

Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2023 - 06:43 pm GMT

PDB ID	:	7QSP
Title	:	Permutated C-terminal lobe of the ribose binding protein from Thermotoga
		maritima
Authors	:	Shanmugaratnam, S.; Michel, F.; Hocker, B.
Deposited on		
Resolution	:	1.36 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

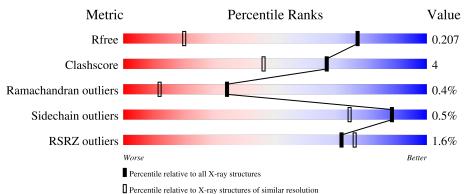
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.36 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1509(1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 <=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	А	151	^{2%} 74%	7% •	19%
1	В	151	% 77%	6%	17%

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	EDO	В	205	-	-	-	Х



7QSP

2 Entry composition (i)

125

В

1

There are 3 unique types of molecules in this entry. The entry contains 4334 atoms, of which 2026 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	123	Total 2014	C 670	11	N 165	0 193	S 6	0	7	0
1	Б	105	Total	С	Н	Ν	0	S	0		0

169

192

7

• Molecule 1 is a protein called Ribose ABC transporter, periplasmic ribose-binding protein.

A116VAL-linkerUNP Q9X053A117GLY-linkerUNP Q9X053A118HIS-linkerUNP Q9X053A119ASN-linkerUNP Q9X053A120HIS-linkerUNP Q9X053A128ALAMETconflictUNP Q9X053A143GLY-expression tagUNP Q9X053A144GLY-expression tagUNP Q9X053A145HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B116VAL-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY </th <th>Chain</th> <th>Residue</th> <th>Modelled</th> <th>Actual</th> <th>Comment</th> <th>Reference</th>	Chain	Residue	Modelled	Actual	Comment	Reference
A117GLY-linkerUNP Q9X053A118HIS-linkerUNP Q9X053A119ASN-linkerUNP Q9X053A120HIS-linkerUNP Q9X053A128ALAMETconflictUNP Q9X053A143GLY-expression tagUNP Q9X053A144GLY-expression tagUNP Q9X053A145HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	0	MET	-	initiating methionine	UNP Q9X053
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$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	117	GLY	-	linker	UNP Q9X053
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	118	HIS	-	linker	UNP Q9X053
A128ALAMETconflictUNP Q9X053A143GLY-expression tagUNP Q9X053A144GLY-expression tagUNP Q9X053A145HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	119	ASN	-	linker	UNP Q9X053
A143GLY-expression tagUNP Q9X053A144GLY-expression tagUNP Q9X053A145HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	120	HIS	-	linker	UNP Q9X053
A144 GLY -expression tagUNP Q9X053A145HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	128	ALA	MET	conflict	UNP Q9X053
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A146HIS-expression tagUNP Q9X053A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	144	GLY	-	expression tag	UNP Q9X053
A147HIS-expression tagUNP Q9X053A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	145	HIS	-	expression tag	UNP Q9X053
A148HIS-expression tagUNP Q9X053A149HIS-expression tagUNP Q9X053A150HIS-expression tagUNP Q9X053B0MET-initiating methionineUNP Q9X053B116VAL-linkerUNP Q9X053B116VAL-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	146	HIS	-	expression tag	UNP Q9X053
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B116VAL-linkerUNP Q9X053B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	А	150	HIS	-	expression tag	UNP Q9X053
B117GLY-linkerUNP Q9X053B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	0	MET	-	initiating methionine	UNP Q9X053
B118HIS-linkerUNP Q9X053B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	116	VAL	-	linker	UNP Q9X053
B119ASN-linkerUNP Q9X053B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	117	GLY	-	linker	UNP Q9X053
B120HIS-linkerUNP Q9X053B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	118	HIS	-	linker	UNP Q9X053
B128ALAMETconflictUNP Q9X053B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	119	ASN	-	linker	UNP Q9X053
B143GLY-expression tagUNP Q9X053B144GLY-expression tagUNP Q9X053	В	120	HIS	- linker		UNP Q9X053
B 144 GLY - expression tag UNP Q9X053	В	128	ALA	MET conflict		UNP Q9X053
	В	143	GLY	- expression tag		UNP Q9X053
B 145 HIS - expression tag UNP Q9X053		144		-	expression tag	UNP Q9X053
	В	145	HIS	-	expression tag	UNP Q9X053

There are 30 discrepancies between the modelled and reference sequences:

992

671

2031

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0

7

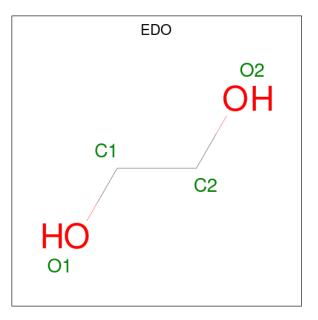
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Contentia	Continued from provous page						
Chain	Residue	Modelled	Actual	Comment	Reference		
В	146	HIS	-	expression tag	UNP Q9X053		
В	147	HIS	-	expression tag	UNP Q9X053		
В	148	HIS	-	expression tag	UNP Q9X053		
В	149	HIS	-	expression tag	UNP Q9X053		
В	150	HIS	-	expression tag	UNP Q9X053		

Continued from previous page...

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C H O 10 2 6 2	0	0
2	А	1	Total C H O 10 2 6 2	0	0
2	А	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0
2	В	1	Total C H O 10 2 6 2	0	0



• Molecule 3 is water.

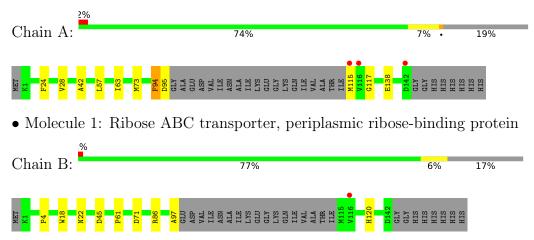
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	89	Total O 90 90	0	1
3	В	107	Total O 109 109	0	2



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: Ribose ABC transporter, periplasmic ribose-binding protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	99.0 (39.76 - 1.36)	Depositor
(in resolution range)	99.0 (40.00-1.35)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.97 (at 1.35 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	2100 reflections $(4.13%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 34.9	EDS
L-test for twinning ²	$< L >=0.43, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.076 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4334	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.07% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/1074	0.68	0/1451	
1	В	0.46	0/1086	0.67	1/1467~(0.1%)	
All	All	0.43	0/2160	0.67	1/2918~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	В	71	ASP	CB-CG-OD2	-5.32	113.51	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	А	1034	980	982	6	0
1	В	1039	992	997	8	0
2	А	12	18	18	0	0
2	В	24	36	36	4	0
3	А	90	0	0	2	0
3	В	109	0	0	4	0
All	All	2308	2026	2033	16	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 4.

All (16) 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:120[B]:HIS:NE2	3:B:301:HOH:O	2.21	0.64
1:B:120[C]:HIS:CE1	3:B:314:HOH:O	2.59	0.55
1:A:57:LEU:HD23	1:A:63[B]:ILE:HD11	1.95	0.48
1:B:4[B]:PRO:HG3	3:B:322:HOH:O	2.14	0.47
1:B:120[C]:HIS:CD2	1:B:120[C]:HIS:H	2.29	0.47
1:B:22:ASN:OD1	2:B:203:EDO:H22	2.16	0.46
1:B:61:PRO:O	1:B:86:ARG:NH1	2.42	0.45
1:A:138:GLU:HG3	3:A:323:HOH:O	2.17	0.44
3:A:356:HOH:O	2:B:203:EDO:C1	2.65	0.44
1:B:97:ALA:H	1:B:120[B]:HIS:CE1	2.36	0.44
2:B:203:EDO:H22	3:B:317[A]:HOH:O	2.19	0.42
1:A:115:MET:HG2	1:A:117:GLY:O	2.19	0.42
1:A:24:PHE:CZ	1:A:28:VAL:HG21	2.55	0.41
1:A:94[B]:PHE:HD1	1:A:95[B]:ASP:H	1.69	0.41
1:B:45:ASP:OD1	2:B:205:EDO:H12	2.21	0.40
1:A:42:ALA:HB3	1:A:73:MET:SD	2.62	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	А	125/151~(83%)	122~(98%)	1 (1%)	2(2%)	9 1
1	В	129/151~(85%)	128 (99%)	1 (1%)	0	100 100
All	All	254/302~(84%)	250 (98%)	2(1%)	2(1%)	34 3

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	94[A]	PHE
1	А	94[B]	PHE

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	А	106/120~(88%)	106 (100%)	0	100 100
1	В	107/120~(89%)	106~(99%)	1 (1%)	78 53
All	All	213/240~(89%)	212 (100%)	1 (0%)	88 74

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	18	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

9 ligands are modelled in this entry.



7QSP

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	Turne	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
	Type	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	EDO	В	202	-	3,3,3	0.46	0	2,2,2	0.26	0
2	EDO	В	201	-	3,3,3	0.59	0	2,2,2	0.13	0
2	EDO	А	203	-	3,3,3	0.51	0	2,2,2	0.19	0
2	EDO	В	206	-	3,3,3	0.58	0	2,2,2	0.04	0
2	EDO	А	201	-	3,3,3	0.51	0	$2,\!2,\!2$	0.21	0
2	EDO	А	202	-	3,3,3	0.48	0	2,2,2	0.19	0
2	EDO	В	205	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	В	203	-	3,3,3	0.56	0	2,2,2	0.05	0
2	EDO	В	204	-	3,3,3	0.50	0	$2,\!2,\!2$	0.32	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	В	202	-	-	0/1/1/1	-
2	EDO	В	201	-	-	0/1/1/1	-
2	EDO	А	203	-	-	0/1/1/1	-
2	EDO	В	206	-	-	0/1/1/1	-
2	EDO	А	201	-	-	1/1/1/1	-
2	EDO	А	202	-	-	1/1/1/1	-
2	EDO	В	205	-	-	1/1/1/1	-
2	EDO	В	203	-	-	0/1/1/1	-
2	EDO	В	204	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

	Mol	Chain	Res	Type	Atoms
2 A 202 EDO 01-C1-C2-C	2	А	202	EDO	O1-C1-C2-O2

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α \cdot \cdot \cdot	C		
Continued	trom	previous	page
0 0	$J \cdot \cdot \cdot \cdot \cdot$	P · · · · · · · · · · · · · · · · · · ·	<i>P</i> •• <i>J</i> ••••

Mol	Chain	Res	Type	Atoms
2	В	204	EDO	O1-C1-C2-O2
2	А	201	EDO	O1-C1-C2-O2
2	В	205	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	205	EDO	1	0
2	В	203	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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q} {<} 0.9$	
1	А	123/151~(81%)	-0.23	3(2%)	59	65	14, 23, 43, 73	0
1	В	125/151~(82%)	-0.42	1 (0%)	86	89	13, 19, 33, 53	0
All	All	248/302~(82%)	-0.32	4 (1%)	72	76	13, 21, 40, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	116	VAL	6.2
1	А	115	MET	5.5
1	А	142	ASP	3.5
1	В	116	VAL	2.2

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^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
2	EDO	В	203	4/4	0.60	0.18	$39,\!49,\!58,\!65$	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	EDO	А	203	4/4	0.73	0.29	40,52,65,74	0
2	EDO	А	201	4/4	0.74	0.25	35,42,58,61	0
2	EDO	В	205	4/4	0.76	0.47	38,51,69,82	0
2	EDO	В	204	4/4	0.77	0.32	36,44,62,66	0
2	EDO	В	202	4/4	0.78	0.33	40,48,60,66	0
2	EDO	В	206	4/4	0.79	0.21	33,47,67,67	0
2	EDO	В	201	4/4	0.86	0.19	31,38,57,57	0
2	EDO	А	202	4/4	0.86	0.23	29,40,48,53	0

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6.5 Other polymers (i)

There are no such residues in this entry.

