



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2025 – 12:09 pm GMT

PDB ID : 9I4F  
Title : Blood Type B-converting alpha-1,3-galactosidase PpaGal from *Pedobacter panaciterrae* in its apo form  
Authors : Schmoeker, O.; Moeller, C.; Terholsen, H.; Girbardt, B.; Palm, G.J.; Hoppen, J.; Lammers, M.; Bornscheuer, U.T.  
Deposited on : 2025-01-24  
Resolution : 2.75 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

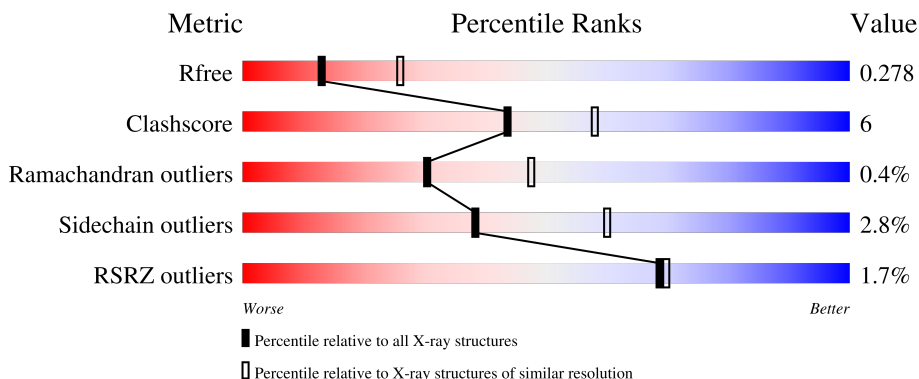
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	584	 85% 14% .
1	B	584	 83% 15% .
1	C	584	 83% 15% .
1	D	584	 82% 16% .

## 2 Entry composition [i](#)

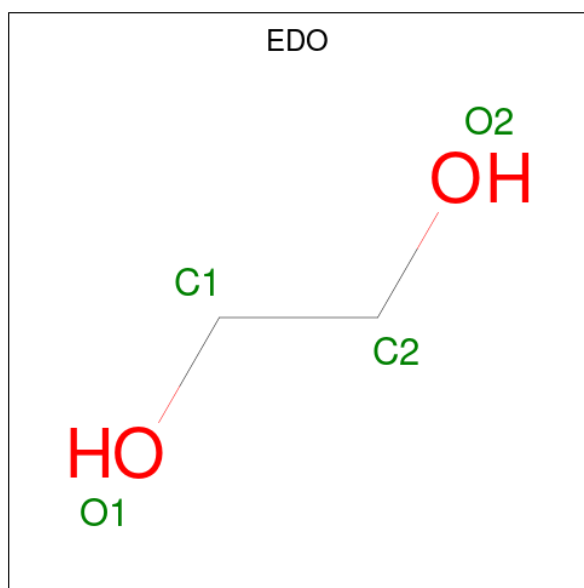
There are 3 unique types of molecules in this entry. The entry contains 37156 atoms, of which 18534 are hydrogens and 0 are deuteriums.

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 Alpha-1,3-galactosidase PpaGal.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	584	Total	C	H	N	O	S	135	0	0
			9271	2964	4632	784	873	18			
1	B	584	Total	C	H	N	O	S	135	0	0
			9271	2964	4632	784	873	18			
1	C	584	Total	C	H	N	O	S	135	0	0
			9271	2964	4632	784	873	18			
1	D	584	Total	C	H	N	O	S	135	0	0
			9271	2964	4632	784	873	18			

- Molecule 2 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
2	B	1	Total	C	H	O	1	0
			10	2	6	2		

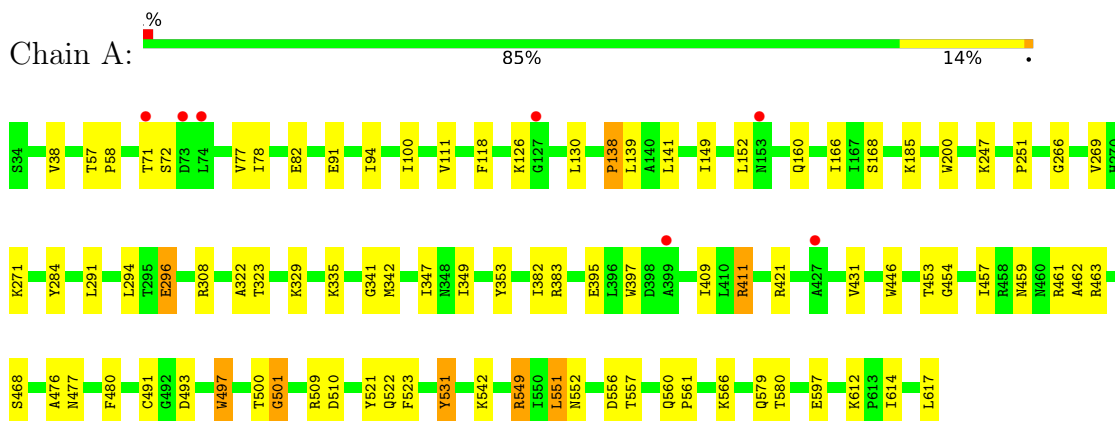
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	17	Total 17	O 17	0	0
3	C	8	Total 8	O 8	0	0
3	D	17	Total 17	O 17	0	0

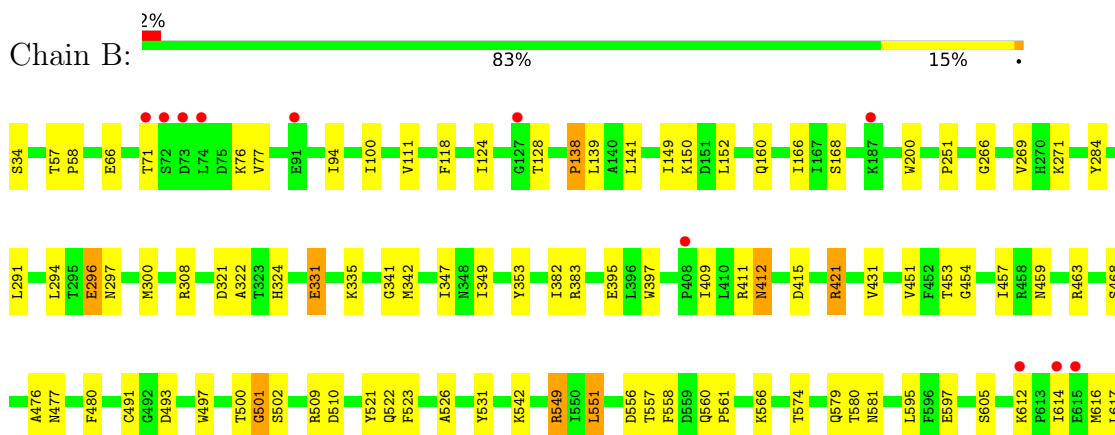
### 3 Residue-property plots

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 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.

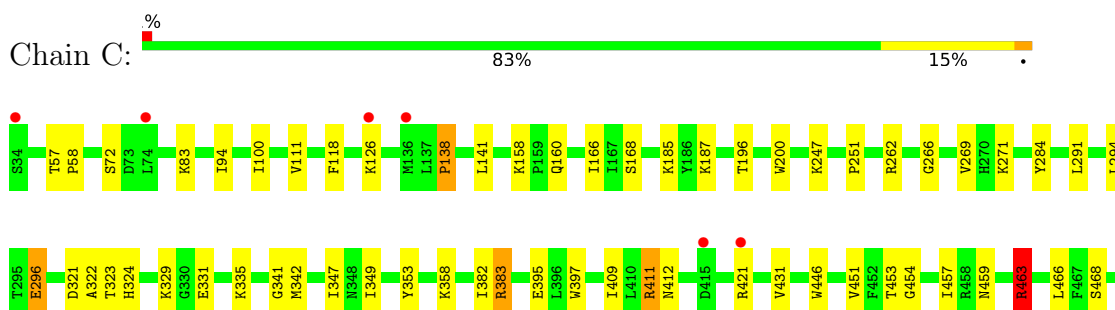
#### • Molecule 1: Alpha-1,3-galactosidase PpaGal

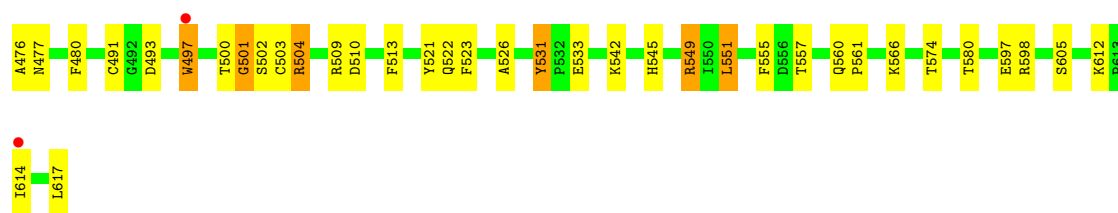


#### • Molecule 1: Alpha-1,3-galactosidase PpaGal

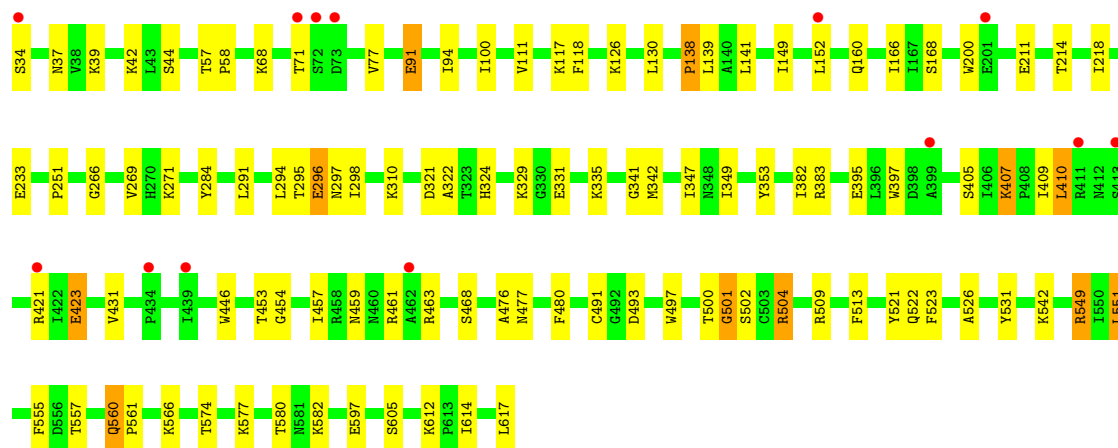
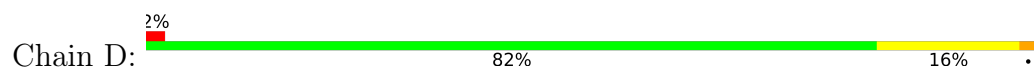


#### • Molecule 1: Alpha-1,3-galactosidase PpaGal





● Molecule 1: Alpha-1,3-galactosidase PpaGal



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.13Å 129.03Å 108.30Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	107.13 – 2.75 107.13 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.2 (107.13-2.75) 95.2 (107.13-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.251 , 0.285 0.240 , 0.278	Depositor DCC
$R_{free}$ test set	3655 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	1.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.044 for h,-k,-l 0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	37156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9874e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	0.75	1/4746 (0.0%)	1.04	8/6416 (0.1%)
1	B	0.76	1/4746 (0.0%)	1.04	8/6416 (0.1%)
1	C	0.75	1/4746 (0.0%)	1.06	9/6416 (0.1%)
1	D	0.78	4/4746 (0.1%)	1.03	8/6416 (0.1%)
All	All	0.76	7/18984 (0.0%)	1.04	33/25664 (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
1	A	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	GLU	CD-OE1	-8.22	1.16	1.25
1	D	331	GLU	CD-OE2	6.05	1.32	1.25
1	D	233	GLU	CD-OE1	-5.90	1.19	1.25
1	B	331	GLU	CD-OE2	5.63	1.31	1.25
1	C	331	GLU	CD-OE2	5.45	1.31	1.25

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	ARG	NE-CZ-NH1	13.21	126.90	120.30
1	C	549	ARG	NE-CZ-NH1	12.43	126.52	120.30
1	A	549	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	C	549	ARG	NE-CZ-NH2	-11.36	114.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	549	ARG	NE-CZ-NH1	10.99	125.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	552	ASN	Sidechain

## 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	4639	4632	4615	50	2
1	B	4639	4632	4615	59	1
1	C	4639	4632	4615	56	1
1	D	4639	4632	4615	60	2
2	B	4	6	6	0	0
3	A	20	0	0	0	0
3	B	17	0	0	1	0
3	C	8	0	0	0	0
3	D	17	0	0	0	0
All	All	18622	18534	18466	223	3

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 6.

The worst 5 of 223 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:C:463:ARG:HG3	1:C:466:LEU:CD1	2.20	0.72
1:D:42:LYS:HE3	1:D:44:SER:OG	1.90	0.70
1:C:463:ARG:HG3	1:C:466:LEU:HD11	1.74	0.70
1:C:100:ILE:HG23	1:C:291:LEU:HD22	1.74	0.70
1:D:100:ILE:HG23	1:D:291:LEU:HD22	1.74	0.70

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:O	1:D:34:SER:HG[2_655]	1.31	0.29
1:A:411:ARG:O	1:D:34:SER:OG[2_655]	2.12	0.08
1:B:66:GLU:OE2	1:C:411:ARG:HH22[1_455]	1.59	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	582/584 (100%)	542 (93%)	38 (6%)	2 (0%)	37	55
1	B	582/584 (100%)	541 (93%)	39 (7%)	2 (0%)	37	55
1	C	582/584 (100%)	541 (93%)	39 (7%)	2 (0%)	37	55
1	D	582/584 (100%)	539 (93%)	40 (7%)	3 (0%)	25	41
All	All	2328/2336 (100%)	2163 (93%)	156 (7%)	9 (0%)	30	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	GLY
1	B	501	GLY
1	D	501	GLY
1	C	501	GLY
1	C	138	PRO

### 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	513/513 (100%)	499 (97%)	14 (3%)	40	61
1	B	513/513 (100%)	502 (98%)	11 (2%)	48	69
1	C	513/513 (100%)	497 (97%)	16 (3%)	35	56
1	D	513/513 (100%)	496 (97%)	17 (3%)	33	55
All	All	2052/2052 (100%)	1994 (97%)	58 (3%)	38	60

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	LYS
1	D	612	LYS
1	C	531	TYR
1	D	582	LYS
1	D	502	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	437	GLN
1	D	390	GLN
1	C	522	GLN
1	B	412	ASN
1	C	545	HIS

### 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

1 ligand is 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	$\# Z  > 2$
2	EDO	B	701	-	3,3,3	0.32	0	2,2,2	0.62	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
2	EDO	B	701	-	-	0/1/1/1	-

There are no bond length outliers.

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	584/584 (100%)	0.21	7 (1%) 76 78	26, 36, 52, 76	0
1	B	584/584 (100%)	0.20	11 (1%) 66 67	23, 35, 53, 88	0
1	C	584/584 (100%)	0.24	8 (1%) 73 75	23, 34, 52, 69	0
1	D	584/584 (100%)	0.27	13 (2%) 62 62	23, 35, 51, 96	0
All	All	2336/2336 (100%)	0.23	39 (1%) 69 70	23, 35, 52, 96	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	3.3
1	D	421	ARG	3.2
1	D	72	SER	3.2
1	B	72	SER	3.1
1	C	74	LEU	3.0

### 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 monosaccharides 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
2	EDO	B	701	4/4	0.91	0.44	53,55,55,55	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.