



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2021 – 08:12 am GMT

PDB ID : 6ZO0  
Title : 2.23 Å resolution 3,4-dimethylcatechol (3,4-dimethylbenzene-1,2-diol) inhibited *Sporosarcina pasteurii* urease  
Authors : Mazzei, L.; Ciani, M.; Musiani, F.; Ciurli, S.  
Deposited on : 2020-07-07  
Resolution : 2.23 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

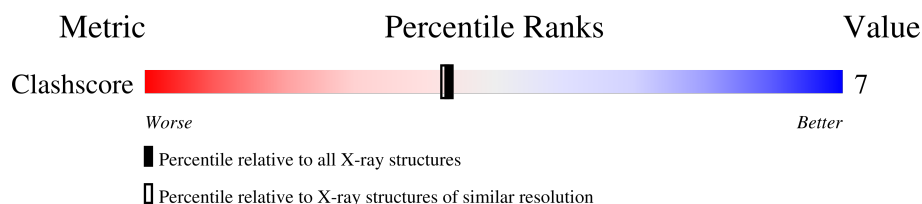
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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))
Clashscore	141614	2539 (2.26-2.22)

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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	100	 86% 14%
2	BBB	122	 89% 11% .
3	CCC	570	 86% 14% .

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	CCC	608	-	-	X	-
4	EDO	CCC	611	-	-	X	-
5	SO4	BBB	203	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6776 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	100	Total	C	N	O	S	0	5	0
			815	512	138	158	7			

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	122	Total	C	N	O	S	0	4	0
			984	607	177	199	1			

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	570	Total	C	N	O	S	0	17	0
			4449	2794	765	864	26			

- 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	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

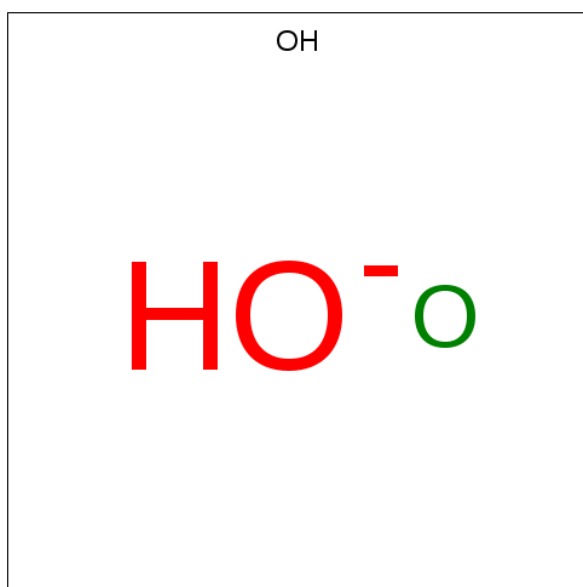


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	CCC	2	Total	Ni	0	0
			2	2		

- Molecule 7 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total	O	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	50	Total	O	0	0
			50	50		
8	BBB	87	Total	O	0	0
			87	87		
8	CCC	255	Total	O	0	0
			255	255		

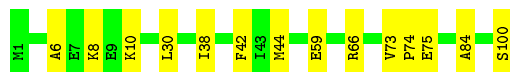
### 3 Residue-property plots [i](#)

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.

Note EDS failed to run properly.

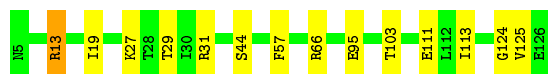
- Molecule 1: Urease subunit gamma

Chain AAA:  86% 14%



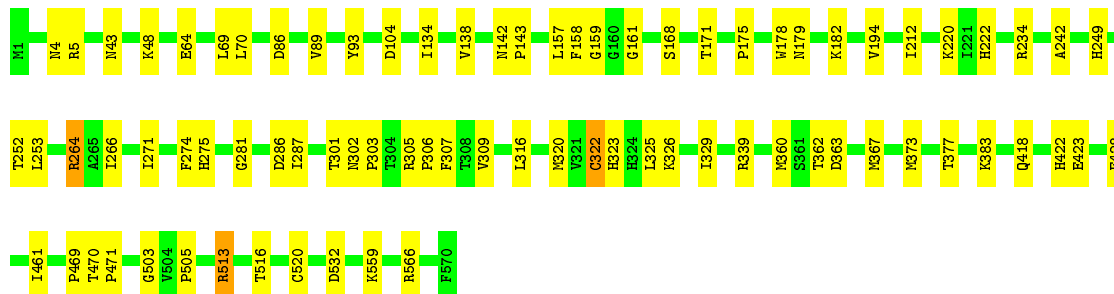
- Molecule 2: Urease subunit beta

Chain BBB:  89% 11%



- Molecule 3: Urease subunit alpha

Chain CCC:  86% 14%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.50Å 131.50Å 188.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.88 – 2.23	Depositor
% Data completeness (in resolution range)	100.0 (113.88-2.23)	Depositor
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.161 , 0.216	Depositor
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.577	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OH, CXM, KCX, SO4, QO8, NI, EDO

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	AAA	0.50	0/821	0.86	0/1104
2	BBB	0.53	0/999	0.95	2/1342 (0.1%)
3	CCC	0.51	1/4525 (0.0%)	0.91	7/6125 (0.1%)
All	All	0.52	1/6345 (0.0%)	0.91	9/8571 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BBB	0	1
3	CCC	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	428	GLU	CD-OE1	-5.94	1.19	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	234	ARG	CG-CD-NE	-7.12	96.85	111.80
3	CCC	264	ARG	CG-CD-NE	6.75	125.98	111.80
3	CCC	520	CYS	CB-CA-C	-6.73	96.94	110.40
3	CCC	513[A]	ARG	CG-CD-NE	-6.71	97.72	111.80
3	CCC	513[B]	ARG	CG-CD-NE	-6.71	97.72	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	125	VAL	Peptide
3	CCC	322	QO8	Mainchain

## 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	AAA	815	0	831	11	0
2	BBB	984	0	964	12	0
3	CCC	4449	0	4418	63	0
4	AAA	16	0	24	2	0
4	BBB	8	0	12	0	0
4	CCC	64	0	96	17	0
5	BBB	15	0	0	2	0
5	CCC	30	0	0	1	0
6	CCC	2	0	0	0	0
7	CCC	1	0	0	1	0
8	AAA	50	0	0	0	0
8	BBB	87	0	0	5	0
8	CCC	255	0	0	5	0
All	All	6776	0	6345	85	0

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

The worst 5 of 85 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)
3:CCC:513[A]:ARG:HH21	4:CCC:611:EDO:C1	1.52	1.21
3:CCC:513[A]:ARG:NH2	4:CCC:611:EDO:H12	1.62	1.15
2:BBB:111[A]:GLU:OE2	8:BBB:301:HOH:O	1.70	1.09
3:CCC:513[A]:ARG:NH2	4:CCC:611:EDO:C1	2.19	1.02
3:CCC:513[A]:ARG:HH21	4:CCC:611:EDO:H12	0.79	0.93

There are no symmetry-related clashes.

## 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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	$\# Z  > 2$
3	KCX	CCC	220	3,6	7,11,12	0.61	0	4,12,14	0.57	0
3	QO8	CCC	322	3	16,16,17	1.66	3 (18%)	14,22,24	2.19	5 (35%)
1	CXM	AAA	1	1	6,10,11	0.57	0	5,11,13	1.05	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
3	KCX	CCC	220	3,6	-	0/7/10/12	-
3	QO8	CCC	322	3	-	3/7/7/9	0/1/1/1
1	CXM	AAA	1	1	-	1/7/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	322	QO8	O-C	-4.19	1.24	1.42
3	CCC	322	QO8	C2-SG	-2.85	1.73	1.77
3	CCC	322	QO8	CB-SG	-2.48	1.76	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	322	QO8	CB-SG-C2	5.43	114.67	102.27
3	CCC	322	QO8	O4-C4-C5	2.71	125.25	118.10
3	CCC	322	QO8	C7-C6-C5	2.35	124.83	121.17
3	CCC	322	QO8	C1-C2-C3	-2.11	118.19	120.08
3	CCC	322	QO8	C7-C6-C1	-2.04	115.72	119.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	CXM	O-C-CA-CB
3	CCC	322	QO8	O-C-CA-N
3	CCC	322	QO8	O-C-CA-CB
3	CCC	322	QO8	CA-CB-SG-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	220	KCX	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 31 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	SO4	CCC	623	-	4,4,4	0.33	0	6,6,6	0.13	0
4	EDO	CCC	620	-	3,3,3	0.63	0	2,2,2	0.20	0
4	EDO	AAA	203	-	3,3,3	0.51	0	2,2,2	0.76	0
4	EDO	BBB	202	-	3,3,3	0.47	0	2,2,2	0.61	0
4	EDO	CCC	611	-	3,3,3	0.67	0	2,2,2	1.82	1 (50%)
4	EDO	CCC	614	-	3,3,3	0.60	0	2,2,2	0.23	0
4	EDO	CCC	607	-	3,3,3	0.48	0	2,2,2	1.01	0
5	SO4	BBB	203	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	BBB	205	-	4,4,4	0.29	0	6,6,6	0.06	0
4	EDO	AAA	204	-	3,3,3	0.48	0	2,2,2	0.49	0
4	EDO	CCC	618	-	3,3,3	0.67	0	2,2,2	0.73	0
4	EDO	AAA	202	-	3,3,3	0.68	0	2,2,2	0.11	0
4	EDO	BBB	201	-	3,3,3	0.54	0	2,2,2	0.92	0
5	SO4	CCC	622	-	4,4,4	0.32	0	6,6,6	0.12	0
4	EDO	CCC	612	-	3,3,3	0.75	0	2,2,2	0.16	0
5	SO4	CCC	625	-	4,4,4	0.31	0	6,6,6	0.06	0
4	EDO	CCC	613	-	3,3,3	0.49	0	2,2,2	0.43	0
5	SO4	CCC	621	-	4,4,4	0.35	0	6,6,6	0.19	0
4	EDO	CCC	606	-	3,3,3	0.68	0	2,2,2	0.73	0
4	EDO	AAA	201	-	3,3,3	1.02	0	2,2,2	0.37	0
4	EDO	CCC	610	-	3,3,3	0.41	0	2,2,2	0.84	0
4	EDO	CCC	619	-	3,3,3	0.86	0	2,2,2	0.51	0
4	EDO	CCC	604	-	3,3,3	0.33	0	2,2,2	1.41	0
4	EDO	CCC	616	-	3,3,3	0.56	0	2,2,2	0.58	0
4	EDO	CCC	608	-	3,3,3	0.67	0	2,2,2	0.82	0
4	EDO	CCC	605	-	3,3,3	1.18	0	2,2,2	0.33	0
5	SO4	CCC	624	-	4,4,4	0.30	0	6,6,6	0.17	0
5	SO4	BBB	204	-	4,4,4	0.33	0	6,6,6	0.17	0
4	EDO	CCC	615	-	3,3,3	0.65	0	2,2,2	0.27	0
5	SO4	CCC	626	-	4,4,4	0.38	0	6,6,6	0.05	0
4	EDO	CCC	609	-	3,3,3	0.71	0	2,2,2	0.04	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	CCC	620	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	AAA	203	-	-	0/1/1/1	-
4	EDO	BBB	202	-	-	1/1/1/1	-
4	EDO	CCC	611	-	-	1/1/1/1	-
4	EDO	CCC	614	-	-	1/1/1/1	-
4	EDO	CCC	607	-	-	1/1/1/1	-
4	EDO	AAA	204	-	-	1/1/1/1	-
4	EDO	CCC	618	-	-	1/1/1/1	-
4	EDO	AAA	202	-	-	0/1/1/1	-
4	EDO	BBB	201	-	-	1/1/1/1	-
4	EDO	CCC	612	-	-	1/1/1/1	-
4	EDO	CCC	613	-	-	1/1/1/1	-
4	EDO	CCC	606	-	-	1/1/1/1	-
4	EDO	AAA	201	-	-	0/1/1/1	-
4	EDO	CCC	610	-	-	0/1/1/1	-
4	EDO	CCC	619	-	-	1/1/1/1	-
4	EDO	CCC	604	-	-	1/1/1/1	-
4	EDO	CCC	616	-	-	0/1/1/1	-
4	EDO	CCC	608	-	-	0/1/1/1	-
4	EDO	CCC	605	-	-	1/1/1/1	-
4	EDO	CCC	615	-	-	1/1/1/1	-
4	EDO	CCC	609	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	CCC	611	EDO	O2-C2-C1	-2.55	93.59	111.91

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CCC	605	EDO	O1-C1-C2-O2
4	CCC	606	EDO	O1-C1-C2-O2
4	CCC	609	EDO	O1-C1-C2-O2
4	CCC	612	EDO	O1-C1-C2-O2
4	CCC	614	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	611	EDO	7	0
5	BBB	203	SO4	2	0
4	CCC	618	EDO	1	0
4	AAA	202	EDO	2	0
5	CCC	622	SO4	1	0
4	CCC	608	EDO	5	0
4	CCC	605	EDO	1	0
4	CCC	609	EDO	3	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 ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.