



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 7C71 / pdb\_00007c71  
Title : Crystal structure of beta-glycosides-binding protein (E117A) of ABC transporter in an open state  
Authors : Kanaujia, S.P.; Chandravanshi, M.; Samanta, R.  
Deposited on : 2020-05-22  
Resolution : 2.10 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.

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 : 4-5-2 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

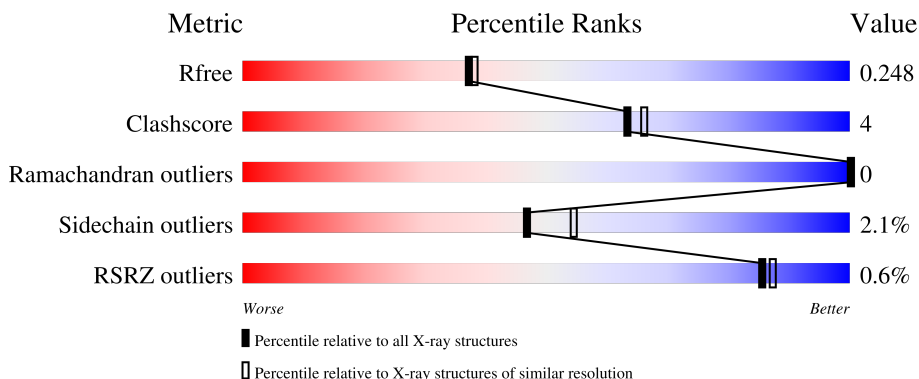
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

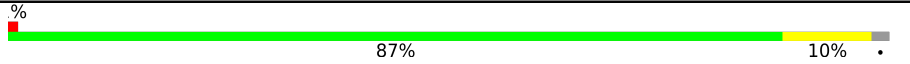

The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\leq 5\%$ . 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	423	 87% 10% .
1	B	423	 88% 10% ..

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7026 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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3182	2048	549	575	10	0	2	0
1	B	415	3179	2045	548	576	10	0	2	0

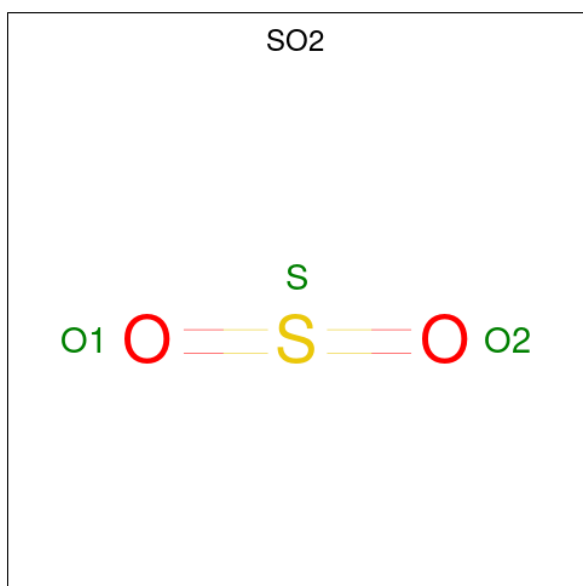
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q53W80
A	117	ALA	GLU	engineered mutation	UNP Q53W80
A	417	HIS	-	expression tag	UNP Q53W80
A	418	HIS	-	expression tag	UNP Q53W80
A	419	HIS	-	expression tag	UNP Q53W80
A	420	HIS	-	expression tag	UNP Q53W80
A	421	HIS	-	expression tag	UNP Q53W80
A	422	HIS	-	expression tag	UNP Q53W80
B	0	MET	-	initiating methionine	UNP Q53W80
B	117	ALA	GLU	engineered mutation	UNP Q53W80
B	417	HIS	-	expression tag	UNP Q53W80
B	418	HIS	-	expression tag	UNP Q53W80
B	419	HIS	-	expression tag	UNP Q53W80
B	420	HIS	-	expression tag	UNP Q53W80
B	421	HIS	-	expression tag	UNP Q53W80
B	422	HIS	-	expression tag	UNP Q53W80

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

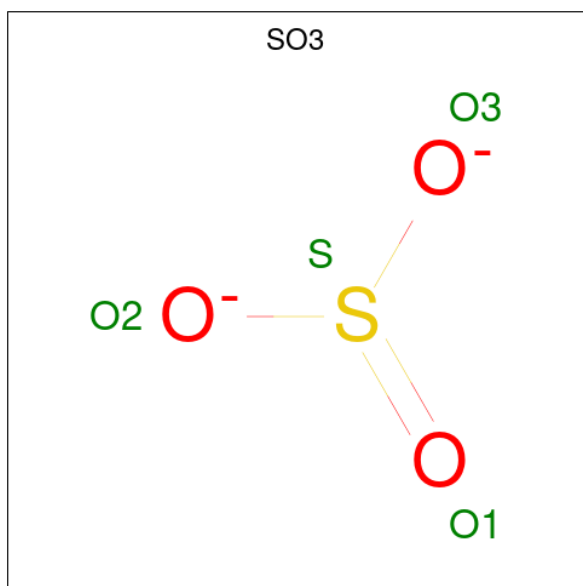
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SULFUR DIOXIDE (CCD ID: SO2) (formula: O<sub>2</sub>S).



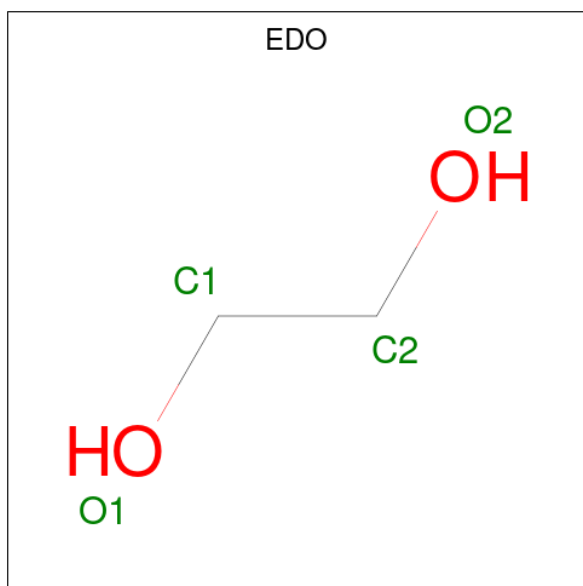
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			3	2	1		
3	A	1	Total	O	S	0	0
			3	2	1		
3	B	1	Total	O	S	0	0
			3	2	1		

- Molecule 4 is SULFITE ION (CCD ID: SO3) (formula: O<sub>3</sub>S).



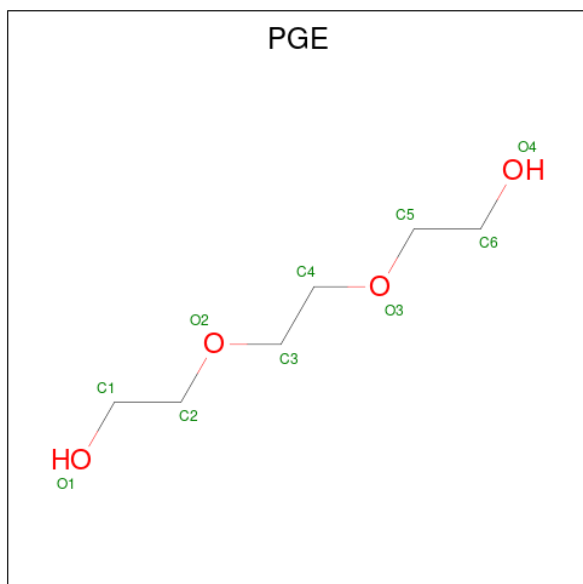
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			4	3	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

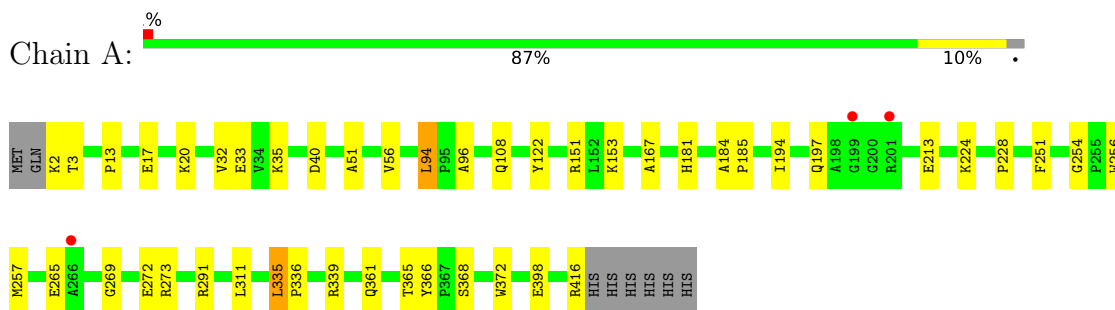
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	310	Total O 310 310	0	0
7	B	301	Total O 301 301	0	0

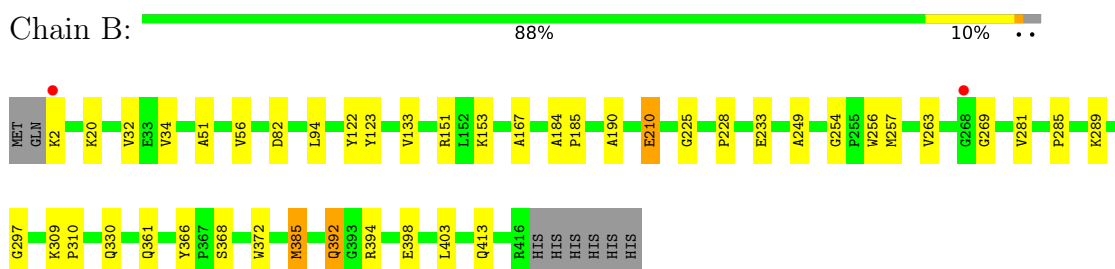
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Sugar ABC transporter, periplasmic sugar-binding protein



- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.40Å 100.96Å 66.52Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	55.55 – 2.10 55.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.55-2.10) 100.0 (55.55-2.10)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.179 , 0.244 0.186 , 0.248	Depositor DCC
$R_{free}$ test set	2149 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: SO3, EDO, PGE, CL, SO2

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	1.16	3/3276 (0.1%)	1.38	3/4459 (0.1%)
1	B	1.13	2/3273 (0.1%)	1.36	3/4456 (0.1%)
All	All	1.14	5/6549 (0.1%)	1.37	6/8915 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	PRO	C-O	-6.98	1.15	1.23
1	B	281	VAL	C-O	6.51	1.30	1.24
1	A	13	PRO	C-O	-5.46	1.17	1.24
1	A	181	HIS	CE1-NE2	5.33	1.37	1.32
1	A	269	GLY	N-CA	5.04	1.48	1.44

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	361	GLN	CB-CG-CD	5.94	122.70	112.60
1	A	40	ASP	CB-CA-C	5.43	118.73	109.72
1	A	269	GLY	CA-C-O	-5.21	115.50	122.23
1	B	392	GLN	CB-CG-CD	-5.11	103.92	112.60

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	3182	0	3157	28	0
1	B	3179	0	3149	24	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	1	0
3	B	3	0	0	0	0
4	A	4	0	0	0	0
5	A	8	0	12	0	0
6	A	10	0	14	0	0
6	B	20	0	28	1	0
7	A	310	0	0	10	1
7	B	301	0	0	2	1
All	All	7026	0	6360	51	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 4.

The worst 5 of 51 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:210:GLU:HG2	7:B:812:HOH:O	1.78	0.82
1:A:265:GLU:OE1	1:A:273:ARG:HD3	1.90	0.72
1:B:385:MET:HE3	1:B:403:LEU:HD22	1.74	0.69
1:A:108:GLN:NE2	7:A:602:HOH:O	2.24	0.69
1:A:94:LEU:HD13	1:A:339:ARG:HD3	1.77	0.66

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)
7:A:731:HOH:O	7:B:793:HOH:O[1_556]	2.14	0.06

## 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	415/423 (98%)	410 (99%)	5 (1%)	0	100	100
1	B	415/423 (98%)	411 (99%)	4 (1%)	0	100	100
All	All	830/846 (98%)	821 (99%)	9 (1%)	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	315/321 (98%)	308 (98%)	7 (2%)	45	53
1	B	315/321 (98%)	309 (98%)	6 (2%)	50	58
All	All	630/642 (98%)	617 (98%)	13 (2%)	47	54

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	LEU
1	B	210	GLU
1	B	413	GLN
1	B	385	MET
1	B	398	GLU

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

Mol	Chain	Res	Type
1	A	358	GLN
1	A	377	ASN
1	B	108	GLN
1	B	197	GLN
1	B	377	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	SO3	A	504	-	1,3,3	1.21	0	0,3,3	-	-
3	SO2	A	503	-	2,2,2	0.21	0	1,1,1	0.03	0
6	PGE	B	504	-	9,9,9	0.23	0	8,8,8	0.18	0
3	SO2	A	502	-	2,2,2	0.35	0	1,1,1	0.23	0
5	EDO	A	506	-	3,3,3	0.07	0	2,2,2	0.19	0
5	EDO	A	505	-	3,3,3	0.09	0	2,2,2	0.56	0
6	PGE	A	507	-	9,9,9	0.29	0	8,8,8	0.14	0
6	PGE	B	505	-	9,9,9	0.26	0	8,8,8	0.26	0
3	SO2	B	503	-	2,2,2	0.31	0	1,1,1	0.02	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
6	PGE	B	504	-	-	3/7/7/7	-
5	EDO	A	506	-	-	1/1/1/1	-
5	EDO	A	505	-	-	1/1/1/1	-
6	PGE	A	507	-	-	5/7/7/7	-
6	PGE	B	505	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	505	PGE	O1-C1-C2-O2
6	B	505	PGE	O3-C5-C6-O4
6	A	507	PGE	O1-C1-C2-O2
6	B	505	PGE	C1-C2-O2-C3
6	A	507	PGE	O3-C5-C6-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	SO2	1	0
6	B	505	PGE	1	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, 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	A	415/423 (98%)	-0.17	3 (0%) 84 86	8, 15, 31, 57	2 (0%)
1	B	415/423 (98%)	-0.12	2 (0%) 87 88	10, 17, 29, 45	2 (0%)
All	All	830/846 (98%)	-0.14	5 (0%) 85 87	8, 16, 30, 57	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	4.2
1	B	268	GLY	2.7
1	A	199	GLY	2.2
1	B	2	LYS	2.1
1	A	201	ARG	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](#)

There are no oligosaccharides in this entry.

### 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( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	505	4/4	0.79	0.17	32,33,34,37	0
6	PGE	B	505	10/10	0.81	0.16	38,41,45,46	0
6	PGE	B	504	10/10	0.84	0.12	36,38,41,42	0
6	PGE	A	507	10/10	0.86	0.11	33,34,38,38	0
5	EDO	A	506	4/4	0.89	0.16	32,32,32,34	0
3	SO2	B	503	3/3	0.89	0.09	49,49,53,55	0
3	SO2	A	502	3/3	0.91	0.09	44,44,45,48	0
4	SO3	A	504	4/4	0.92	0.10	47,48,48,49	0
3	SO2	A	503	3/3	0.94	0.08	39,39,39,43	0
2	CL	A	501	1/1	0.99	0.01	10,10,10,10	0
2	CL	B	501	1/1	0.99	0.04	14,14,14,14	0
2	CL	B	502	1/1	0.99	0.09	19,19,19,19	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.