



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 10:02 AM EST

PDB ID : 1PMH  
Title : Crystal structure of Caldicellulosiruptor saccharolyticus CBM27-1 in complex with mannohexaose  
Authors : Roske, Y.; Sunna, A.; Heinemann, U.  
Deposited on : 2003-06-11  
Resolution : 1.06 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

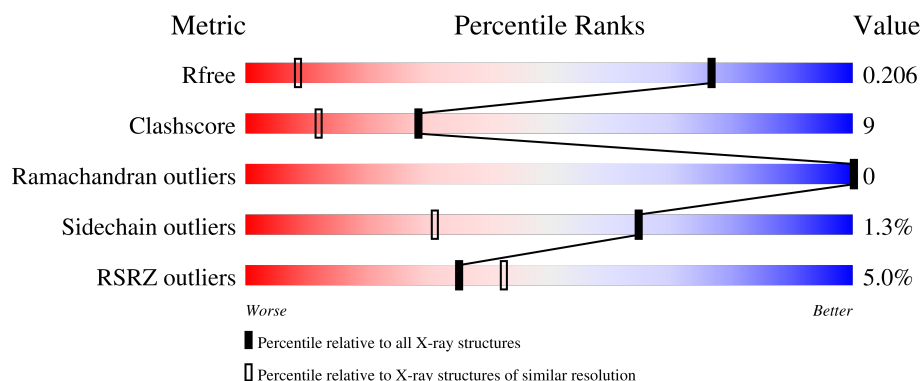
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.06 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	1027 (1.08-1.04)
Clashscore	180529	1152 (1.08-1.04)
Ramachandran outliers	177936	1127 (1.08-1.04)
Sidechain outliers	177891	1128 (1.08-1.04)
RSRZ outliers	164620	1026 (1.08-1.04)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	X	185	
2	A	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
4	EDO	X	403	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1904 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 beta-1,4-mannanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	183	Total	C	N	O	S	Se	0	18	0
			1528	984	250	291	1	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	17	MSE	MET	modified residue	GB 1491795
X	69	ILE	PHE	SEE REMARK 999	GB 1491795
X	89	MSE	MET	modified residue	GB 1491795
X	104	ALA	PRO	SEE REMARK 999	GB 1491795

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	A	6	Total	C	O	0	2	0
			80	43	37			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

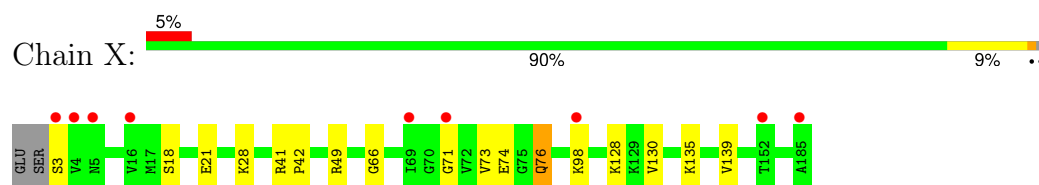
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	279	Total	O	0	0
			279	279		

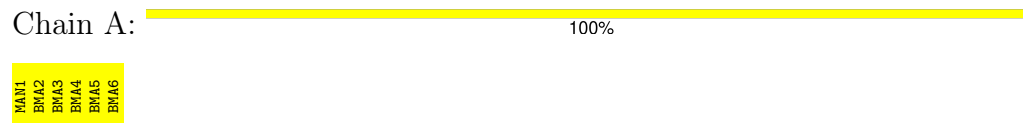
### 3 Residue-property plots [i](#)

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. 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. 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: beta-1,4-mannanase



- Molecule 2: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.28Å 45.70Å 110.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.00 – 1.06 23.00 – 1.06	Depositor EDS
% Data completeness (in resolution range)	95.9 (23.00-1.06) 95.9 (23.00-1.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.06Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.141 , 0.173 0.186 , 0.206	Depositor DCC
$R_{free}$ test set	4226 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, EDO, CA, MAN

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	X	0.65	0/1636	0.96	1/2200 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	X	49	ARG	NE-CZ-NH2	-7.41	116.60	120.30

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	X	1528	0	1481	26	1
2	A	80	0	66	0	0
3	X	1	0	0	0	0
4	X	16	0	24	11	0
5	X	279	0	0	5	1
All	All	1904	0	1571	28	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 9.



All (28) 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)
4:X:402:EDO:H12	5:X:661:HOH:O	1.58	1.01
1:X:128:LYS:HG3	1:X:139[B]:VAL:CG1	1.99	0.91
1:X:66:GLY:O	4:X:404:EDO:H11	1.89	0.72
1:X:71:GLY:HA2	4:X:403:EDO:H12	1.72	0.70
1:X:71:GLY:CA	4:X:403:EDO:H12	2.23	0.68
1:X:128:LYS:CG	1:X:139[B]:VAL:HG13	2.25	0.66
1:X:128:LYS:HG3	1:X:139[B]:VAL:HG13	1.78	0.65
1:X:130[B]:VAL:HG11	1:X:139[B]:VAL:HG11	1.79	0.63
1:X:28[B]:LYS:HD2	5:X:504:HOH:O	1.98	0.62
1:X:73:VAL:CG2	4:X:403:EDO:H22	2.32	0.59
1:X:128:LYS:CG	1:X:139[B]:VAL:CG1	2.76	0.58
1:X:21:GLU:O	4:X:404:EDO:H12	2.05	0.57
1:X:135:LYS:NZ	5:X:497:HOH:O	2.33	0.56
1:X:128:LYS:O	1:X:139[B]:VAL:HG12	2.06	0.56
1:X:130[B]:VAL:CG1	1:X:139[B]:VAL:HG11	2.36	0.56
1:X:130[B]:VAL:HG13	1:X:139[B]:VAL:HG12	1.90	0.54
1:X:18[B]:SER:HB2	4:X:403:EDO:H11	1.89	0.53
1:X:73:VAL:HG22	4:X:403:EDO:H22	1.91	0.53
1:X:128:LYS:HG2	1:X:139[B]:VAL:HG13	1.91	0.52
1:X:130[B]:VAL:HG13	1:X:139[B]:VAL:CG1	2.43	0.49
1:X:73:VAL:HG12	1:X:74[B]:GLU:HG2	1.97	0.47
1:X:130[B]:VAL:CG1	1:X:139[B]:VAL:CG1	2.93	0.47
1:X:71:GLY:O	4:X:403:EDO:H12	2.16	0.46
1:X:128:LYS:HG3	1:X:139[B]:VAL:HG12	1.90	0.45
1:X:73:VAL:HG23	4:X:403:EDO:H22	2.02	0.42
1:X:3:SER:N	5:X:683:HOH:O	2.54	0.41
4:X:404:EDO:H21	5:X:578:HOH:O	2.20	0.41
1:X:41:ARG:HB2	1:X:42:PRO:CD	2.50	0.41

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:X:76[A]:GLN:NE2	5:X:413:HOH:O[3_555]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	199/185 (108%)	193 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	172/154 (112%)	168 (98%)	4 (2%)	45	10

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	76[A]	GLN
1	X	76[B]	GLN
1	X	98[A]	LYS
1	X	98[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	37	GLN
1	X	40	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 ⓘ

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	MAN	A	1	2	12,12,12	0.46	0	17,17,17	1.32	2 (11%)
2	BMA	A	2	2	11,11,12	0.83	1 (9%)	15,15,17	1.13	2 (13%)
2	BMA	A	3	2	11,11,12	0.78	0	15,15,17	1.10	1 (6%)
2	BMA	A	4	2	11,11,12	0.76	0	15,15,17	1.40	1 (6%)
2	BMA	A	5[A]	-	11,11,12	0.82	0	15,15,17	1.74	4 (26%)
2	BMA	A	5[B]	-	11,11,12	0.83	0	15,15,17	1.68	4 (26%)
2	BMA	A	6[A]	2	11,11,12	0.56	0	15,15,17	2.31	2 (13%)
2	BMA	A	6[B]	2	11,11,12	0.57	0	15,15,17	1.41	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	MAN	A	1	2	-	0/2/22/22	0/1/1/1
2	BMA	A	2	2	-	0/2/19/22	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	BMA	A	4	2	-	0/2/19/22	0/1/1/1
2	BMA	A	5[A]	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	A	5[B]	-	-	0/2/19/22	0/1/1/1
2	BMA	A	6[A]	2	-	0/2/19/22	0/1/1/1
2	BMA	A	6[B]	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	A	2	BMA	O5-C1	-2.32	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6[A]	BMA	C1-O5-C5	8.14	123.10	112.19
2	A	5[A]	BMA	C1-O5-C5	3.68	117.12	112.19
2	A	5[B]	BMA	C1-O5-C5	3.68	117.12	112.19
2	A	4	BMA	C1-C2-C3	-3.57	104.44	109.64
2	A	1	MAN	O1-C1-O5	3.33	120.31	110.41
2	A	6[B]	BMA	O5-C1-C2	-3.02	103.59	110.79
2	A	6[B]	BMA	C1-O5-C5	2.89	116.06	112.19
2	A	5[A]	BMA	O2-C2-C3	2.82	116.00	110.15
2	A	5[B]	BMA	O2-C2-C3	2.82	116.00	110.15
2	A	3	BMA	O4-C4-C5	-2.54	103.08	109.32
2	A	2	BMA	O4-C4-C3	-2.36	104.81	110.38
2	A	5[A]	BMA	C2-C3-C4	-2.23	106.94	110.86
2	A	5[B]	BMA	C2-C3-C4	-2.23	106.94	110.86
2	A	1	MAN	O4-C4-C5	-2.18	103.96	109.32
2	A	2	BMA	O5-C1-C2	2.15	115.93	110.79
2	A	5[A]	BMA	O4-C4-C5	-2.12	104.11	109.32
2	A	5[B]	BMA	O4-C4-C5	-2.12	104.11	109.32
2	A	6[A]	BMA	C1-C2-C3	2.10	112.71	109.64

There are no chirality outliers.

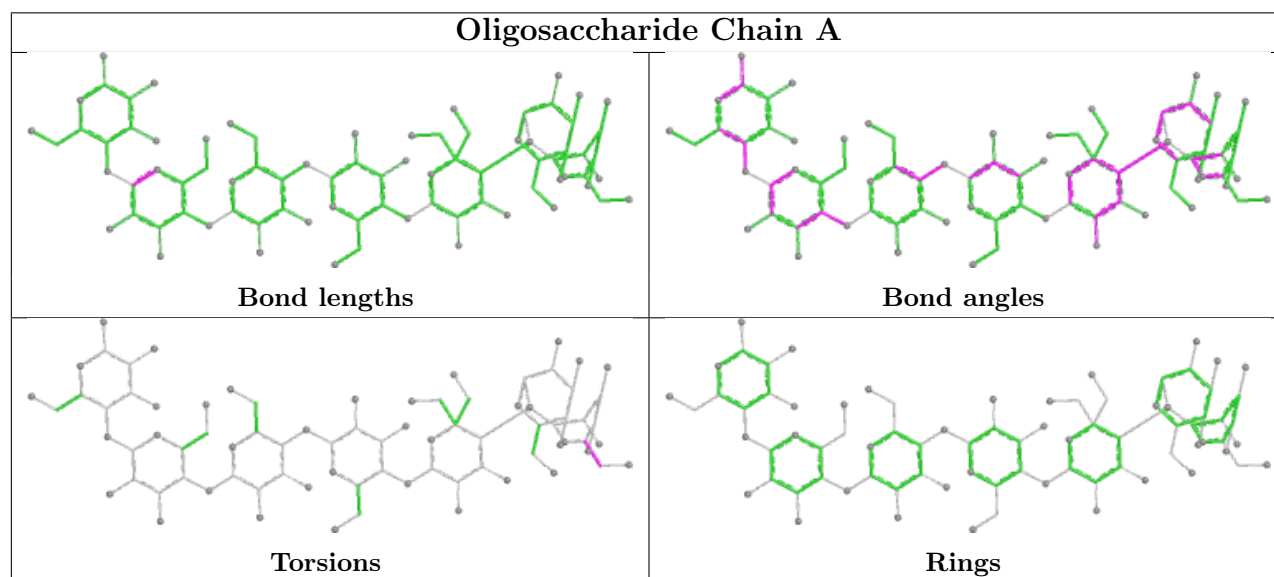
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6[B]	BMA	O5-C5-C6-O6
2	A	6[B]	BMA	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	X	401	-	3,3,3	0.33	0	2,2,2	1.50	0
4	EDO	X	404	-	3,3,3	0.34	0	2,2,2	0.45	0
4	EDO	X	402	-	3,3,3	0.32	0	2,2,2	0.18	0
4	EDO	X	403	-	3,3,3	0.25	0	2,2,2	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	X	401	-	-	1/1/1/1	-
4	EDO	X	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	X	402	-	-	1/1/1/1	-
4	EDO	X	403	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	401	EDO	O1-C1-C2-O2
4	X	402	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	404	EDO	3	0
4	X	402	EDO	1	0
4	X	403	EDO	7	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

**Warning:** The R factor obtained from EDS is 0.2039, which does not match the depositor's R factor of 0.14132. Please interpret the results in this section carefully.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	181/185 (97%)	0.65	9 (4%) 35 42	11, 18, 25, 47	21 (11%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	3	SER	3.5
1	X	69[A]	ILE	3.5
1	X	4	VAL	2.8
1	X	5	ASN	2.6
1	X	152	THR	2.4
1	X	185	ALA	2.4
1	X	71	GLY	2.3
1	X	16	VAL	2.0
1	X	98[A]	LYS	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](#)

SUGAR-RSR INFOmissingINFO

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	X	402	4/4	0.77	0.14	31,35,40,41	0
4	EDO	X	401	4/4	0.87	0.11	31,31,35,42	0
4	EDO	X	404	4/4	0.91	0.10	22,25,28,34	0
4	EDO	X	403	4/4	0.92	0.10	26,32,34,38	0
3	CA	X	300	1/1	0.99	0.03	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.