



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 11:57 AM BST

PDB ID : 2HMK  
Title : Crystal Structure of Naphthalene 1,2-Dioxygenase Bound to Phenanthrene  
Authors : Ferraro, D.J.; Okerlund, A.L.; Mowers, J.C.; Ramaswamy, S.  
Deposited on : 2006-07-11  
Resolution : 1.65 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.

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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 : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

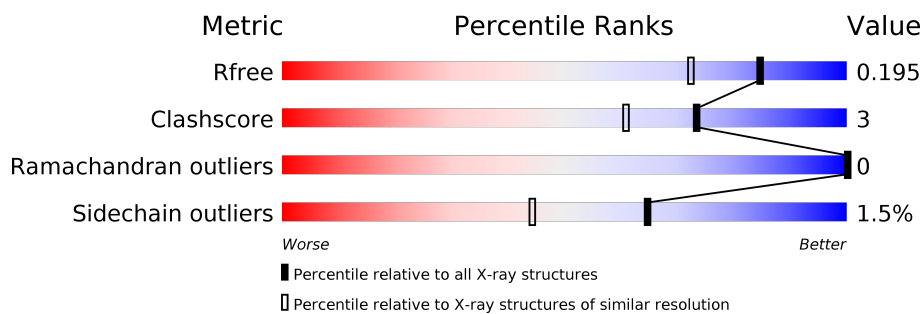
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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  $\geq 3$ , 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	A	449	 94% 6% •
2	B	194	 90% 8% ••

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5882 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 Naphthalene 1,2-dioxygenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	6	0
			3507	2223	599	668	17			

- Molecule 2 is a protein called Naphthalene 1,2-dioxygenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1600	1002	301	292	5			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

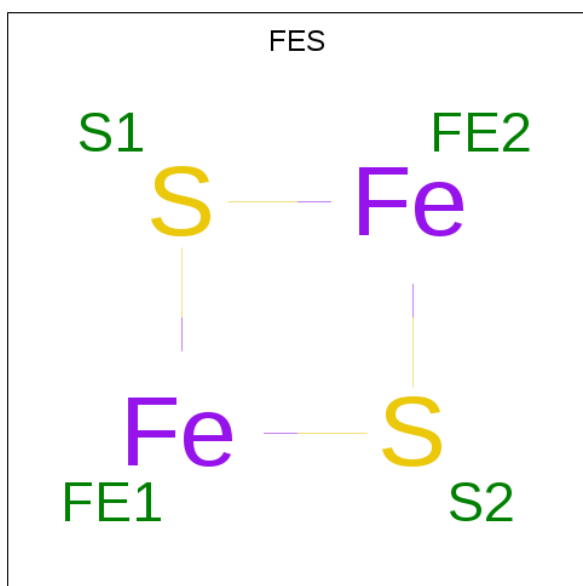
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

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



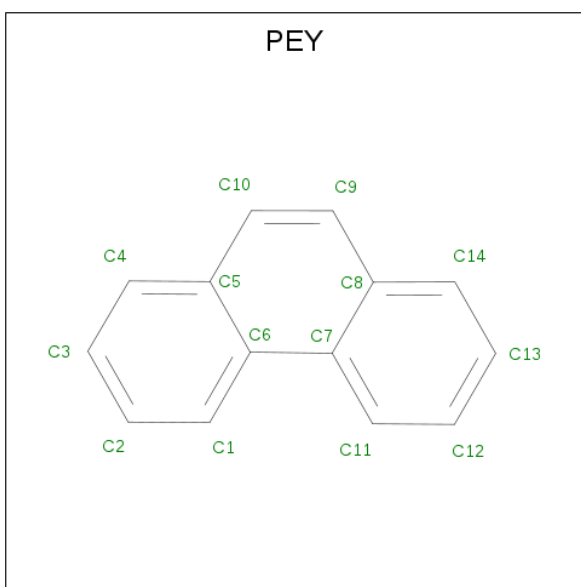
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe S 4 2 2	0	0

- Molecule 6 is PHENANTHRENE (three-letter code: PEY) (formula:  $\text{C}_{14}\text{H}_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C		0	0
			14	14			

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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

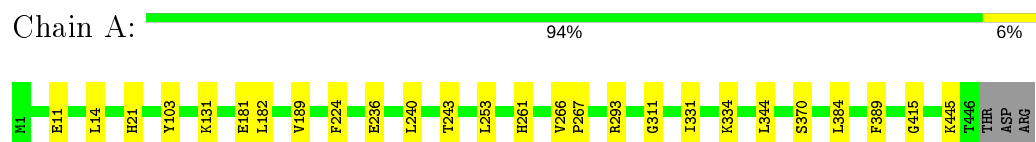
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	457	Total O 457 457	0	0
8	B	194	Total O 194 194	0	0

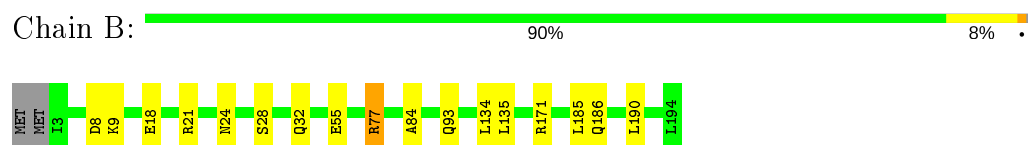
### 3 Residue-property plots

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. 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: Naphthalene 1,2-dioxygenase alpha subunit



- Molecule 2: Naphthalene 1,2-dioxygenase beta subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.95Å 139.95Å 208.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.51 – 1.65 39.43 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.51-1.65) 99.3 (39.43-1.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.158 , 0.183 0.170 , 0.195	Depositor DCC
$R_{free}$ test set	4696 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 31.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: SO4, EDO, FE, FES, PEY

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	0.51	0/3608	0.64	0/4887
2	B	0.54	0/1630	0.74	2/2199 (0.1%)
All	All	0.52	0/5238	0.67	2/7086 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	ASN	N-CA-C	9.12	135.63	111.00
2	B	24	ASN	CB-CA-C	-6.90	96.60	110.40

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	3507	0	3356	18	0
2	B	1600	0	1574	14	0
3	A	1	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
5	A	4	0	0	0	0
6	A	14	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	56	0	84	0	0
7	B	24	0	36	3	0
8	A	457	0	0	2	0
8	B	194	0	0	8	0
All	All	5882	0	5060	34	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 3.

All (34) 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:224:PHE:CE1	1:A:253:LEU:HD23	2.17	0.78
1:A:11:GLU:OE2	1:A:445:LYS:NZ	2.23	0.72
1:A:181:GLU:HG3	1:A:334:LYS:HG2	1.77	0.66
1:A:224:PHE:CD2	6:A:701:PEY:H13	2.32	0.65
2:B:186:GLN:HG2	8:B:829:HOH:O	2.06	0.56
2:B:77:ARG:H	2:B:77:ARG:NE	2.06	0.53
1:A:384:LEU:HD21	8:A:1060:HOH:O	2.08	0.52
2:B:55:GLU:HG3	8:B:830:HOH:O	2.09	0.52
2:B:134:LEU:HD23	2:B:135:LEU:N	2.27	0.49
2:B:84:ALA:HB3	7:B:703:EDO:H22	1.94	0.49
1:A:224:PHE:CE1	1:A:253:LEU:CD2	2.96	0.47
1:A:189[B]:VAL:HG12	2:B:185:LEU:HB2	1.97	0.47
2:B:134:LEU:C	2:B:134:LEU:HD23	2.37	0.45
1:A:261:HIS:CE1	1:A:344:LEU:HD12	2.51	0.45
1:A:311:GLY:HA2	1:A:331:ILE:HG13	1.99	0.45
6:A:701:PEY:H1	6:A:701:PEY:H11	1.74	0.44
8:A:1100:HOH:O	7:B:718:EDO:H22	2.17	0.44
1:A:224:PHE:CZ	1:A:253:LEU:HD23	2.53	0.44
1:A:14:LEU:HD21	1:A:389:PHE:CG	2.53	0.43
7:B:703:EDO:H11	8:B:864:HOH:O	2.19	0.43
1:A:182:LEU:HD12	1:A:331:ILE:HG23	2.00	0.43
1:A:21:HIS:HB3	1:A:370:SER:HA	2.01	0.43
1:A:266:VAL:HB	1:A:267:PRO:HD3	2.01	0.42
1:A:243:THR:OG1	1:A:415:GLY:HA3	2.18	0.42
2:B:9:LYS:NZ	8:B:902:HOH:O	2.51	0.42
1:A:261:HIS:NE2	1:A:344:LEU:HD11	2.35	0.42
2:B:28:SER:O	2:B:32:GLN:NE2	2.52	0.42
2:B:186:GLN:CG	8:B:829:HOH:O	2.65	0.41
2:B:32:GLN:NE2	8:B:885:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:GLN:CD	8:B:885:HOH:O	2.59	0.41
2:B:18:GLU:OE2	2:B:21:ARG:NH1	2.53	0.41
2:B:93:GLN:HG2	8:B:813:HOH:O	2.20	0.40
1:A:182:LEU:HD12	1:A:331:ILE:CG2	2.52	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	450/449 (100%)	437 (97%)	13 (3%)	0	100	100
2	B	190/194 (98%)	183 (96%)	7 (4%)	0	100	100
All	All	640/643 (100%)	620 (97%)	20 (3%)	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	372/369 (101%)	368 (99%)	4 (1%)	73	57
2	B	171/173 (99%)	167 (98%)	4 (2%)	50	25
All	All	543/542 (100%)	535 (98%)	8 (2%)	65	44

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	131	LYS
1	A	236	GLU
1	A	293	ARG
2	B	8	ASP
2	B	77	ARG
2	B	171	ARG
2	B	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	115	GLN
2	B	14	HIS
2	B	32	GLN
2	B	82	ASN
2	B	186	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	$\# Z  > 2$
7	EDO	A	719	-	3,3,3	0.47	0	2,2,2	0.15	0
7	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.32	0
7	EDO	B	718	-	3,3,3	0.54	0	2,2,2	0.03	0
7	EDO	A	716	-	3,3,3	0.44	0	2,2,2	0.41	0
7	EDO	B	702	-	3,3,3	0.56	0	2,2,2	0.37	0
7	EDO	A	726	-	3,3,3	0.52	0	2,2,2	0.12	0
4	SO4	A	453	-	4,4,4	0.12	0	6,6,6	0.15	0
5	FES	A	454	1	0,4,4	0.00	-	-	-	-
7	EDO	B	722	-	3,3,3	0.46	0	2,2,2	0.07	0
7	EDO	A	720	-	3,3,3	0.56	0	2,2,2	0.46	0
4	SO4	B	195	-	4,4,4	0.19	0	6,6,6	0.19	0
7	EDO	A	724	-	3,3,3	0.54	0	2,2,2	0.12	0
7	EDO	A	710	-	3,3,3	0.48	0	2,2,2	0.40	0
7	EDO	B	721	-	3,3,3	0.50	0	2,2,2	0.09	0
4	SO4	B	197	-	4,4,4	0.17	0	6,6,6	0.27	0
6	PEY	A	701	-	16,16,16	1.60	5 (31%)	22,22,22	0.99	0
7	EDO	A	711	-	3,3,3	0.56	0	2,2,2	0.19	0
7	EDO	B	703	-	3,3,3	0.89	0	2,2,2	0.50	0
7	EDO	A	712	-	3,3,3	0.40	0	2,2,2	0.40	0
4	SO4	A	452	-	4,4,4	0.15	0	6,6,6	0.33	0
7	EDO	A	717	-	3,3,3	0.38	0	2,2,2	0.65	0
7	EDO	A	723	-	3,3,3	0.73	0	2,2,2	0.24	0
4	SO4	B	196	-	4,4,4	0.20	0	6,6,6	0.44	0
7	EDO	A	709	-	3,3,3	0.43	0	2,2,2	0.23	0
7	EDO	A	725	-	3,3,3	0.41	0	2,2,2	0.44	0
7	EDO	B	706	-	3,3,3	0.54	0	2,2,2	0.19	0
7	EDO	A	715	-	3,3,3	0.54	0	2,2,2	0.19	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
7	EDO	A	719	-	-	0/1/1/1	-
7	EDO	A	714	-	-	0/1/1/1	-
7	EDO	B	718	-	-	1/1/1/1	-
7	EDO	A	716	-	-	1/1/1/1	-
7	EDO	A	709	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	726	-	-	1/1/1/1	-
5	FES	A	454	1	-	-	0/1/1/1
7	EDO	B	722	-	-	0/1/1/1	-
7	EDO	A	720	-	-	1/1/1/1	-
7	EDO	A	724	-	-	0/1/1/1	-
7	EDO	A	710	-	-	0/1/1/1	-
7	EDO	B	721	-	-	1/1/1/1	-
6	PEY	A	701	-	-	-	0/3/3/3
7	EDO	A	711	-	-	0/1/1/1	-
7	EDO	B	703	-	-	1/1/1/1	-
7	EDO	A	712	-	-	0/1/1/1	-
7	EDO	A	717	-	-	1/1/1/1	-
7	EDO	A	723	-	-	0/1/1/1	-
7	EDO	B	702	-	-	1/1/1/1	-
7	EDO	A	725	-	-	1/1/1/1	-
7	EDO	B	706	-	-	0/1/1/1	-
7	EDO	A	715	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	PEY	C6-C5	-2.77	1.36	1.42
6	A	701	PEY	C7-C6	-2.49	1.37	1.45
6	A	701	PEY	C9-C8	-2.47	1.36	1.41
6	A	701	PEY	C7-C8	-2.39	1.37	1.42
6	A	701	PEY	C10-C5	-2.04	1.37	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	718	EDO	O1-C1-C2-O2
7	B	703	EDO	O1-C1-C2-O2
7	A	725	EDO	O1-C1-C2-O2
7	A	726	EDO	O1-C1-C2-O2
7	A	720	EDO	O1-C1-C2-O2
7	A	715	EDO	O1-C1-C2-O2
7	A	716	EDO	O1-C1-C2-O2
7	A	717	EDO	O1-C1-C2-O2
7	B	702	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	721	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	718	EDO	1	0
6	A	701	PEY	2	0
7	B	703	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.