

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	6KXK
Title	:	BON1
Authors	:	Wang, Q.C.; Jiang, M.Q.; Isupov, M.N.; Sun, L.F.; Wu, Y.K.
Deposited on	:	2019-09-12
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	$2.14.4.\mathrm{dev1}$
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)	:	$2.14.4.\mathrm{dev1}$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	$5346\ (2.50-2.50)$		
Ramachandran outliers	138981	5231(2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559(2.50-2.50)		

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 >=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		~ ~ 0	3%		
	A	553	83%	14%	•
	~		2%		_
1		553	85%	13%	•
	_		2%		_
1	D	553	84%	14%	•
	_		5%		_
1	F F	553	83%	14%	•
_			5%		_
2	В	528	82%	15%	••
			11%		
3	Е	550	82%	15%	• ••



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Mol	Chain	\mathbf{Length}	Quality of chain		
4	G	527	9%	1.4%	
1	ŭ	021	10%		••
5	H	553	84%	13%	••

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
6	PEG	А	807	-	-	-	Х
6	PEG	D	611	-	-	Х	Х
6	PEG	D	614	-	-	Х	-
7	EDO	А	804	-	-	Х	-
7	EDO	А	805	-	-	Х	-
7	EDO	А	813	-	-	-	Х
7	EDO	А	817	-	-	Х	-
7	EDO	В	601	-	-	-	Х
7	EDO	В	603	-	-	-	Х
7	EDO	В	608	-	-	Х	-
7	EDO	В	609	-	-	Х	-
7	EDO	В	616	-	-	-	Х
7	EDO	D	612	-	-	Х	-
7	EDO	D	621	-	-	-	Х
7	EDO	F	1705	-	-	Х	-
7	EDO	F	1707	-	-	-	Х
7	EDO	F	1719	-	-	Х	-
7	EDO	F	1720	-	-	-	Х
8	GOL	В	607	-	-	-	Х



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 35097 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	Δ	559	552	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	000	4299	2735	719	832	13	0	0	U	
1	C	552	Total	С	Ν	Ο	S	0	0	0	
		000	4299	2735	719	832	13			0	
1	П	552	Total	С	Ν	Ο	S	0	0	0	
		000	4299	2735	719	832	13			0	
1	1 F	552	Total	С	Ν	Ο	S	0	0	0	
		553	4299	2735	719	832	13			U	

• Molecule 1 is a protein called Protein BONZAI 1.

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-9	GLY	-	expression tag	UNP Q941L3
А	-8	THR	-	expression tag	UNP Q941L3
A	-7	SER	-	expression tag	UNP Q941L3
A	-6	SER	-	expression tag	UNP Q941L3
A	-5	MET	-	expression tag	UNP Q941L3
A	-4	ALA	-	expression tag	UNP Q941L3
A	-3	ASP	-	expression tag	UNP Q941L3
A	-2	ILE	-	expression tag	UNP Q941L3
А	-1	GLY	-	expression tag	UNP Q941L3
A	0	SER	-	expression tag	UNP Q941L3
С	-9	GLY	-	expression tag	UNP Q941L3
C	-8	THR	-	expression tag	UNP Q941L3
С	-7	SER	-	expression tag	UNP Q941L3
C	-6	SER	-	expression tag	UNP Q941L3
С	-5	MET	-	expression tag	UNP Q941L3
С	-4	ALA	-	expression tag	UNP Q941L3
С	-3	ASP	-	expression tag	UNP Q941L3
С	-2	ILE	-	expression tag	UNP Q941L3
C	-1	GLY	-	expression tag	UNP Q941L3
С	0	SER	-	expression tag	UNP Q941L3
D	-9	GLY	-	expression tag	UNP Q941L3



Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	THR	-	expression tag	UNP Q941L3
D	-7	SER	-	expression tag	UNP Q941L3
D	-6	SER	-	expression tag	UNP Q941L3
D	-5	MET	-	expression tag	UNP Q941L3
D	-4	ALA	-	expression tag	UNP Q941L3
D	-3	ASP	-	expression tag	UNP Q941L3
D	-2	ILE	-	expression tag	UNP Q941L3
D	-1	GLY	-	expression tag	UNP Q941L3
D	0	SER	-	expression tag	UNP Q941L3
F	-9	GLY	-	expression tag	UNP Q941L3
F	-8	THR	-	expression tag	UNP Q941L3
F	-7	SER	-	expression tag	UNP Q941L3
F	-6	SER	-	expression tag	UNP Q941L3
F	-5	MET	-	expression tag	UNP Q941L3
F	-4	ALA	-	expression tag	UNP Q941L3
F	-3	ASP	-	expression tag	UNP Q941L3
F	-2	ILE	-	expression tag	UNP Q941L3
F	-1	GLY	-	expression tag	UNP Q941L3
F	0	SER	-	expression tag	UNP Q941L3

• Molecule 2 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	528	Total 4114	C 2621	N 690	O 791	S 12	0	0	0

• Molecule 3 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Е	547	Total 4259	C 2711	N 712	O 823	S 13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	-6	SER	-	expression tag	UNP Q941L3
E	-5	MET	-	expression tag	UNP Q941L3
E	-4	ALA	-	expression tag	UNP Q941L3
E	-3	ASP	-	expression tag	UNP Q941L3
E	-2	ILE	-	expression tag	UNP Q941L3
Е	-1	GLY	-	expression tag	UNP Q941L3
E	0	SER	-	expression tag	UNP Q941L3



• Molecule 4 is a protein called Protein BONZAI 1.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
4	G	508	Total 3963	C 2524	N 667	O 760	S 12	0	0	0

• Molecule 5 is a protein called Protein BONZAI 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	Н	550	Total 4277	C 2721	N 715	O 828	S 13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	-9	GLY	-	expression tag	UNP Q941L3
Н	-8	THR	-	expression tag	UNP Q941L3
Н	-7	SER	-	expression tag	UNP Q941L3
Н	-6	SER	-	expression tag	UNP Q941L3
Н	-5	MET	-	expression tag	UNP Q941L3
Н	-4	ALA	-	expression tag	UNP Q941L3
Н	-3	ASP	-	expression tag	UNP Q941L3
Н	-2	ILE	-	expression tag	UNP Q941L3
Н	-1	GLY	-	expression tag	UNP Q941L3
Н	0	THR	-	expression tag	UNP Q941L3

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





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Mol	Chain	Residues	\mathbf{Atoms}	ZeroOcc	AltConf
6	А	1	Total C O 7 4 3	0	0
6	А	1	Total C O 7 4 3	0	0
6	А	1	Total C O 7 4 3	0	0
6	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	Е	1	$\begin{array}{c cc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ \hline 7 & 4 & 3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
6	F	1	TotalCO743	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{c cc} \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{c cc} \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	С	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Е	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	TotalCO422	0	0
7	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	G	1	$\begin{array}{c c} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	G	1	$\begin{array}{c cc} \overline{\text{Total}} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Н	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
7	Н	1	TotalCO422	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Η	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	Η	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	D	1	Total C O 6 3 3	0	0
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	D	1	Total C O 6 3 3	0	0
8	Ε	1	Total C O 6 3 3	0	0
8	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	F	1	Total C O 6 3 3	0	0
8	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	G	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ 6 & 3 & 3 \end{array}$	0	0
8	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
8	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total C O 10 6 4	0	0
9	А	1	Total C O 10 6 4	0	0
9	В	1	Total C O 10 6 4	0	0
9	С	1	Total C O 10 6 4	0	0
9	F	1	Total C O 10 6 4	0	0

• Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total C O 13 8 5	0	0
10	D	1	Total C O 13 8 5	0	0

• Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Cl 1 1	0	0
11	С	1	Total Cl 1 1	0	0

• Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total Ca 1 1	0	0
12	F	1	Total Ca 1 1	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	126	Total O 126 126	0	0
13	В	89	Total O 89 89	0	0
13	С	76	Total O 76 76	0	0
13	D	95	Total O 95 95	0	0
13	Е	46	$\begin{array}{cc} \text{Total} & \text{O} \\ 46 & 46 \end{array}$	0	0
13	F	86	Total O 86 86	0	0
13	G	38	Total O 38 38	0	0
13	Н	47	TotalO4747	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: Protein BONZAI 1







• Molecule 4: Protein BONZAI 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	122.28Å 118.72Å 222.25Å	Deneiten
a, b, c, α , β , γ	90.00° 90.20° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}\left(\hat{\boldsymbol{\lambda}}\right)$	48.21 - 2.50	Depositor
Resolution (A)	48.16 - 2.50	EDS
% Data completeness	98.0 (48.21-2.50)	Depositor
(in resolution range)	$97.1 \ (48.16 - 2.50)$	EDS
R _{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.55 \;({\rm at}\; 2.51{\rm \AA})$	Xtriage
Refinement program	REFMAC $5.8.0238$	Depositor
R R.	0.227 , 0.266	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.227 , 0.266	DCC
R_{free} test set	10856 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.5	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 37.8	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
	0.000 for k,h,-l	
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
	$0.099 {\rm for} {\rm h,-k,-l}$	
F_o, F_c correlation	0.95	EDS
Total number of atoms	35097	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	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 35.11 % 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 6.1375e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: GOL, PGE, CL, CA, EDO, PG4, PEG

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).

Mal	Chain	Bond	lengths	B	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/4382	0.78	5/5929~(0.1%)
1	С	0.42	0/4382	0.75	4/5929~(0.1%)
1	D	0.44	0/4382	0.81	6/5929~(0.1%)
1	F	0.43	0/4382	0.75	2/5929~(0.0%)
2	В	0.45	0/4194	0.85	13/5676~(0.2%)
3	Е	0.43	0/4340	0.76	5/5871~(0.1%)
4	G	0.41	0/4035	0.74	1/5452~(0.0%)
5	Н	0.41	0/4358	0.74	1/5896~(0.0%)
All	All	0.43	0/34455	0.77	$37/46611 \ (0.1\%)$

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	D	0	1
1	F	0	1
2	В	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	540	ARG	CG-CD-NE	-9.88	91.06	111.80
4	G	138	ARG	CB-CG-CD	-9.24	87.58	111.60
1	D	540	ARG	CG-CD-NE	-8.58	93.79	111.80
1	D	346	ARG	CG-CD-NE	8.24	129.12	111.80
1	А	340	ARG	CG-CD-NE	-7.75	95.53	111.80



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
2	В	198	GLY	Peptide
2	В	514	ARG	Peptide
1	D	12	LYS	Peptide
1	F	11	SER	Peptide

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	4299	0	4300	64	0
1	С	4299	0	4300	50	0
1	D	4299	0	4300	56	0
1	F	4299	0	4300	66	0
2	В	4114	0	4125	58	0
3	Е	4259	0	4266	55	0
4	G	3963	0	3986	45	0
5	Н	4277	0	4283	49	0
6	А	35	0	50	6	0
6	В	7	0	10	0	0
6	С	21	0	30	4	0
6	D	35	0	50	10	0
6	Ε	14	0	20	3	0
6	F	7	0	10	2	0
7	А	48	0	72	21	0
7	В	52	0	78	16	0
7	С	40	0	60	4	0
7	D	56	0	84	7	0
7	Ε	20	0	30	2	0
7	F	68	0	102	17	0
7	G	16	0	24	0	0
7	Н	24	0	36	3	0
8	A	36	0	48	0	0
8	В	6	0	8	0	0
8	С	24	0	32	3	0
8	D	24	0	32	5	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Е	30	0	40	2	0
8	F	24	0	32	2	0
8	G	6	0	8	1	0
8	Н	12	0	16	1	0
9	А	20	0	28	2	0
9	В	10	0	14	2	0
9	С	10	0	14	1	0
9	F	10	0	14	5	0
10	В	13	0	18	3	0
10	D	13	0	18	3	0
11	С	1	0	0	0	0
11	D	1	0	0	0	0
12	D	1	0	0	0	0
12	F	1	0	0	0	0
13	А	126	0	0	8	0
13	В	89	0	0	3	0
13	С	76	0	0	2	0
13	D	95	0	0	7	0
13	Е	46	0	0	2	0
13	F	86	0	0	6	0
13	G	38	0	0	1	0
13	Н	47	0	0	0	0
All	All	35097	0	34838	457	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 7.

The worst 5 of 457 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)	
4:G:249:LEU:O	4:G:249:LEU:HD12	1.52	1.10	
3:E:10:LYS:HD3	3:E:541:ILE:HD11	1.35	1.06	
2:B:85:GLN:H	7:B:609:EDO:H12	1.11	1.05	
4:G:249:LEU:HD13	4:G:274:LEU:CD2	1.90	1.01	
1:F:99:GLN:HA	7:F:1705:EDO:H12	1.39	1.01	

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	Perc	$\mathbf{entiles}$
1	А	551/553~(100%)	525~(95%)	22~(4%)	4 (1%)	22	39
1	С	551/553~(100%)	521~(95%)	24~(4%)	6 (1%)	14	26
1	D	551/553~(100%)	524 (95%)	21 (4%)	6 (1%)	14	26
1	F	551/553~(100%)	524~(95%)	21 (4%)	6 (1%)	14	26
2	В	526/528~(100%)	501~(95%)	20~(4%)	5 (1%)	15	28
3	Ε	543/550~(99%)	505~(93%)	31~(6%)	7 (1%)	12	21
4	G	498/527~(94%)	477 (96%)	19 (4%)	2(0%)	34	54
5	Η	546/553~(99%)	514 (94%)	25~(5%)	7 (1%)	12	21
All	All	4317/4370 (99%)	4091 (95%)	183 (4%)	43 (1%)	15	28

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	278	ALA
1	А	514	ARG
2	В	36	LEU
2	В	144	PRO
1	С	145	GLN

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	$481/481 \ (100\%)$	449 (93%)	32~(7%)	16 31		



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	С	481/481~(100%)	458~(95%)	23~(5%)	25	48	
1	D	481/481~(100%)	456~(95%)	25~(5%)	23	44	
1	F	481/481~(100%)	454 (94%)	27~(6%)	21	40	
2	В	461/461~(100%)	433~(94%)	28~(6%)	18	36	
3	Ε	477/479~(100%)	444~(93%)	33~(7%)	15	30	
4	G	446/461~(97%)	421 (94%)	25~(6%)	21	40	
5	Н	479/481~(100%)	444 (93%)	35~(7%)	14	27	
All	All	3787/3806~(100%)	$3559\ (94\%)$	228 (6%)	19	37	

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	515	ASP
3	Е	276	THR
5	Н	252	LYS
1	D	533	SER
3	Е	70	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	29	ASN
1	D	281	ASN
5	Н	225	GLN
1	D	65	ASN
1	D	147	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 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 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).

Mal	Iol Type Chain		Ros Link	Bo	ond leng	\mathbf{ths}	Bond angles			
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
7	EDO	C	611	-	3,3,3	0.07	0	2,2,2	0.13	0
7	EDO	F	1715	-	3, 3, 3	0.09	0	2,2,2	0.33	0
7	EDO	В	608	-	3, 3, 3	0.11	0	2,2,2	0.87	0
6	PEG	А	825	-	$6,\!6,\!6$	0.16	0	$5,\!5,\!5$	0.08	0
7	EDO	A	819	-	3,3,3	0.07	0	2,2,2	0.30	0
8	GOL	F	1714	-	5, 5, 5	0.14	0	$5,\!5,\!5$	0.65	0
6	PEG	D	611	-	6,6,6	0.15	0	$5,\!5,\!5$	0.10	0
7	EDO	C	604	-	3,3,3	0.19	0	$2,\!2,\!2$	0.30	0
7	EDO	В	604	-	3,3,3	0.09	0	$2,\!2,\!2$	0.36	0
7	EDO	D	607	-	3,3,3	0.12	0	$2,\!2,\!2$	0.22	0
7	EDO	В	605	-	3,3,3	0.10	0	$2,\!2,\!2$	0.19	0
7	EDO	Н	607	-	3,3,3	0.12	0	2,2,2	0.62	0
6	PEG	E	2001	-	6,6,6	0.12	0	$5,\!5,\!5$	0.12	0
7	EDO	G	604	-	3, 3, 3	0.14	0	2,2,2	0.06	0
8	GOL	E	2004	-	5, 5, 5	0.17	0	$5,\!5,\!5$	0.48	0
9	PGE	В	612	-	$9,\!9,\!9$	0.29	0	8,8,8	0.29	0
7	EDO	G	603	-	3,3,3	0.10	0	$2,\!2,\!2$	0.22	0
8	GOL	В	607	-	5, 5, 5	0.17	0	$5,\!5,\!5$	0.48	0
7	EDO	С	608	-	3,3,3	0.17	0	$2,\!2,\!2$	0.16	0
7	EDO	D	622	-	3,3,3	0.15	0	$2,\!2,\!2$	0.02	0
7	EDO	В	616	-	3,3,3	0.12	0	$2,\!2,\!2$	0.27	0
8	GOL	С	618	-	5, 5, 5	0.10	0	$5,\!5,\!5$	0.42	0
9	PGE	F	1718	-	$9,\!9,\!9$	0.27	0	8,8,8	0.13	0
7	EDO	F	1723	-	3,3,3	0.10	0	2,2,2	0.31	0
6	PEG	C	605	-	$6,\!6,\!6$	0.18	0	5, 5, 5	0.13	0
7	EDO	F	1719	-	3, 3, 3	0.18	0	2,2,2	0.23	0
7	EDO	F	1717	-	3,3,3	0.10	0	2,2,2	0.15	0



N.T1	T	<u>(1)</u>	Der	т. 1	Bond lengths		Bond angles			
IVI01	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	В	615	-	3,3,3	0.02	0	2,2,2	0.29	0
7	EDO	А	804	-	3, 3, 3	0.11	0	2,2,2	0.49	0
8	GOL	D	609	-	5, 5, 5	0.11	0	$5,\!5,\!5$	0.50	0
7	EDO	D	616	-	3, 3, 3	0.07	0	$2,\!2,\!2$	0.04	0
7	EDO	А	812	-	3, 3, 3	0.18	0	2,2,2	0.56	0
7	EDO	D	608	-	3, 3, 3	0.11	0	2,2,2	0.11	0
7	EDO	D	603	-	3,3,3	0.07	0	2,2,2	0.19	0
7	EDO	F	1702	-	3, 3, 3	0.08	0	$2,\!2,\!2$	0.26	0
7	EDO	С	601	-	3,3,3	0.18	0	$2,\!2,\!2$	0.36	0
7	EDO	В	602	-	3,3,3	0.06	0	$2,\!2,\!2$	0.16	0
7	EDO	С	613	-	3, 3, 3	0.15	0	2,2,2	0.17	0
8	GOL	G	605	-	5, 5, 5	0.11	0	$5,\!5,\!5$	0.40	0
7	EDO	В	609	-	3,3,3	0.28	0	2,2,2	0.17	0
8	GOL	Η	606	-	5, 5, 5	0.18	0	$5,\!5,\!5$	0.55	0
8	GOL	D	610	-	5, 5, 5	0.07	0	$5,\!5,\!5$	0.30	0
7	EDO	В	613	-	3, 3, 3	0.13	0	2,2,2	0.52	0
7	EDO	D	621	-	3, 3, 3	0.21	0	2,2,2	0.44	0
7	EDO	F	1707	-	3,3,3	0.31	0	2,2,2	1.01	0
7	EDO	А	806	-	3, 3, 3	0.06	0	2,2,2	0.28	0
7	EDO	F	1720	-	3, 3, 3	0.14	0	2,2,2	0.22	0
7	EDO	С	614	-	3, 3, 3	0.09	0	2,2,2	0.31	0
7	EDO	D	606	-	3, 3, 3	0.14	0	2,2,2	0.35	0
7	EDO	Е	2002	-	3,3,3	0.07	0	2,2,2	0.23	0
7	EDO	А	808	-	3, 3, 3	0.05	0	2,2,2	0.13	0
6	PEG	F	1712	-	$6,\!6,\!6$	0.17	0	$5,\!5,\!5$	0.15	0
7	EDO	D	612	-	3, 3, 3	0.30	0	$2,\!2,\!2$	1.11	0
7	EDO	А	823	-	3, 3, 3	0.15	0	2,2,2	0.20	0
7	EDO	F	1706	-	3, 3, 3	0.15	0	2,2,2	0.35	0
7	EDO	В	617	-	3, 3, 3	0.11	0	2,2,2	0.18	0
7	EDO	F	1710	-	3,3,3	0.10	0	2,2,2	1.04	0
7	EDO	G	602	-	3,3,3	0.15	0	$2,\!2,\!2$	0.11	0
8	GOL	F	1708	-	5, 5, 5	0.09	0	$5,\!5,\!5$	0.34	0
8	GOL	Ε	2006	-	5, 5, 5	0.14	0	$5,\!5,\!5$	0.41	0
7	EDO	Ε	2009	-	3, 3, 3	0.13	0	$2,\!2,\!2$	0.19	0
10	PG4	D	613	-	12,12,12	0.24	0	$11,\!11,\!11$	0.21	0
7	EDO	С	616	-	3,3,3	0.12	0	2,2,2	0.26	0
8	GOL	C	602		5, 5, 5	0.16	0	5, 5, 5	0.48	0
7	EDO	С	610	-	$3,\!3,\!3$	0.11	0	$2,\!2,\!2$	0.44	0
8	GOL	C	612		5, 5, 5	0.14	0	5, 5, 5	0.45	0
8	GOL	A	815	-	5, 5, 5	0.17	0	5, 5, 5	0.28	0
7	EDO	H	608	-	3,3,3	0.09	0	2,2,2	0.05	0
7	EDO	В	601	-	3,3,3	0.26	0	2,2,2	0.96	0
7	EDO	D	615	-	3,3,3	0.12	0	$2,\!2,\!2$	0.26	0



Ъ <i>Т</i> -1	m	Cl	D	τ. ι	Bo	ond leng	$_{\rm ths}$	Bond angles		
	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	А	821	-	5, 5, 5	0.09	0	$5,\!5,\!5$	0.39	0
8	GOL	А	822	-	5, 5, 5	0.14	0	$5,\!5,\!5$	0.41	0
6	PEG	А	801	-	$6,\!6,\!6$	0.25	0	$5,\!5,\!5$	0.21	0
7	EDO	Е	2010	-	3,3,3	0.08	0	2,2,2	0.18	0
7	EDO	А	809	-	3,3,3	0.05	0	2,2,2	0.23	0
6	PEG	А	802	-	$6,\!6,\!6$	0.21	0	$5,\!5,\!5$	0.12	0
7	EDO	F	1709	-	3,3,3	0.10	0	2,2,2	0.37	0
8	GOL	Е	2008	-	5, 5, 5	0.10	0	$5,\!5,\!5$	0.35	0
10	PG4	В	610	-	12,12,12	0.35	0	11,11,11	0.26	0
7	EDO	А	813	-	3,3,3	0.07	0	2,2,2	0.08	0
7	EDO	F	1713	-	3,3,3	0.14	0	2,2,2	0.42	0
7	EDO	D	605	-	3,3,3	0.15	0	2,2,2	0.40	0
7	EDO	F	1705	-	3, 3, 3	0.12	0	2,2,2	0.80	0
7	EDO	С	609	-	3, 3, 3	0.16	0	2,2,2	0.48	0
7	EDO	Н	602	-	3, 3, 3	0.06	0	2,2,2	0.25	0
6	PEG	D	620	-	$6,\!6,\!6$	0.20	0	$5,\!5,\!5$	0.24	0
7	EDO	Е	2003	-	3, 3, 3	0.09	0	2,2,2	0.10	0
7	EDO	F	1704	-	3, 3, 3	0.04	0	2,2,2	0.07	0
7	EDO	А	817	-	3, 3, 3	0.24	0	2,2,2	0.24	0
7	EDO	Н	603	-	3, 3, 3	0.05	0	2,2,2	0.43	0
7	EDO	А	805	-	3, 3, 3	0.57	0	2,2,2	0.25	0
8	GOL	Н	601	-	5, 5, 5	0.09	0	$5,\!5,\!5$	0.25	0
6	PEG	А	811	-	$6,\!6,\!6$	0.16	0	5, 5, 5	0.07	0
6	PEG	В	611	-	$6,\!6,\!6$	0.35	0	$5,\!5,\!5$	0.24	0
7	EDO	Н	604	-	3, 3, 3	0.10	0	2,2,2	0.28	0
8	GOL	С	607	-	5, 5, 5	0.14	0	5, 5, 5	0.74	0
9	PGE	А	824	-	9, 9, 9	0.23	0	8,8,8	0.13	0
8	GOL	F	1716	-	5, 5, 5	0.07	0	5, 5, 5	0.40	0
7	EDO	D	618	-	3,3,3	0.09	0	2,2,2	0.11	0
8	GOL	D	604	-	5, 5, 5	0.12	0	$5,\!5,\!5$	0.39	0
6	PEG	С	606	-	$6,\!6,\!6$	0.17	0	$5,\!5,\!5$	0.10	0
6	PEG	D	614	-	6,6,6	0.11	0	$5,\!5,\!5$	0.10	0
8	GOL	А	818	-	5, 5, 5	0.12	0	$5,\!5,\!5$	0.52	0
8	GOL	Е	2005	-	5, 5, 5	0.16	0	$5,\!5,\!5$	0.47	0
7	EDO	G	601	-	3, 3, 3	0.28	0	2,2,2	0.47	0
7	EDO	В	603	-	3, 3, 3	0.20	0	2,2,2	0.71	0
7	EDO	F	1703	-	3, 3, 3	0.13	0	$2,\!2,\!2$	0.22	0
7	EDO	D	623	-	3, 3, 3	0.06	0	2,2,2	0.07	0
7	EDO	F	1701	-	3,3,3	0.11	0	2,2,2	0.58	0
7	EDO	В	606	-	3,3,3	0.17	0	2,2,2	0.39	0
7	EDO	F	1721	-	3,3,3	0.08	0	2,2,2	0.15	0
6	PEG	А	807	-	6,6,6	0.16	0	$5,\!5,\!5$	0.09	0
8	GOL	А	810	-	5, 5, 5	0.10	0	$5,\!5,\!5$	0.37	0



Mal	Tune	Chain	Dog	Link	Bo	Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
8	GOL	D	602	-	5, 5, 5	0.13	0	$5,\!5,\!5$	0.43	0	
7	EDO	А	803	-	3,3,3	0.61	0	2,2,2	1.92	1 (50%)	
7	EDO	F	1711	-	3,3,3	0.14	0	2,2,2	0.33	0	
7	EDO	Н	605	-	3, 3, 3	0.21	0	2,2,2	0.82	0	
7	EDO	С	615	-	3, 3, 3	0.13	0	2,2,2	0.12	0	
6	PEG	D	601	-	6,6,6	0.11	0	$5,\!5,\!5$	0.19	0	
7	EDO	Е	2011	-	3, 3, 3	0.15	0	$2,\!2,\!2$	0.34	0	
9	PGE	А	814	-	9, 9, 9	0.25	0	8,8,8	0.11	0	
9	PGE	С	617	-	$9,\!9,\!9$	0.20	0	8,8,8	0.20	0	
7	EDO	D	624	-	3, 3, 3	0.09	0	2,2,2	0.11	0	
6	PEG	Е	2007	-	$6,\!6,\!6$	0.18	0	$5,\!5,\!5$	0.13	0	
7	EDO	В	614	-	3, 3, 3	0.15	0	$2,\!2,\!2$	0.50	0	
7	EDO	D	619	-	3, 3, 3	0.12	0	$2,\!2,\!2$	0.64	0	
8	GOL	А	820	-	5, 5, 5	0.17	0	$5,\!5,\!5$	0.55	0	
8	GOL	F	1722	-	5, 5, 5	0.09	0	$5,\!5,\!5$	0.35	0	
6	PEG	C	603	-	6,6,6	0.32	0	$5,\!5,\!5$	0.27	0	
6	PEG	D	617	-	$6,\!6,\!6$	0.20	0	5, 5, 5	0.10	0	
8	GOL	E	2012	-	5, 5, 5	0.10	0	5, 5, 5	0.34	0	
7	EDO	A	816	-	3, 3, 3	0.12	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	С	611	-	-	1/1/1/1	-
7	EDO	F	1715	-	-	1/1/1/1	-
7	EDO	В	608	-	-	1/1/1/1	-
6	PEG	А	825	-	-	3/4/4/4	-
7	EDO	А	819	-	-	1/1/1/1	-
8	GOL	F	1714	-	-	4/4/4/4	-
6	PEG	D	611	-	-	2/4/4/4	-
7	EDO	С	604	-	-	1/1/1/1	-
7	EDO	В	604	-	-	0/1/1/1	-
7	EDO	D	607	-	-	0/1/1/1	-
7	EDO	В	605	-	-	1/1/1/1	-
7	EDO	Н	607	-	-	1/1/1/1	-
6	PEG	Е	2001	-	-	1/4/4/4	-
7	EDO	G	604	-	-	1/1/1/1	-
8	GOL	E	2004	_	_	2/4/4/4	_



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PGE	В	612	_	_	$\frac{4}{7}/7/7$	-
7	EDO	G	603	_	_	0/1/1/1	_
8	GOL	В	607	_	_	1/4/4/4	-
7	EDO	С	608	_	-	0/1/1/1	-
7	EDO	D	622	-	-	0/1/1/1	-
7	EDO	В	616	-	-	1/1/1/1	-
8	GOL	С	618	-	-	2/4/4/4	-
9	PGE	F	1718	-	-	4/7/7/7	_
7	EDO	F	1723	-	-	0/1/1/1	-
6	PEG	С	605	-	-	2/4/4/4	-
7	EDO	F	1719	-	-	0/1/1/1	-
7	EDO	F	1717	-	-	1/1/1/1	-
7	EDO	В	615	-	_	0/1/1/1	-
7	EDO	А	804	-	-	1/1/1/1	-
8	GOL	D	609	-	-	4/4/4/4	-
7	EDO	D	616	-	-	0/1/1/1	-
7	EDO	А	812	-	-	0/1/1/1	-
7	EDO	D	608	-	-	1/1/1/1	-
7	EDO	D	603	-	-	0/1/1/1	-
7	EDO	F	1702	-	-	0/1/1/1	-
7	EDO	C	601	-	-	1/1/1/1	-
7	EDO	В	602	-	-	0/1/1/1	-
7	EDO	С	613	-	-	0/1/1/1	-
8	GOL	G	605	-	-	2/4/4/4	-
7	EDO	В	609	-	_	0/1/1/1	-
8	GOL	Н	606	-	-	$\frac{4}{4} \frac{4}{4}$	-
8	GOL	D	610	-	-	2/4/4/4	-
7	EDO	В	613	-	-	1/1/1/1	-
7	EDO	D	621	-	-	1/1/1/1	-
7	EDO	F	1707	-	_	0/1/1/1	-
7	EDO	A	806	-	-	0/1/1/1	-
7	EDO	F	1720	-	-	1/1/1/1	-
7	EDO	C	614	-	-	0/1/1/1	-
7	EDO	D	606	-	-	1/1/1/1	-
7	EDO	E	2002	-	-	0/1/1/1	-
7	EDO	A	808	-	-	0/1/1/1	-
6	PEG	F	1712	-	-	2/4/4/4	-
7	EDO	D	612	-	-	0/1/1/1	-
7	EDO	A	823	-	-	1/1/1/1	-
7	EDO	F	1706	-		0/1/1/1	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	В	617	-	-	1/1/1/1	-
7	EDO	F	1710	-	-	1/1/1/1	-
7	EDO	G	602	-	-	1/1/1/1	-
8	GOL	\mathbf{F}	1708	-	-	2/4/4/4	-
8	GOL	Ε	2006	-	-	3/4/4/4	-
7	EDO	Е	2009	-	_	1/1/1/1	-
10	PG4	D	613	-	-	4/10/10/10	-
7	EDO	С	616	-	-	1/1/1/1	-
8	GOL	С	602	-	-	2/4/4/4	-
7	EDO	С	610	-	-	0/1/1/1	-
8	GOL	С	612	-	-	0/4/4/4	-
8	GOL	А	815	-	-	2/4/4/4	-
7	EDO	Η	608	-	-	1/1/1/1	-
7	EDO	В	601	-	-	1/1/1/1	-
7	EDO	D	615	-	-	1/1/1/1	-
8	GOL	А	821	-	-	4/4/4/4	-
8	GOL	А	822	-	-	2/4/4/4	-
6	PEG	А	801	-	-	$\frac{4}{4}/\frac{4}{4}$	-
7	EDO	Е	2010	-	-	1/1/1/1	-
7	EDO	А	809	-	-	0/1/1/1	-
6	PEG	А	802	_	_	2/4/4/4	-
7	EDO	F	1709	-	-	1/1/1/1	-
8	GOL	Е	2008	_	-	4/4/4/4	-
10	PG4	В	610	-	-	6/10/10/10	-
7	EDO	А	813	_	_	0/1/1/1	-
7	EDO	F	1713	-	-	1/1/1/1	-
7	EDO	D	605	-	-	0/1/1/1	-
7	EDO	F	1705	-	-	0/1/1/1	-
7	EDO	C	609	-	-	1/1/1/1	-
7	EDO	<u>H</u>	602	-	-	0/1/1/1	-
6	PEG	D	620	-	-	2/4/4/4	-
7	EDO	E	2003	-	_	1/1/1/1	-
7	EDO	F'	1704	-	-	$\frac{1/1/1/1}{0/1/1/1}$	-
7	EDO	A U	602	-	-	$\frac{U/1/1/1}{1/1/1}$	-
$\frac{1}{7}$	EDO	Π Δ	003 805	-	-	$\frac{1/1/1/1}{0/1/1/1}$	
1 8	GOL	 Н	601		-		
6		11	011		-	$\frac{1}{2}$	
0			011	-	-		-
6	PEG	В	611	-	-	$\frac{4}{4}/\frac{4}{4}$	-



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Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
7	EDO	Н	604	_	_	0/1/1/1	-
8	GOL	С	607		-	1/4/4/4	-
9	PGE	А	824	-	-	7/7/7/7	-
8	GOL	F	1716	_	-	2/4/4/4	-
7	EDO	D	618	-	-	0/1/1/1	-
8	GOL	D	604	-	-	4/4/4/4	-
6	PEG	С	606	-	-	3/4/4/4	-
6	PEG	D	614	-	-	2/4/4/4	-
8	GOL	А	818	-	-	2/4/4/4	-
8	GOL	Е	2005	-	-	2/4/4/4	-
7	EDO	G	601	-	-	1/1/1/1	-
7	EDO	В	603	-	_	0/1/1/1	-
7	EDO	F	1703	-	-	1/1/1/1	-
7	EDO	D	623	-	-	0/1/1/1	-
7	EDO	F	1701	-	-	1/1/1/1	-
7	EDO	В	606	-	-	0/1/1/1	-
7	EDO	F	1721	-	-	1/1/1/1	-
6	PEG	А	807	-	-	2/4/4/4	-
8	GOL	A	810	_	_	0/4/4/4	-
8	GOL	D	602	-	-	2/4/4/4	-
7	EDO	А	803	-	_	1/1/1/1	-
7	EDO	F	1711	-	-	0/1/1/1	-
7	EDO	Н	605	-	-	0/1/1/1	-
7	EDO	С	615	-	-	1/1/1/1	-
6	PEG	D	601	-	-	2/4/4/4	-
7	EDO	E	2011	-	-	1/1/1/1	-
9	PGE	А	814	-	-	5/7/7/7	-
9	PGE	С	617	-	_	4/7/7/7	-
7	EDO	D	624	_	_	1/1/1/1	-
6	PEG	Е	2007	-	-	2/4/4/4	-
7	EDO	В	614	-	-	1/1/1/1	-
7	EDO	D	619	-	-	0/1/1/1	-
8	GOL	А	820	-	-	0/4/4/4	-
8	GOL	F	1722	-	-	2/4/4/4	-
6	PEG	C	603	-	-	2/4/4/4	-
6	PEG	D	617	-	-	3/4/4/4	-
8	GOL	Е	2012	-	_	2/4/4/4	_
7	EDO	A	816	_	_	1/1/1/1	_



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	А	803	EDO	O2-C2-C1	-2.54	93.62	111.91

There are no chirality outliers.

5 of 178 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	1714	GOL	O1-C1-C2-O2
8	F	1714	GOL	O1-C1-C2-C3
8	Е	2004	GOL	O1-C1-C2-C3
8	С	618	GOL	C1-C2-C3-O3
8	D	609	GOL	O1-C1-C2-C3

There are no ring outliers.

49 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	С	611	EDO	1	0
7	В	608	EDO	6	0
6	А	825	PEG	1	0
8	F	1714	GOL	2	0
6	D	611	PEG	4	0
7	В	604	EDO	2	0
9	В	612	PGE	2	0
7	D	622	EDO	1	0
9	F	1718	PGE	5	0
7	F	1723	EDO	2	0
6	С	605	PEG	1	0
7	F	1719	EDO	5	0
7	А	804	EDO	5	0
7	D	608	EDO	1	0
8	G	605	GOL	1	0
7	В	609	EDO	7	0
7	F	1707	EDO	2	0
7	С	614	EDO	2	0
6	F	1712	PEG	2	0
7	D	612	EDO	5	0
10	D	613	PG4	3	0
7	С	610	EDO	1	0
8	С	612	GOL	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	В	601	EDO	3	0
6	А	801	PEG	2	0
7	Е	2010	EDO	2	0
7	А	809	EDO	2	0
6	А	802	PEG	3	0
10	В	610	PG4	3	0
7	F	1705	EDO	6	0
6	D	620	PEG	1	0
7	А	817	EDO	4	0
7	Н	603	EDO	3	0
7	А	805	EDO	10	0
8	Н	601	GOL	1	0
8	С	607	GOL	2	0
9	А	824	PGE	1	0
8	D	604	GOL	2	0
6	D	614	PEG	4	0
8	Е	2005	GOL	1	0
7	F	1721	EDO	2	0
8	D	602	GOL	3	0
6	D	601	PEG	1	0
9	A	814	PGE	1	0
9	С	617	PGE	1	0
6	Е	2007	PEG	3	0
6	С	603	PEG	3	0
8	Е	2012	GOL	1	0
7	A	816	EDO	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^{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	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	553/553~(100%)	0.14	15 (2%) 54 58	27, 53, 112, 173	0
1	C	553/553~(100%)	0.14	11 (1%) 65 68	35, 56, 118, 183	0
1	D	553/553~(100%)	0.11	11 (1%) 65 68	25, 55, 123, 163	0
1	F	553/553~(100%)	0.26	26 (4%) 31 33	27, 58, 128, 200	0
2	В	528/528~(100%)	0.32	25 (4%) 31 33	27, 54, 130, 173	0
3	Е	547/550~(99%)	0.53	59 (10%) 5 5	29, 60, 154, 199	0
4	G	508/527~(96%)	0.41	45 (8%) 9 9	35, 65, 144, 187	0
5	Н	550/553~(99%)	0.56	57 (10%) 6 6	39, 66, 165, 204	0
All	All	4345/4370 (99%)	0.31	249 (5%) 23 25	25, 58, 143, 204	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Н	35	VAL	17.3
2	В	16	GLY	12.0
3	Е	143	ALA	10.7
5	Н	198	GLY	10.6
2	В	521	ILE	10.0

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^{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	${f B}$ -factors(Å ²)	Q<0.9
7	EDO	С	615	4/4	0.60	0.26	76,79,79,80	4
6	PEG	А	811	7/7	0.60	0.33	59,71,82,83	7
12	CA	F	1724	1/1	0.61	0.13	86,86,86,86	0
8	GOL	А	820	6/6	0.62	0.32	66,81,84,84	0
7	EDO	С	616	4/4	0.65	0.27	67,71,77,78	0
7	EDO	А	812	4/4	0.67	0.28	76,81,82,87	0
10	PG4	D	613	13/13	0.68	0.39	$57,\!85,\!95,\!100$	13
7	EDO	Н	605	4/4	0.68	0.24	$56,\!61,\!65,\!66$	0
8	GOL	С	618	6/6	0.68	0.20	70,78,80,82	0
7	EDO	D	621	4/4	0.69	0.40	$54,\!55,\!63,\!64$	4
8	GOL	В	607	6/6	0.69	0.40	62,70,80,80	6
6	PEG	D	620	7/7	0.70	0.26	$60,\!66,\!69,\!69$	7
7	EDO	С	609	4/4	0.70	0.29	71,72,73,74	4
7	EDO	F	1702	4/4	0.71	0.23	78,88,92,94	0
7	EDO	В	616	4/4	0.72	0.41	$79,\!84,\!93,\!95$	0
6	PEG	С	606	7/7	0.72	0.27	59,70,77,79	7
9	PGE	А	824	10/10	0.73	0.36	$85,\!88,\!93,\!95$	0
7	EDO	В	613	4/4	0.73	0.33	78,88,92,96	0
6	PEG	А	807	7/7	0.73	0.43	$57,\!63,\!68,\!74$	7
8	GOL	А	810	6/6	0.73	0.29	79,82,88,88	0
7	EDO	Е	2009	4/4	0.73	0.29	67,75,77,80	4
7	EDO	Н	608	4/4	0.73	0.16	77,79,80,81	4
7	EDO	F	1720	4/4	0.74	0.40	72,76,83,87	0
7	EDO	В	603	4/4	0.74	0.49	$59,\!69,\!72,\!75$	0
10	PG4	В	610	13/13	0.74	0.24	73,84,88,90	13
7	EDO	С	604	4/4	0.75	0.22	$90,\!92,\!93,\!104$	4
7	EDO	F	1707	4/4	0.75	0.40	$63,\!65,\!68,\!72$	0
6	PEG	D	601	7/7	0.75	0.28	$81,\!85,\!97,\!99$	0
8	GOL	D	609	6/6	0.75	0.18	$82,\!91,\!97,\!100$	0
7	EDO	Е	2002	4/4	0.76	0.22	$63,\!68,\!68,\!72$	4
7	EDO	С	610	4/4	0.76	0.37	72,73,78,80	0
9	PGE	F	1718	10/10	0.76	0.34	63,78,80,84	10
8	GOL	D	610	6/6	0.76	0.33	$60,\!68,\!77,\!78$	6
7	EDO	D	618	4/4	0.76	0.27	79,86,88,90	0
7	EDO	D	624	4/4	0.76	0.25	66,78,79,82	4
7	EDO	A	813	4/4	0.76	0.72	72,74,74,79	4
6	PEG	A	801	7/7	0.77	0.21	61,69,71,76	7



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
7	EDO	С	611	4/4	0.78	0.21	74,85,91,95	0
7	EDO	F	1701	4/4	0.78	0.26	94,97,104,109	0
6	PEG	D	614	7/7	0.78	0.37	75,80,89,92	7
8	GOL	Е	2005	6/6	0.78	0.35	61,71,75,77	0
7	EDO	В	601	4/4	0.79	0.41	50,54,59,66	0
6	PEG	D	611	7/7	0.80	0.42	72,77,85,89	7
8	GOL	Н	606	6/6	0.80	0.25	71,75,85,89	0
7	EDO	В	617	4/4	0.80	0.29	60,70,72,73	4
8	GOL	С	612	6/6	0.80	0.21	$53,\!61,\!62,\!66$	6
7	EDO	А	819	4/4	0.80	0.24	$53,\!53,\!61,\!61$	4
7	EDO	А	804	4/4	0.81	0.40	64,74,76,76	0
7	EDO	D	606	4/4	0.81	0.65	67, 75, 76, 85	0
7	EDO	D	619	4/4	0.81	0.47	69,79,80,81	0
6	PEG	С	605	7/7	0.81	0.19	$56,\!64,\!71,\!71$	7
7	EDO	С	613	4/4	0.82	0.15	64,73,74,78	4
7	EDO	D	623	4/4	0.82	0.29	$64,\!65,\!66,\!67$	4
7	EDO	Н	607	4/4	0.82	0.81	79,81,84,87	0
6	PEG	Е	2001	7/7	0.82	0.21	74,85,93,93	0
7	EDO	F	1713	4/4	0.82	0.18	71,77,84,92	0
7	EDO	Е	2010	4/4	0.83	0.21	$67,\!68,\!71,\!71$	4
7	EDO	В	605	4/4	0.83	0.20	77, 78, 82, 85	0
6	PEG	D	617	7/7	0.83	0.50	82,84,93,94	0
7	EDO	F	1704	4/4	0.84	0.23	$61,\!63,\!66,\!66$	4
7	EDO	А	808	4/4	0.85	0.34	77, 77, 86, 88	0
7	EDO	Ε	2003	4/4	0.85	0.15	$96,\!96,\!103,\!103$	0
7	EDO	В	604	4/4	0.85	0.50	$91,\!92,\!94,\!102$	0
7	EDO	F	1719	4/4	0.85	0.40	$80,\!81,\!81,\!83$	4
6	PEG	F	1712	7/7	0.86	0.22	58,77,83,87	7
8	GOL	D	602	6/6	0.86	0.29	78,85,87,92	0
7	EDO	В	615	4/4	0.86	0.18	78,82,82,89	0
8	GOL	H	601	6/6	0.86	0.13	62,70,73,74	0
8	GOL	A	821	6/6	0.86	0.25	69,86,92,93	0
6	PEG	E	2007	7/7	0.86	0.39	55,72,76,76	0
6	PEG	В	611	7/7	0.86	0.29	65,77,81,86	0
8	GOL	F	1708	6/6	0.86	0.25	74,80,81,86	0
7	EDO	F	1715	4/4	0.86	0.12	73,78,81,82	0
6	PEG	A	802	7/7	0.87	0.28	75,86,92,93	0
7	EDO	D	615	4/4	0.87	0.26	68,72,80,82	0
9	PGE	В	612	10/10	0.87	0.29	58,72,77,79	0
7	EDO	E	2011	4/4	0.87	0.14	59,68,73,76	0
9	PGE	С	617	10/10	0.87	0.16	56,68,74,78	10
8	GOL	A	822	6/6	0.87	0.17	78,81,87,88	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
7	EDO	D	605	4/4	0.87	0.23	$55,\!69,\!70,\!79$	0
7	EDO	В	614	4/4	0.87	0.24	$76,\!91,\!91,\!96$	0
7	EDO	С	614	4/4	0.87	0.22	$76,\!82,\!83,\!88$	0
8	GOL	F	1716	6/6	0.87	0.24	72,82,84,86	0
7	EDO	G	604	4/4	0.87	0.25	$64,\!65,\!75,\!75$	0
9	PGE	А	814	10/10	0.88	0.21	56,73,82,83	10
7	EDO	F	1706	4/4	0.88	0.23	$57,\!63,\!70,\!72$	0
7	EDO	С	608	4/4	0.88	0.17	$51,\!53,\!58,\!61$	4
8	GOL	F	1722	6/6	0.88	0.27	$67,\!90,\!92,\!96$	0
7	EDO	F	1723	4/4	0.88	0.41	$76,\!80,\!80,\!81$	0
7	EDO	А	816	4/4	0.88	0.42	64,73,73,77	0
7	EDO	F	1717	4/4	0.89	0.24	$61,\!69,\!71,\!73$	4
8	GOL	Е	2012	6/6	0.89	0.39	$66,\!69,\!73,\!76$	0
8	GOL	А	818	6/6	0.89	0.17	54,61,67,69	0
7	EDO	F	1721	4/4	0.90	0.17	75,78,80,87	0
7	EDO	F	1709	4/4	0.90	0.17	$55,\!64,\!66,\!68$	0
7	EDO	F	1705	4/4	0.90	0.59	52, 59, 59, 64	0
8	GOL	Е	2008	6/6	0.90	0.37	62,73,76,77	0
7	EDO	Н	604	4/4	0.90	0.23	82,92,93,95	0
7	EDO	D	616	4/4	0.90	0.46	67,68,73,74	0
8	GOL	Е	2006	6/6	0.90	0.15	90, 94, 96, 103	0
7	EDO	D	622	4/4	0.90	0.21	$62,\!69,\!70,\!72$	0
7	EDO	В	606	4/4	0.90	0.40	66,70,82,86	0
7	EDO	D	607	4/4	0.91	0.13	70,71,72,74	0
8	GOL	Е	2004	6/6	0.91	0.27	$75,\!85,\!91,\!93$	0
8	GOL	С	607	6/6	0.91	0.30	$53,\!67,\!71,\!75$	0
7	EDO	F	1703	4/4	0.91	0.19	88,90,90,91	0
7	EDO	А	809	4/4	0.91	0.22	68,77,90,94	0
7	EDO	D	612	4/4	0.92	0.51	58,62,66,72	0
7	EDO	В	602	4/4	0.92	0.23	71,71,78,82	0
7	EDO	Н	603	4/4	0.92	0.44	68,70,73,74	0
7	EDO	А	806	4/4	0.92	0.16	$64,\!65,\!70,\!71$	0
6	PEG	С	603	7/7	0.92	0.30	66,79,88,90	0
7	EDO	Н	602	4/4	0.92	0.11	$63,\!68,\!73,\!75$	0
7	EDO	F	1710	4/4	0.92	0.33	37,40,45,63	0
7	EDO	А	803	4/4	0.92	0.19	43,45,48,49	0
8	GOL	D	604	6/6	0.93	0.28	$76,\!89,\!92,\!92$	0
8	GOL	А	815	6/6	0.93	0.16	52, 56, 59, 64	0
7	EDO	F	1711	4/4	0.93	0.09	67,71,72,75	0
8	GOL	G	605	6/6	0.93	0.12	$60,\!69,\!69,\!71$	0
7	EDO	В	608	4/4	0.93	0.42	$66,\!67,\!69,\!71$	0
8	GOL	С	602	6/6	0.93	0.28	58,70,73,73	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors ($Å^2$)	Q<0.9
7	EDO	A	823	4/4	0.93	0.15	64,65,69,69	0
7	EDO	G	601	4/4	0.93	0.12	60,61,62,63	0
7	EDO	G	603	4/4	0.93	0.32	$66,\!83,\!85,\!86$	0
7	EDO	G	602	4/4	0.94	0.14	71,73,73,75	0
8	GOL	F	1714	6/6	0.94	0.17	$61,\!66,\!68,\!70$	0
7	EDO	D	608	4/4	0.94	0.25	$53,\!64,\!65,\!69$	0
7	EDO	D	603	4/4	0.94	0.15	77,80,81,84	0
7	EDO	С	601	4/4	0.96	0.11	62,62,63,64	0
7	EDO	А	817	4/4	0.96	0.30	$33,\!49,\!50,\!57$	0
11	CL	D	625	1/1	0.96	0.13	$62,\!62,\!62,\!62$	0
11	CL	С	619	1/1	0.97	0.14	58, 58, 58, 58, 58	0
12	CA	D	626	1/1	0.97	0.17	55, 55, 55, 55	0
7	EDO	А	805	4/4	0.97	0.33	$40,\!41,\!44,\!47$	0
6	PEG	A	825	7/7	0.97	0.28	56, 58, 63, 68	0
7	EDO	В	609	4/4	0.97	0.41	52, 52, 55, 58	0

6.5 Other polymers (i)

There are no such residues in this entry.

