



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:54 PM UTC

PDB ID : 7Q84 / pdb_00007q84
Title : Crystal structure of human peroxisomal acyl-Co-A oxidase 1a, apo-form
Authors : Sonani, R.R.; Blat, A.; Dubin, G.
Deposited on : 2021-11-10
Resolution : 2.00 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 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

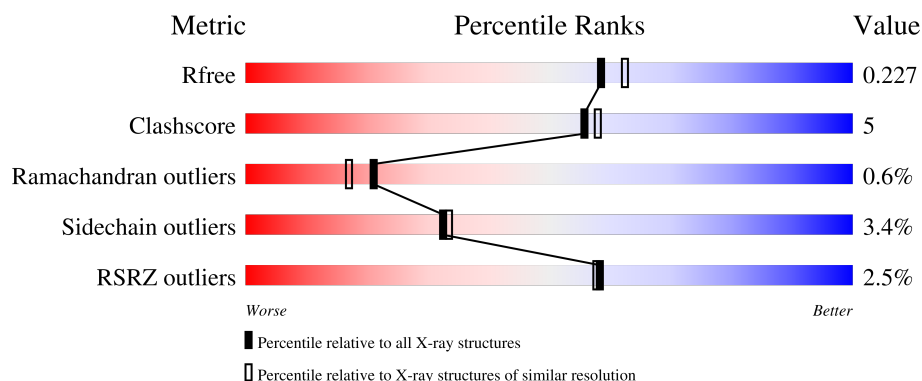
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

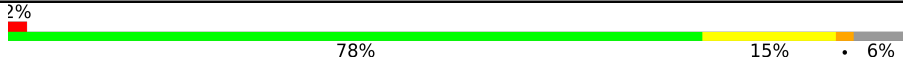
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	667	
1	B	667	

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
2	PGE	A	701	-	-	X	-

2 Entry composition [i](#)

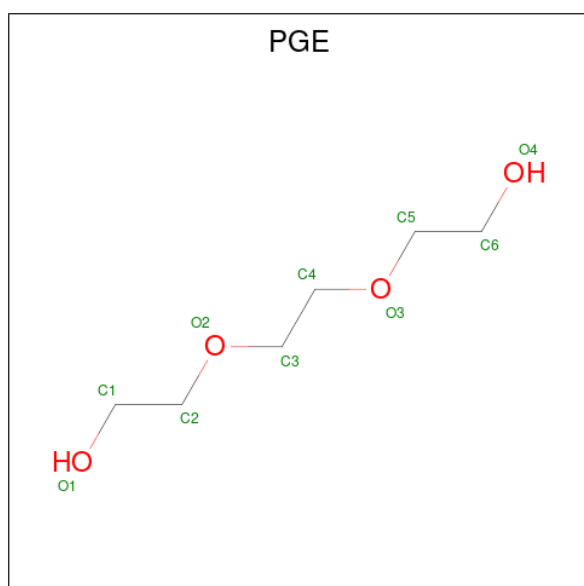
There are 6 unique types of molecules in this entry. The entry contains 10556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			5002	3185	868	920	29			
1	B	625	Total	C	N	O	S	0	0	0
			4977	3169	863	916	29			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total 221	O 221	0	0
6	B	271	Total 271	O 271	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.87Å 133.22Å 139.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.00 48.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.23-2.00) 99.1 (48.23-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.220 0.192 , 0.227	Depositor DCC
R_{free} test set	5573 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10556	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: CSO, PGE, GOL, PEG, 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	1.32	19/5099 (0.4%)	1.51	19/6896 (0.3%)
1	B	1.30	19/5073 (0.4%)	1.50	28/6861 (0.4%)
All	All	1.31	38/10172 (0.4%)	1.50	47/13757 (0.3%)

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	HIS	CE1-NE2	8.27	1.40	1.32
1	B	298	THR	C-O	7.50	1.32	1.24
1	A	48	HIS	CE1-NE2	7.12	1.39	1.32
1	A	387	THR	C-O	-6.98	1.16	1.24
1	A	594	GLU	C-O	-6.77	1.15	1.24

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	HIS	CA-CB-CG	-9.52	104.28	113.80
1	B	155	THR	CB-CA-C	7.58	122.23	109.80
1	B	94	ARG	CA-C-O	-7.25	113.17	121.65
1	B	283	SER	CA-C-N	6.86	129.77	120.38
1	B	283	SER	C-N-CA	6.86	129.77	120.38

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	5002	0	4973	51	0
1	B	4977	0	4945	45	0
2	A	10	0	14	6	0
2	B	10	0	14	4	0
3	A	24	0	36	3	0
3	B	16	0	24	0	0
4	A	7	0	10	0	0
5	A	6	0	8	2	0
5	B	12	0	16	1	0
6	A	221	0	0	5	0
6	B	271	0	0	4	0
All	All	10556	0	10040	94	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 5.

The worst 5 of 94 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:348:MET:HE1	1:A:374:THR:HG22	1.20	1.12
1:A:307:ARG:HE	2:A:701:PGE:H12	1.45	0.79
1:A:309:GLN:HG2	2:A:701:PGE:H2	1.73	0.71
1:A:103:HIS:HD2	1:A:134:GLY:H	1.39	0.70
1:A:143:HIS:ND1	6:A:801:HOH:O	2.29	0.66

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	618/667 (93%)	593 (96%)	21 (3%)	4 (1%)	21	17
1	B	615/667 (92%)	597 (97%)	15 (2%)	3 (0%)	24	21
All	All	1233/1334 (92%)	1190 (96%)	36 (3%)	7 (1%)	21	17

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	A	473	THR
1	B	176	TRP
1	B	473	THR
1	A	365	SER

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	A	539/576 (94%)	516 (96%)	23 (4%)	26	25
1	B	536/576 (93%)	522 (97%)	14 (3%)	40	44
All	All	1075/1152 (93%)	1038 (97%)	37 (3%)	32	33

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	357	GLU
1	B	591	ARG
1	B	366	GLU
1	B	457	ASP
1	A	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	430	GLN

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Mol	Chain	Res	Type
1	B	576	GLN
1	B	627	ASN
1	A	441	GLN
1	A	430	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	$\# Z > 2$
1	CSO	B	449	1	3,6,7	1.22	1 (33%)	1,6,8	0.40	0
1	CSO	A	449	1	3,6,7	1.29	1 (33%)	1,6,8	0.49	0
1	CSO	A	199	1	3,6,7	1.40	1 (33%)	1,6,8	0.30	0
1	CSO	B	199	1	3,6,7	1.20	0	1,6,8	0.53	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
1	CSO	B	449	1	-	0/1/5/7	-
1	CSO	A	449	1	-	0/1/5/7	-
1	CSO	A	199	1	-	0/1/5/7	-
1	CSO	B	199	1	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	CSO	O-C	2.30	1.28	1.20
1	A	449	CSO	O-C	2.08	1.27	1.20
1	B	449	CSO	O-C	2.04	1.27	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands 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	EDO	A	708	-	3,3,3	0.62	0	2,2,2	0.32	0
3	EDO	A	709	-	3,3,3	0.21	0	2,2,2	0.32	0
3	EDO	B	704	-	3,3,3	0.79	0	2,2,2	0.49	0
4	PEG	A	704	-	6,6,6	0.77	0	5,5,5	0.41	0
5	GOL	A	707	-	5,5,5	0.27	0	5,5,5	0.59	0
2	PGE	A	701	-	9,9,9	0.61	0	8,8,8	1.08	2 (25%)
3	EDO	B	703	-	3,3,3	1.11	0	2,2,2	0.52	0
3	EDO	B	706	-	3,3,3	0.14	0	2,2,2	0.35	0
3	EDO	B	702	-	3,3,3	1.34	0	2,2,2	0.86	0
3	EDO	A	705	-	3,3,3	0.73	0	2,2,2	0.30	0
2	PGE	B	701	-	9,9,9	0.86	0	8,8,8	0.94	0
5	GOL	B	705	-	5,5,5	0.16	0	5,5,5	0.44	0
3	EDO	A	702	-	3,3,3	1.31	0	2,2,2	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	706	-	3,3,3	0.26	0	2,2,2	0.38	0
3	EDO	A	703	-	3,3,3	0.77	0	2,2,2	0.92	0
5	GOL	B	707	-	5,5,5	0.20	0	5,5,5	0.51	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	EDO	A	708	-	-	1/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
4	PEG	A	704	-	-	3/4/4/4	-
5	GOL	A	707	-	-	0/4/4/4	-
2	PGE	A	701	-	-	3/7/7/7	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	B	706	-	-	1/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
2	PGE	B	701	-	-	4/7/7/7	-
5	GOL	B	705	-	-	4/4/4/4	-
3	EDO	A	702	-	-	1/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
5	GOL	B	707	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PGE	C3-O2-C2	-2.09	104.10	113.26
2	A	701	PGE	O2-C2-C1	-2.04	101.14	110.11

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	705	GOL	O1-C1-C2-O2
5	B	705	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	705	GOL	C1-C2-C3-O3
2	B	701	PGE	O2-C3-C4-O3
4	A	704	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	GOL	2	0
2	A	701	PGE	6	0
2	B	701	PGE	4	0
5	B	705	GOL	1	0
3	A	702	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 [i](#)

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

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	626/667 (93%)	0.14	16 (2%) 57 56	30, 48, 81, 145	0
1	B	623/667 (93%)	0.08	15 (2%) 59 59	29, 45, 79, 125	0
All	All	1249/1334 (93%)	0.11	31 (2%) 58 58	29, 47, 80, 145	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	LEU	4.8
1	B	458	LEU	4.6
1	A	472	PRO	4.2
1	A	653	LEU	3.8
1	B	278	MET	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	B	449	7/8	0.83	0.32	20,20,20,20	0
1	CSO	A	449	7/8	0.84	0.25	20,20,20,20	0
1	CSO	A	199	7/8	0.90	0.27	20,20,20,20	0
1	CSO	B	199	7/8	0.93	0.25	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	EDO	B	703	4/4	0.82	0.17	52,57,57,61	0
3	EDO	A	708	4/4	0.83	0.18	63,68,70,73	0
3	EDO	B	704	4/4	0.85	0.15	42,58,62,63	0
3	EDO	B	706	4/4	0.85	0.17	49,59,62,65	0
3	EDO	A	702	4/4	0.87	0.15	44,52,52,54	0
3	EDO	A	705	4/4	0.87	0.16	53,60,67,69	0
2	PGE	B	701	10/10	0.88	0.19	41,64,72,77	0
3	EDO	A	706	4/4	0.88	0.14	50,53,57,57	0
2	PGE	A	701	10/10	0.88	0.20	43,54,64,70	0
4	PEG	A	704	7/7	0.88	0.18	61,65,72,75	0
3	EDO	B	702	4/4	0.89	0.23	38,50,59,59	0
5	GOL	A	707	6/6	0.89	0.12	63,65,72,73	0
5	GOL	B	707	6/6	0.90	0.10	54,58,59,64	0
3	EDO	A	703	4/4	0.91	0.12	36,48,50,54	0
3	EDO	A	709	4/4	0.92	0.14	59,64,67,72	0
5	GOL	B	705	6/6	0.94	0.11	63,70,75,77	0

6.5 Other polymers

There are no such residues in this entry.