



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:30 pm BST

PDB ID : 1I0B
Title : HIGH RESOLUTION STRUCTURE OF THE MANGANESE-CONTAINING PHOSPHOTRIESTERASE FROM PSEUDOMONAS DIMINUTA
Authors : Holden, H.M.; Benning, M.M.; Raushel, F.M.; Shim, H.
Deposited on : 2001-01-29
Resolution : 1.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.11

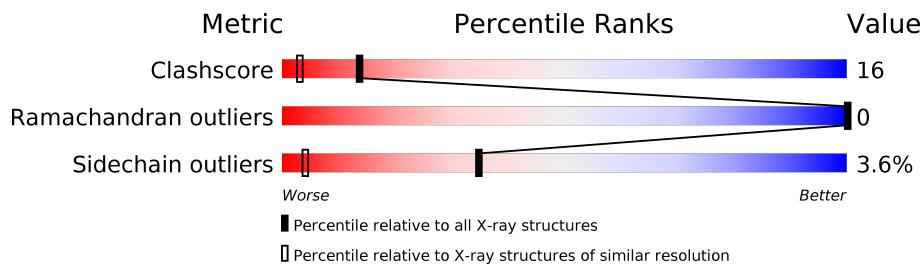
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	332	
1	B	332	

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	A	417	-	-	X	-
4	EDO	A	419	-	-	X	-
4	EDO	A	420	-	-	X	-
4	EDO	A	432	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	414	-	-	X	-
4	EDO	B	416	-	-	X	-
4	EDO	B	418	-	-	X	-
4	EDO	B	421	-	-	X	-
4	EDO	B	422	-	-	X	-
4	EDO	B	426	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5917 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 PHOSPHOTRIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	Total 2549	C 1610	N 453	O 479	S 7	0	8	0
1	B	331	Total 2538	C 1603	N 455	O 473	S 7	0	7	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



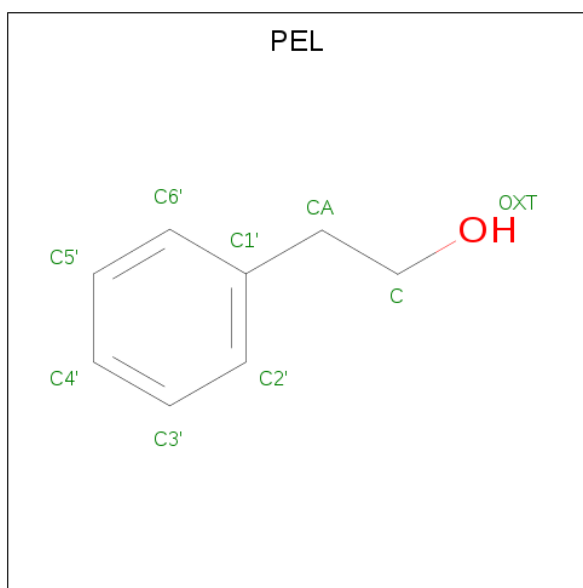
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 2 3	0	1
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	1
4	B	1	Total C O 4 2 2	0	0

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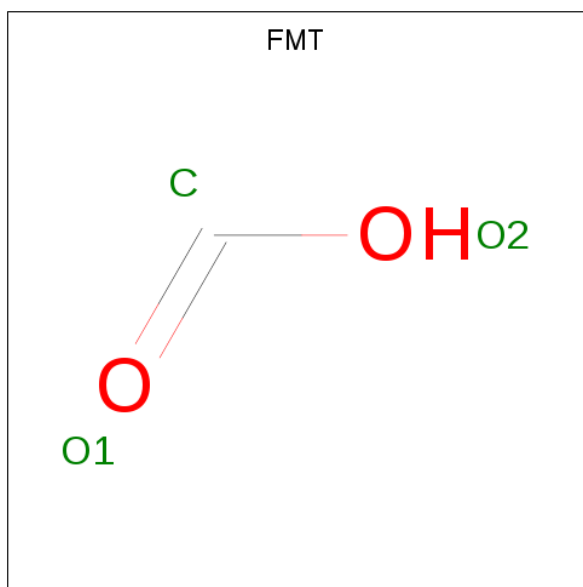
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0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

- Molecule 5 is 2-PHENYL-ETHANOL (three-letter code: PEL) (formula: C₈H₁₀O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 8 1	0	0
5	B	1	Total C O 9 8 1	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	333	Total O 333 333	0	0
7	B	362	Total O 362 362	0	0

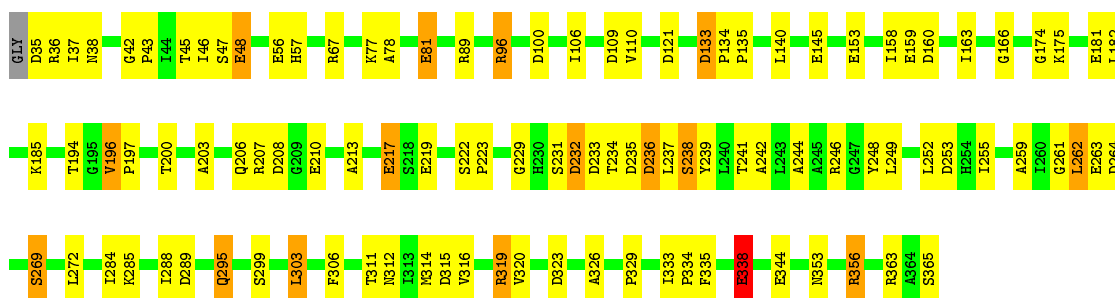
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 was not executed.

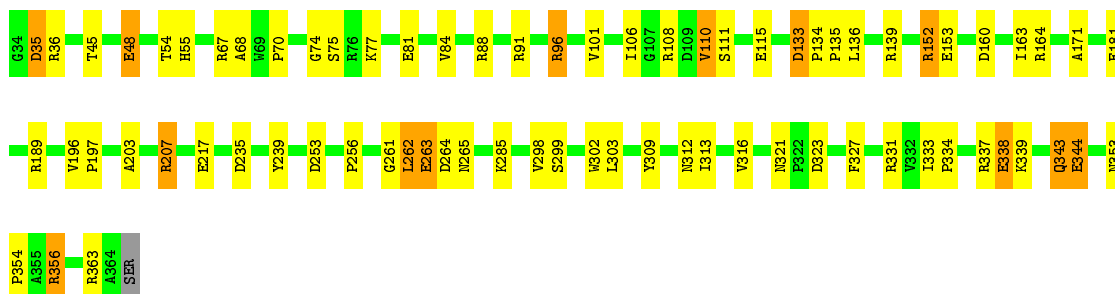
- Molecule 1: PHOSPHOTRIESTERASE

Chain A: 



- Molecule 1: PHOSPHOTRIESTERASE

Chain B: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.44Å 90.03Å 68.39Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	30.00 – 1.30	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.222 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5917	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: PEL, NA, FMT, MN, 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	A	2.25	13/2640 (0.5%)	1.33	31/3587 (0.9%)
1	B	0.88	8/2626 (0.3%)	1.30	25/3566 (0.7%)
All	All	1.71	21/5266 (0.4%)	1.32	56/7153 (0.8%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	SER	C-OXT	106.28	3.25	1.23
1	A	153	GLU	CD-OE2	6.84	1.33	1.25
1	A	56	GLU	CD-OE2	6.70	1.33	1.25
1	B	263	GLU	CD-OE2	6.10	1.32	1.25
1	B	48	GLU	CD-OE2	6.09	1.32	1.25

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	B	253	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	331	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	253	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	133	ASP	CB-CG-OD2	-7.53	111.53	118.30

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	A	2549	0	2578	90	1
1	B	2538	0	2560	72	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	49	0	72	33	0
4	B	56	0	81	42	0
5	A	9	0	10	1	0
5	B	9	0	10	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	333	0	0	8	0
7	B	362	0	0	14	0
All	All	5917	0	5311	168	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 16.

The worst 5 of 168 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:96:ARG:HH11	4:B:418:EDO:H21	1.19	1.04
1:B:337:ARG:HH12	1:B:343:GLN:HG3	1.24	1.00
1:B:68:ALA:HB2	4:B:426:EDO:C2	1.97	0.94
1:B:96:ARG:NH1	4:B:418:EDO:H21	1.84	0.92
1:B:135:PRO:HA	4:B:416:EDO:H21	1.51	0.92

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:A:236:ASP:OD1	1:A:236:ASP:OD1[2_656]	2.19	0.01

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	338/332 (102%)	323 (96%)	15 (4%)	0	100	100
1	B	336/332 (101%)	326 (97%)	10 (3%)	0	100	100
All	All	674/664 (102%)	649 (96%)	25 (4%)	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	275/266 (103%)	260 (94%)	15 (6%)	21	1
1	B	272/266 (102%)	263 (97%)	9 (3%)	38	5
All	All	547/532 (103%)	523 (96%)	24 (4%)	35	2

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295[C]	GLN
1	A	319	ARG
1	B	343	GLN
1	A	299	SER
1	A	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	212	GLN
1	B	38	ASN
1	B	212	GLN
1	B	343	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 6 are monoatomic - 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	$\# Z > 2$
4	EDO	B	422	-	3,3,3	0.43	0	2,2,2	0.43	0
4	EDO	B	415	-	3,3,3	0.36	0	2,2,2	0.88	0
4	EDO	B	418	-	3,3,3	0.42	0	2,2,2	0.34	0
5	PEL	A	434	-	9,9,9	0.97	0	10,10,10	0.62	0
5	PEL	B	433	-	9,9,9	0.94	0	10,10,10	0.74	0
4	EDO	A	410	-	3,3,3	0.56	0	2,2,2	0.17	0
4	EDO	A	430	-	3,3,3	0.37	0	2,2,2	0.43	0
4	EDO	A	408[B]	-	3,3,3	0.50	0	2,2,2	0.40	0
4	EDO	B	414	-	3,3,3	0.47	0	2,2,2	0.25	0
4	EDO	A	424	-	3,3,3	0.44	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	426	-	3,3,3	0.37	0	2,2,2	0.30	0
4	EDO	A	411	-	3,3,3	0.40	0	2,2,2	0.50	0
6	FMT	A	369	1,2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	423	-	3,3,3	0.44	0	2,2,2	0.30	0
4	EDO	B	409	-	3,3,3	0.35	0	2,2,2	0.32	0
4	EDO	A	413	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	B	428	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	B	421	-	3,3,3	0.35	0	2,2,2	0.31	0
4	EDO	B	425	-	3,3,3	0.48	0	2,2,2	0.38	0
4	EDO	B	416	-	3,3,3	0.40	0	2,2,2	0.38	0
4	EDO	A	427	-	3,3,3	0.48	0	2,2,2	0.28	0
6	FMT	B	369	1,2	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	429	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	419	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	B	431	-	3,3,3	0.41	0	2,2,2	0.41	0
4	EDO	A	432	-	3,3,3	0.53	0	2,2,2	0.40	0
4	EDO	A	417	-	3,3,3	0.41	0	2,2,2	0.31	0
4	EDO	A	412	-	3,3,3	0.45	0	2,2,2	0.51	0
4	EDO	A	420	-	3,3,3	0.41	0	2,2,2	0.21	0
4	EDO	A	408[A]	-	3,3,3	0.50	0	2,2,2	0.41	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	B	422	-	-	0/1/1/1	-
4	EDO	B	415	-	-	0/1/1/1	-
4	EDO	B	418	-	-	1/1/1/1	-
5	PEL	A	434	-	-	1/3/3/3	0/1/1/1
5	PEL	B	433	-	-	3/3/3/3	0/1/1/1
4	EDO	A	410	-	-	1/1/1/1	-
4	EDO	A	430	-	-	1/1/1/1	-
4	EDO	A	408[B]	-	-	0/1/1/1	-
4	EDO	B	414	-	-	1/1/1/1	-
4	EDO	A	424	-	-	0/1/1/1	-
4	EDO	B	426	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	B	423	-	-	1/1/1/1	-
4	EDO	B	409	-	-	0/1/1/1	-
4	EDO	A	413	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	428	-	-	1/1/1/1	-
4	EDO	B	421	-	-	1/1/1/1	-
4	EDO	B	425	-	-	1/1/1/1	-
4	EDO	B	416	-	-	0/1/1/1	-
4	EDO	A	427	-	-	1/1/1/1	-
4	EDO	B	429	-	-	1/1/1/1	-
4	EDO	A	419	-	-	1/1/1/1	-
4	EDO	B	431	-	-	0/1/1/1	-
4	EDO	A	432	-	-	1/1/1/1	-
4	EDO	A	417	-	-	1/1/1/1	-
4	EDO	A	412	-	-	0/1/1/1	-
4	EDO	A	420	-	-	0/1/1/1	-
4	EDO	A	408[A]	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	433	PEL	OXT-C-CA-C1'
5	A	434	PEL	OXT-C-CA-C1'
4	A	413	EDO	O1-C1-C2-O2
4	B	428	EDO	O1-C1-C2-O2
4	B	421	EDO	O1-C1-C2-O2

There are no ring outliers.

19 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	422	EDO	5	0
4	B	418	EDO	5	0
5	A	434	PEL	1	0
4	A	410	EDO	2	0
4	A	430	EDO	2	0
4	B	414	EDO	4	0
4	A	424	EDO	1	0
4	B	426	EDO	12	0
4	A	411	EDO	1	0
4	B	423	EDO	1	0
4	B	428	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	421	EDO	4	0
4	B	416	EDO	6	0
4	A	427	EDO	1	0
4	B	429	EDO	3	0
4	A	419	EDO	4	0
4	A	432	EDO	10	0
4	A	417	EDO	8	0
4	A	420	EDO	4	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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.