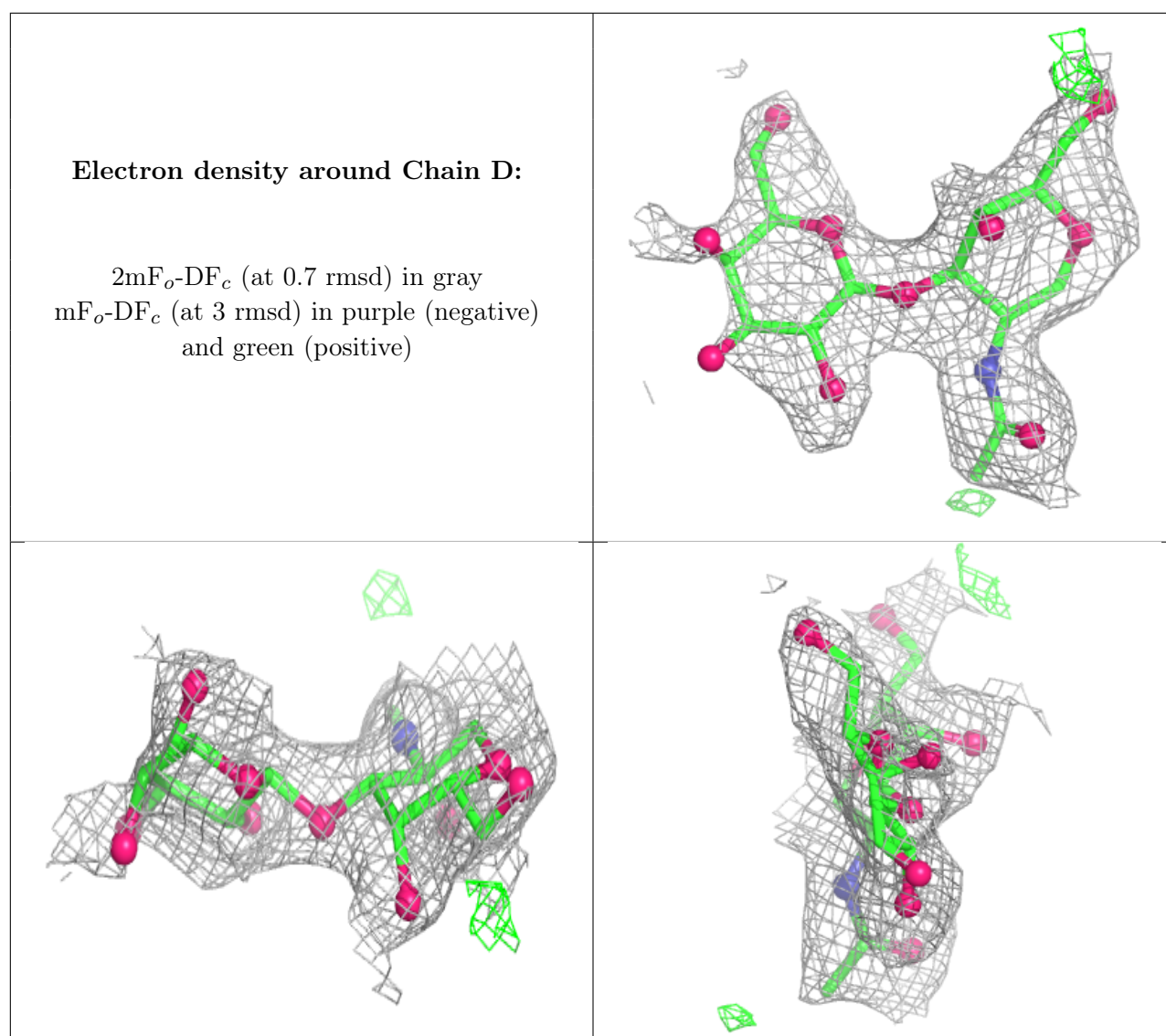
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	C	2	11/12	0.69	0.21	40,43,45,46	11
2	GAL	D	2	11/12	0.74	0.22	42,45,47,47	11
2	A2G	C	1	14/15	0.90	0.11	30,36,39,39	0
2	A2G	D	1	14/15	0.92	0.13	35,41,43,45	0

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 [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	EDO	B	1013	4/4	0.68	0.23	44,47,47,48	0
5	EDO	A	1020	4/4	0.72	0.20	53,53,54,57	0
5	EDO	A	1015	4/4	0.74	0.18	38,38,39,41	0
5	EDO	B	1015	4/4	0.75	0.18	45,45,45,46	0
5	EDO	A	1013	4/4	0.76	0.23	41,42,43,45	0
5	EDO	B	1014	4/4	0.78	0.18	44,45,47,47	0
5	EDO	A	1014	4/4	0.81	0.17	37,39,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	1005	5/5	0.83	0.13	37,38,39,41	1
5	EDO	A	1016	4/4	0.83	0.16	38,40,41,44	0
5	EDO	B	1017	4/4	0.83	0.18	39,41,41,45	0
5	EDO	A	1011	4/4	0.84	0.25	34,35,37,39	0
5	EDO	A	1019	4/4	0.86	0.16	41,43,43,44	0
5	EDO	A	1010	4/4	0.87	0.15	31,36,37,37	0
5	EDO	A	1007	4/4	0.87	0.22	38,39,39,41	0
6	SER	B	1018	7/7	0.88	0.13	36,40,43,43	0
5	EDO	A	1017	4/4	0.89	0.12	34,34,34,35	0
5	EDO	B	1010	4/4	0.89	0.16	34,35,35,35	0
5	EDO	B	1012	4/4	0.89	0.14	37,38,40,42	0
6	SER	A	1021	7/7	0.89	0.10	28,29,33,36	0
3	PO4	A	1003	5/5	0.89	0.18	44,45,47,47	0
5	EDO	A	1006	4/4	0.90	0.19	27,30,30,31	0
5	EDO	A	1018	4/4	0.90	0.12	38,40,41,44	0
3	PO4	B	1003	5/5	0.90	0.15	40,40,42,44	0
5	EDO	A	1012	4/4	0.91	0.14	32,35,35,35	0
5	EDO	B	1011	4/4	0.91	0.10	36,36,37,37	0
5	EDO	B	1016	4/4	0.91	0.11	42,42,43,43	0
3	PO4	A	1004	5/5	0.92	0.12	43,49,50,52	1
5	EDO	B	1008	4/4	0.92	0.14	20,21,21,21	0
5	EDO	A	1008	4/4	0.93	0.15	27,27,28,28	0
5	EDO	B	1009	4/4	0.93	0.16	35,37,37,37	0
5	EDO	B	1007	4/4	0.93	0.12	40,40,41,42	0
5	EDO	A	1009	4/4	0.94	0.12	19,20,21,21	0
3	PO4	B	1004	5/5	0.96	0.12	36,38,39,40	0
4	ZN	A	1005	1/1	0.99	0.02	22,22,22,22	0
4	ZN	B	1006	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.