



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 5YNA / pdb_00005yna
Title : Crystal structure of Pullulanase from *Klebsiella pneumoniae* complex at 1 mM alpha-cyclodextrin
Authors : Saka, N.; Iwamoto, H.; Takahashi, N.; Mizutani, K.; Mikami, B.
Deposited on : 2017-10-24
Resolution : 1.96 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

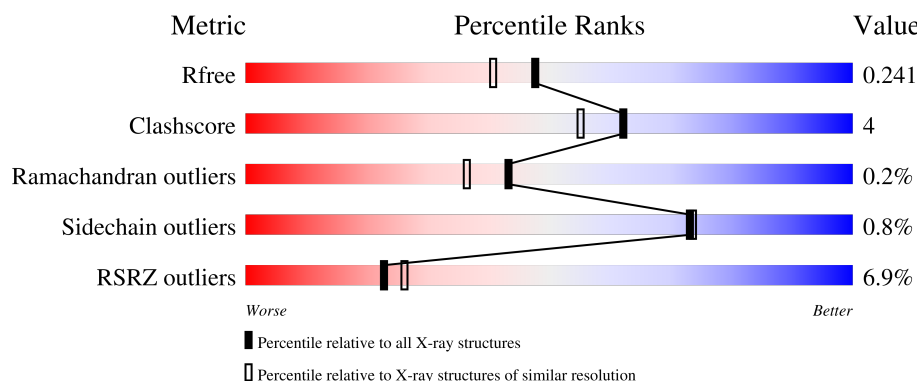
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

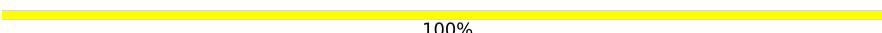
The reported resolution of this entry is 1.96 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	1102	
2	B	6	

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	PEG	A	1108	-	-	X	-
6	ACT	A	1109	-	-	X	-
6	ACT	A	1110	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8783 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.

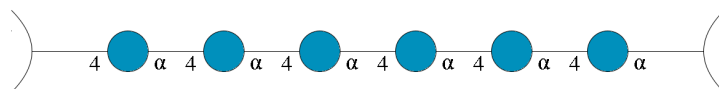
- Molecule 1 is a protein called PulA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1055	Total	C	N	O	S	0	12	0
			8181	5100	1404	1650	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	680	LEU	GLY	conflict	UNP W9BQ28

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	6	Total	C	O	0	0	0
			66	36	30			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

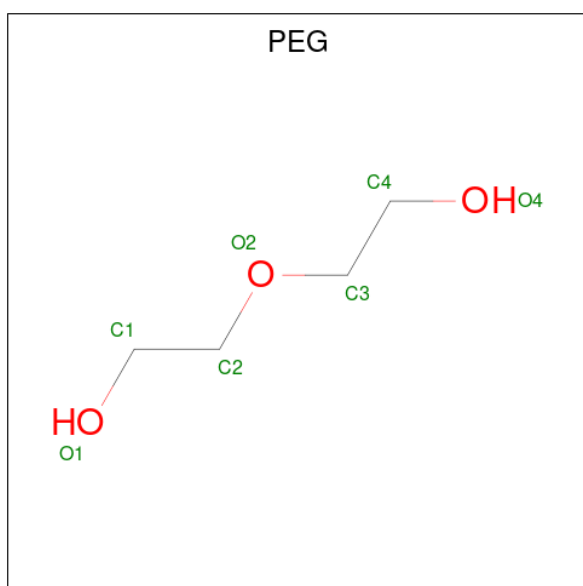
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

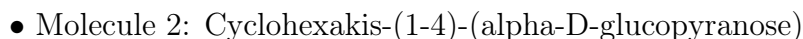


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	496	Total	O	0	8
			504	504		

- Molecule 1: PulA protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.28Å 89.28Å 299.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.15 – 1.96 44.15 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.15-1.96) 99.9 (44.15-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.198 , 0.240 0.199 , 0.241	Depositor DCC
R_{free} test set	4407 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8783	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: CA, ACT, GLC, PEG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/8347	0.50	0/11364

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8181	0	7862	66	0
2	B	66	0	54	0	0
3	A	5	0	0	0	0
4	A	12	0	16	0	0
5	A	7	0	10	4	0
6	A	8	0	6	4	0
7	A	504	0	0	7	0
All	All	8783	0	7948	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:HG3	1:A:916:ARG:HA	1.34	1.05
1:A:680:LEU:HG	1:A:710:SER:HB2	1.51	0.93
1:A:685:ALA:H	5:A:1108:PEG:H41	1.45	0.81
1:A:248:PRO:HB2	1:A:250:ASP:OD2	1.84	0.78
1:A:491:LYS:NZ	7:A:1202:HOH:O	2.26	0.69
1:A:785[A]:ARG:NH2	7:A:1205:HOH:O	2.31	0.63
1:A:1039:ALA:HB3	1:A:1043:SER:HB2	1.81	0.62
1:A:1027:GLY:N	1:A:1053:ASP:O	2.26	0.62
1:A:189:TRP:O	1:A:243:PRO:HG2	2.02	0.60
1:A:615:ASP:HB3	7:A:1483:HOH:O	2.02	0.58
1:A:89:SER:HA	1:A:117:THR:HG23	1.85	0.58
1:A:303:ASP:OD1	1:A:304:SER:N	2.36	0.58
1:A:250:ASP:OD2	1:A:250:ASP:N	2.36	0.58
1:A:708:TRP:CE3	1:A:709:ASP:HB3	2.38	0.58
1:A:680:LEU:HG	1:A:710:SER:CB	2.29	0.57
1:A:685:ALA:H	5:A:1108:PEG:C4	2.14	0.56
1:A:475:GLU:OE2	1:A:675:ARG:HD3	2.05	0.56
1:A:317:GLN:HG2	1:A:362:THR:HB	1.87	0.56
1:A:228:VAL:HG13	1:A:244:ALA:HB2	1.90	0.54
1:A:973:ARG:HG2	1:A:998:ALA:HB1	1.90	0.54
1:A:211:ASP:OD2	1:A:217:SER:OG	2.23	0.54
1:A:405:GLY:H	6:A:1110:ACT:CH3	2.22	0.53
1:A:460:VAL:HG13	1:A:595:LEU:HD21	1.91	0.53
1:A:411[A]:MET:HE3	1:A:698:ASN:HD21	1.76	0.51
1:A:125:VAL:HG13	1:A:139:LEU:HB2	1.93	0.51
1:A:405:GLY:H	6:A:1110:ACT:H2	1.74	0.51
1:A:510:LYS:HG2	7:A:1294:HOH:O	2.10	0.51
1:A:659:ALA:HB1	1:A:693[C]:ARG:HD2	1.93	0.50
1:A:311:TRP:CZ2	1:A:313:PRO:HG3	2.46	0.50
1:A:107:LYS:NZ	7:A:1215:HOH:O	2.43	0.49
1:A:1031:GLN:NE2	1:A:1069:PRO:HG3	2.29	0.48
1:A:875:ASP:OD2	1:A:879:SER:HB2	2.13	0.48
1:A:973:ARG:NH1	1:A:1002:LEU:HG	2.30	0.47
1:A:166:ASP:OD1	1:A:169[A]:ARG:NH2	2.43	0.46
1:A:680:LEU:HD22	1:A:707:GLY:HA3	1.97	0.46
1:A:684:LYS:HB3	5:A:1108:PEG:H42	1.97	0.46
1:A:1025:PHE:HB3	1:A:1028:THR:HG21	1.98	0.46
1:A:881:LEU:O	6:A:1109:ACT:H1	2.16	0.45
1:A:680:LEU:HD22	1:A:707:GLY:CA	2.47	0.45
1:A:675:ARG:HD2	1:A:732:PHE:CE1	2.53	0.44
1:A:752:LEU:HD13	1:A:844:TYR:CZ	2.52	0.44
1:A:685:ALA:HB2	5:A:1108:PEG:H21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:OD1	1:A:255:GLU:HB2	2.18	0.43
1:A:718:ILE:HG13	1:A:720:SER:HB3	1.99	0.43
1:A:495:ILE:HA	1:A:524:VAL:HB	2.00	0.43
1:A:269:ASP:N	1:A:269:ASP:OD1	2.51	0.43
1:A:49:ALA:HB2	1:A:55:VAL:HG23	2.00	0.42
1:A:29:ASP:HA	1:A:30:PRO:HD2	1.84	0.42
1:A:279[B]:GLN:HG3	7:A:1642:HOH:O	2.18	0.42
1:A:908:ASN:HA	6:A:1109:ACT:C	2.50	0.41
1:A:80:TRP:CZ2	1:A:124:ASN:HB3	2.56	0.41
1:A:221:VAL:HG11	1:A:247:LEU:HD23	2.01	0.41
1:A:317:GLN:HG2	1:A:362:THR:CB	2.49	0.41
1:A:449:TYR:CZ	1:A:571:TYR:HB2	2.55	0.41
1:A:119:GLU:HG2	1:A:149:ARG:CZ	2.50	0.41
1:A:967:GLY:O	1:A:971:MET:HG3	2.20	0.41
1:A:557:TRP:CD2	1:A:892:TYR:HA	2.54	0.41
1:A:737:ARG:HG2	1:A:741:ARG:HD3	2.02	0.41
1:A:464:LYS:HG3	1:A:595:LEU:CD2	2.51	0.41
1:A:961:LEU:HB3	1:A:992:ILE:HG21	2.02	0.41
1:A:990:MET:HE2	1:A:990:MET:HB3	1.87	0.41
1:A:680:LEU:HD13	1:A:707:GLY:C	2.46	0.41
1:A:680:LEU:HD21	7:A:1222:HOH:O	2.21	0.41
1:A:183:ASP:HB2	1:A:286:ASP:OD2	2.21	0.40
1:A:308:PHE:O	1:A:345:SER:HA	2.21	0.40
1:A:684:LYS:HE3	1:A:727:THR:HG21	2.03	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	1065/1102 (97%)	1033 (97%)	30 (3%)	2 (0%)	43 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	CYS
1	A	478	PRO

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	881/907 (97%)	874 (99%)	7 (1%)	73 74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	SER
1	A	241	SER
1	A	374	TYR
1	A	391	SER
1	A	482	LEU
1	A	543	GLN
1	A	886	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	231	GLN
1	A	277	GLN
1	A	461	GLN
1	A	593	GLN
1	A	629	GLN
1	A	835	ASN
1	A	944	GLN
1	A	1037	GLN

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 ⓘ

6 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	B	1	2	11,11,12	0.49	0	15,15,17	0.78	1 (6%)
2	GLC	B	2	2	11,11,12	0.73	0	15,15,17	1.01	1 (6%)
2	GLC	B	3	2	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
2	GLC	B	4	2	11,11,12	0.51	0	15,15,17	1.19	1 (6%)
2	GLC	B	5	2	11,11,12	0.56	0	15,15,17	1.14	1 (6%)
2	GLC	B	6	2	11,11,12	0.58	0	15,15,17	1.53	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	B	1	2	-	1/2/19/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	2/2/19/22	0/1/1/1
2	GLC	B	4	2	-	1/2/19/22	0/1/1/1
2	GLC	B	5	2	-	0/2/19/22	0/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	GLC	C1-O5-C5	3.38	116.71	112.19
2	B	6	GLC	C1-O5-C5	3.21	116.49	112.19
2	B	6	GLC	C3-C4-C5	2.95	115.58	110.23
2	B	3	GLC	C2-C3-C4	2.77	115.74	110.86
2	B	5	GLC	C3-C4-C5	2.29	114.39	110.23
2	B	3	GLC	C1-C2-C3	2.24	112.90	109.64
2	B	2	GLC	O4-C4-C3	-2.23	105.13	110.38
2	B	1	GLC	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

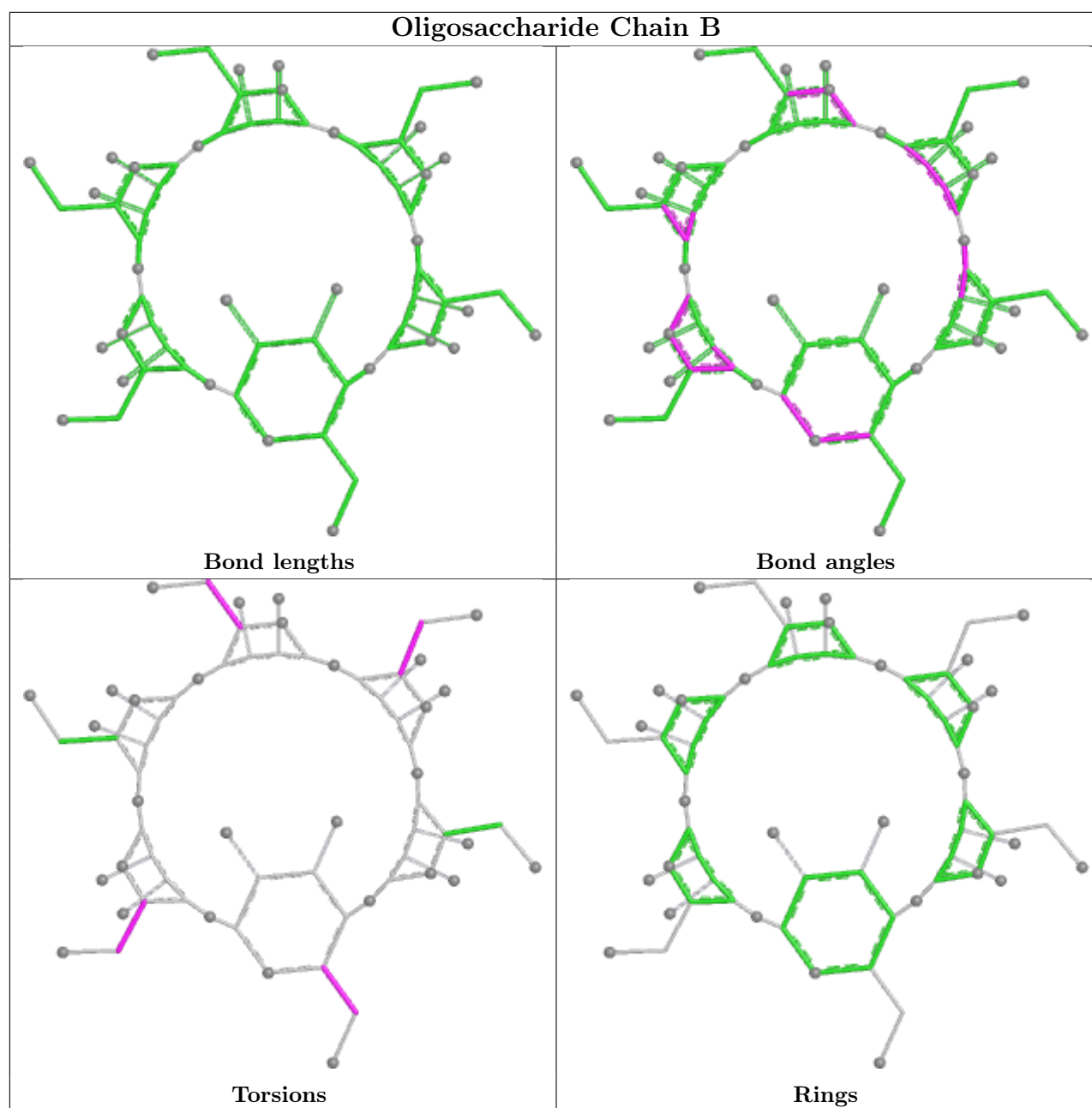
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	GLC	O5-C5-C6-O6
2	B	3	GLC	C4-C5-C6-O6
2	B	6	GLC	C4-C5-C6-O6
2	B	6	GLC	O5-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	4	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
6	ACT	A	1109	-	3,3,3	0.79	0	3,3,3	0.93	0
4	GOL	A	1107	-	5,5,5	0.32	0	5,5,5	0.29	0
5	PEG	A	1108	-	6,6,6	0.45	0	5,5,5	0.68	0
4	GOL	A	1106	-	5,5,5	0.36	0	5,5,5	0.63	0
6	ACT	A	1110	-	3,3,3	0.82	0	3,3,3	1.27	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	PEG	A	1108	-	-	2/4/4/4	-
4	GOL	A	1106	-	-	4/4/4/4	-
4	GOL	A	1107	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1107	GOL	O1-C1-C2-O2
4	A	1107	GOL	O1-C1-C2-C3
4	A	1106	GOL	O1-C1-C2-C3
5	A	1108	PEG	O2-C3-C4-O4
4	A	1106	GOL	O1-C1-C2-O2
4	A	1106	GOL	C1-C2-C3-O3
5	A	1108	PEG	O1-C1-C2-O2
4	A	1107	GOL	O2-C2-C3-O3
4	A	1107	GOL	C1-C2-C3-O3
4	A	1106	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1109	ACT	2	0
5	A	1108	PEG	4	0
6	A	1110	ACT	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	1055/1102 (95%)	0.50	73 (6%)	23 26	14, 36, 62, 94	12 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	5.0
1	A	708	TRP	4.7
1	A	251	VAL	4.0
1	A	68	THR	3.7
1	A	84	THR	3.7
1	A	30	PRO	3.7
1	A	95	TRP	3.4
1	A	93	ALA	3.3
1	A	271	ILE	3.2
1	A	90	ALA	3.2
1	A	194	ASN	3.2
1	A	998	ALA	3.1
1	A	78	TYR	3.0
1	A	262	VAL	3.0
1	A	46	ALA	3.0
1	A	240	ALA	3.0
1	A	92	VAL	2.8
1	A	1006	VAL	2.8
1	A	87	ALA	2.8
1	A	233	SER	2.7
1	A	70	ALA	2.7
1	A	411[A]	MET	2.7
1	A	1068	LEU	2.7
1	A	33	VAL	2.6
1	A	517	TYR	2.6
1	A	38	PRO	2.6
1	A	190	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	303	ASP	2.6
1	A	65	THR	2.6
1	A	518	CYS	2.5
1	A	64	ILE	2.5
1	A	1075	GLY	2.5
1	A	1004[A]	SER	2.5
1	A	125	VAL	2.5
1	A	995	GLY	2.5
1	A	228	VAL	2.5
1	A	234	MET	2.5
1	A	711	ASN	2.4
1	A	67	SER	2.4
1	A	141	VAL	2.4
1	A	239	LEU	2.4
1	A	123	ILE	2.3
1	A	270	GLY	2.3
1	A	707	GLY	2.3
1	A	268	SER	2.3
1	A	159	ALA	2.3
1	A	89	SER	2.3
1	A	174	VAL	2.3
1	A	96	ASN	2.3
1	A	216	PHE	2.2
1	A	236	PHE	2.2
1	A	1007	ASP	2.2
1	A	266	ALA	2.2
1	A	231	GLN	2.2
1	A	347[A]	GLN	2.2
1	A	171	ALA	2.2
1	A	1000	ALA	2.2
1	A	98	VAL	2.1
1	A	273	SER	2.1
1	A	419	ALA	2.1
1	A	968	ALA	2.1
1	A	201	TYR	2.1
1	A	264	ILE	2.1
1	A	709	ASP	2.1
1	A	198	VAL	2.1
1	A	122	CYS	2.1
1	A	245	PHE	2.0
1	A	147	THR	2.0
1	A	237	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	2.0
1	A	189	TRP	2.0
1	A	135	ILE	2.0
1	A	140	ARG	2.0

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

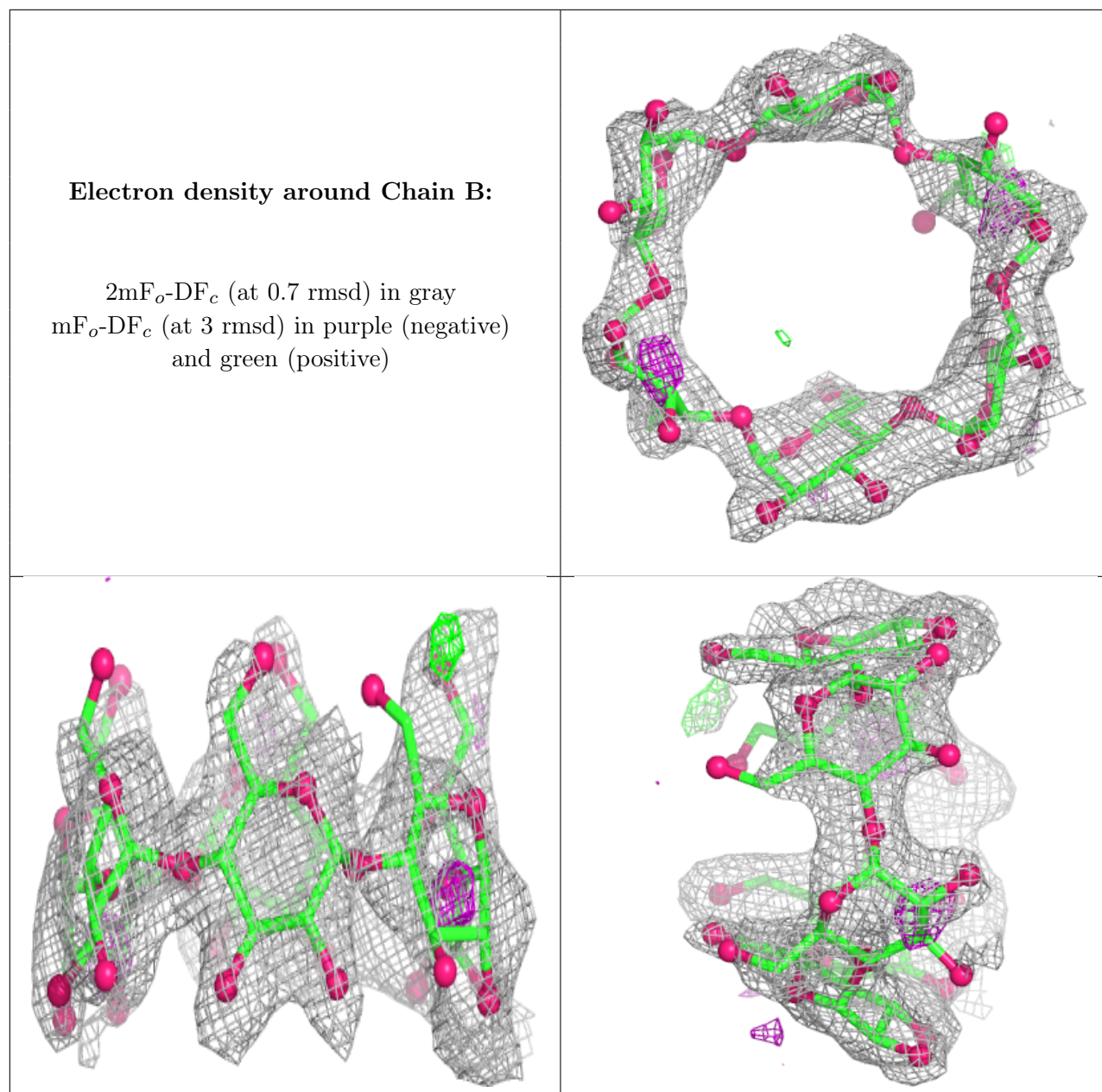
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	GLC	B	3	11/12	0.51	0.14	77,88,90,96	0
2	GLC	B	4	11/12	0.64	0.13	81,86,92,95	0
2	GLC	B	5	11/12	0.64	0.14	77,80,90,92	0
2	GLC	B	6	11/12	0.67	0.15	66,74,83,85	0
2	GLC	B	2	11/12	0.84	0.11	56,67,77,80	0
2	GLC	B	1	11/12	0.85	0.11	62,71,75,79	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.



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($\text{\AA}^2$)	Q<0.9
3	CA	A	1105	1/1	0.54	0.17	85,85,85,85	0
4	GOL	A	1106	6/6	0.71	0.18	44,51,54,58	0
6	ACT	A	1110	4/4	0.77	0.16	40,47,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	1108	7/7	0.80	0.14	37,46,50,56	0
6	ACT	A	1109	4/4	0.84	0.33	30,43,43,44	0
3	CA	A	1104	1/1	0.86	0.10	64,64,64,64	0
4	GOL	A	1107	6/6	0.87	0.12	50,56,60,60	0
3	CA	A	1103	1/1	0.91	0.09	67,67,67,67	0
3	CA	A	1101	1/1	0.99	0.02	29,29,29,29	0
3	CA	A	1102	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.