

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 11, 2023 – 06:19 AM EDT

PDB ID	:	7L9E
Title	:	Crystal structure of apo-alpha glucosidase
Authors	:	Karade, S.S.; Mariuzza, R.A.
Deposited on	:	2021-01-03
Resolution	:	2.29 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

# 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 2.29 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R <sub>free</sub>	130704	5042 (2.30-2.30)		
Clashscore	141614	5643 (2.30-2.30)		
Ramachandran outliers	138981	5575(2.30-2.30)		
Sidechain outliers	138945	5575(2.30-2.30)		
RSRZ outliers	127900	4938 (2.30-2.30)		

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	Е	184	% 71%	8%	•	18%					
1	G	184	68%	15%		17%					
2	F	107	5% 86%			12% •					
2	Н	107	89%			11%					
3	А	609	.% <b>8</b> 9%			8% •					



Mol	Chain	Length	Quality of chain							
3	С	609	2%	90%			8%	·		
	D	104	15%				0,0	_		
4	В	134	10%	61%	•	37%				
4	D	134		58%	••	37%				

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
7	PG4	А	1009	-	-	-	Х



## 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15764 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	Atoms					ZeroOcc	AltConf	Trace
1	F	150	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
		150	1189	748	215	222	4	0	L	0
1	С	152	Total	С	Ν	0	S	0	0	0
	G	199	1183 741 219 219 4 0		0	U				

• Molecule 1 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1.

Chain	Residue	Modelled	Actual	Comment	Reference
Е	2	MET	-	initiating methionine	UNP Q8BHN3
Е	3	GLY	-	expression tag	UNP Q8BHN3
Е	4	ILE	-	expression tag	UNP Q8BHN3
Е	5	LEU	-	expression tag	UNP Q8BHN3
Е	6	PRO	-	expression tag	UNP Q8BHN3
E	7	SER	-	expression tag	UNP Q8BHN3
Е	8	PRO	-	expression tag	UNP Q8BHN3
Е	9	GLY	-	expression tag	UNP Q8BHN3
E	10	MET	-	expression tag	UNP Q8BHN3
E	11	PRO	-	expression tag	UNP Q8BHN3
E	12	ALA	-	expression tag	UNP Q8BHN3
Е	13	LEU	-	expression tag	UNP Q8BHN3
Е	14	LEU	-	expression tag	UNP Q8BHN3
Е	15	SER	-	expression tag	UNP Q8BHN3
Е	16	LEU	-	expression tag	UNP Q8BHN3
E	17	VAL	-	expression tag	UNP Q8BHN3
Е	18	SER	-	expression tag	UNP Q8BHN3
E	19	LEU	-	expression tag	UNP Q8BHN3
Е	20	LEU	-	expression tag	UNP Q8BHN3
Е	21	SER	-	expression tag	UNP Q8BHN3
Е	22	VAL	-	expression tag	UNP Q8BHN3
Е	23	LEU	-	expression tag	UNP Q8BHN3
Е	24	LEU	-	expression tag	UNP Q8BHN3
Е	25	MET	-	expression tag	UNP Q8BHN3
Е	26	GLY	-	expression tag	UNP Q8BHN3

There are 64 discrepancies between the modelled and reference sequences:



Chain Е Е Е Е Е Е Е G G G G G G G G G G G G G G G G G G G G G G G G G G

G

G

G

G

G

G

28

29

30

31

32

97

J	Figure Post			
Residue	Modelled	Actual	Comment	Reference
27	CYS	_	expression tag	UNP Q8BHN3
28	VAL	-	expression tag	UNP Q8BHN3
29	ALA	-	expression tag	UNP Q8BHN3
30	GLU	-	expression tag	UNP Q8BHN3
31	THR	_	expression tag	UNP Q8BHN3
32	GLY	-	expression tag	UNP Q8BHN3
97	ASP	ASN	engineered mutation	UNP Q8BHN3
2	MET	-	initiating methionine	UNP Q8BHN3
3	GLY	-	expression tag	UNP Q8BHN3
4	ILE	_	expression tag	UNP Q8BHN3
5	LEU	-	expression tag	UNP Q8BHN3
6	PRO	-	expression tag	UNP Q8BHN3
7	SER	-	expression tag	UNP Q8BHN3
8	PRO	-	expression tag	UNP Q8BHN3
9	GLY	-	expression tag	UNP Q8BHN3
10	MET	-	expression tag	UNP Q8BHN3
11	PRO	-	expression tag	UNP Q8BHN3
12	ALA	-	expression tag	UNP Q8BHN3
13	LEU	-	expression tag	UNP Q8BHN3
14	LEU	-	expression tag	UNP Q8BHN3
15	SER	-	expression tag	UNP Q8BHN3
16	LEU	-	expression tag	UNP Q8BHN3
17	VAL	-	expression tag	UNP Q8BHN3
18	SER	-	expression tag	UNP Q8BHN3
19	LEU	-	expression tag	UNP Q8BHN3
20	LEU	-	expression tag	UNP Q8BHN3
21	SER	-	expression tag	UNP Q8BHN3
22	VAL	-	expression tag	UNP Q8BHN3
23	LEU	-	expression tag	UNP Q8BHN3
24	LEU	-	expression tag	UNP Q8BHN3
25	MET	-	expression tag	UNP Q8BHN3
26	GLY	-	expression tag	UNP Q8BHN3
27	CYS	-	expression tag	UNP Q8BHN3

Continued from previous page.

• Molecule 2 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2.

expression tag

expression tag

expression tag

expression tag

expression tag

engineered mutation

UNP Q8BHN3

UNP Q8BHN3

UNP Q8BHN3

UNP Q8BHN3

UNP Q8BHN3

UNP Q8BHN3

-

-

-

-

-

ASN

VAL

ALA

 $\operatorname{GLU}$ 

THR

GLY

ASP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	105	Total	С	Ν	0	S	0	0	0
	2 Г	105	828	535	135	156	2	0		
0	п	107	Total	С	Ν	0	S	0	0	0
	11	107	835	538	138	157	2			U

• Molecule 3 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Δ	507	Total	С	Ν	0	$\mathbf{S}$	0	6	0
5	3 A	091	4858	3125	836	875	22	0	0	0
9	C	507	Total	С	Ν	0	S	0	6	0
0	3 C	097	4848	3120	834	872	22			U

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	967	SER	-	expression tag	UNP Q8BHN3
А	968	ALA	-	expression tag	UNP Q8BHN3
А	969	TRP	-	expression tag	UNP Q8BHN3
А	970	SER	-	expression tag	UNP Q8BHN3
А	971	HIS	-	expression tag	UNP Q8BHN3
А	972	PRO	-	expression tag	UNP Q8BHN3
А	973	GLN	-	expression tag	UNP Q8BHN3
А	974	PHE	-	expression tag	UNP Q8BHN3
А	975	GLU	-	expression tag	UNP Q8BHN3
А	976	LYS	-	expression tag	UNP Q8BHN3
А	977	LEU	-	expression tag	UNP Q8BHN3
А	978	GLU	-	expression tag	UNP Q8BHN3
С	967	SER	-	expression tag	UNP Q8BHN3
С	968	ALA	-	expression tag	UNP Q8BHN3
С	969	TRP	-	expression tag	UNP Q8BHN3
С	970	SER	-	expression tag	UNP Q8BHN3
С	971	HIS	-	expression tag	UNP Q8BHN3
С	972	PRO	-	expression tag	UNP Q8BHN3
С	973	GLN	-	expression tag	UNP Q8BHN3
С	974	PHE	-	expression tag	UNP Q8BHN3
С	975	GLU	-	expression tag	UNP Q8BHN3
С	976	LYS	-	expression tag	UNP Q8BHN3
С	977	LEU	-	expression tag	UNP Q8BHN3
C	978	GLU	-	expression tag	UNP Q8BHN3

• Molecule 4 is a protein called Glucosidase 2 subunit beta.



Mol	Chain	Residues		At	toms			ZeroOcc	AltConf	Trace
4	В	85	Total	С	Ν	0	$\mathbf{S}$	0	0	0
4	D	00	603	356	101	136	10	0	AltConf00	0
4	а	84	Total	С	Ν	0	S	0	0	0
4	D	04	595	352	96	137	10	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-16	MET	-	initiating methionine	UNP 008795
В	-15	GLY	-	expression tag	UNP 008795
В	-14	ILE	-	expression tag	UNP 008795
В	-13	LEU	-	expression tag	UNP 008795
В	-12	PRO	-	expression tag	UNP 008795
В	-11	SER	-	expression tag	UNP 008795
В	-10	PRO	-	expression tag	UNP 008795
В	-9	GLY	-	expression tag	UNP 008795
В	-8	MET	-	expression tag	UNP 008795
В	-7	PRO	-	expression tag	UNP 008795
В	-6	ALA	-	expression tag	UNP 008795
В	-5	LEU	-	expression tag	UNP 008795
В	-4	LEU	-	expression tag	UNP 008795
В	-3	SER	-	expression tag	UNP 008795
В	-2	LEU	-	expression tag	UNP 008795
В	-1	VAL	-	expression tag	UNP 008795
В	0	SER	-	expression tag	UNP 008795
В	1	LEU	-	expression tag	UNP 008795
В	2	LEU	-	expression tag	UNP 008795
В	3	SER	-	expression tag	UNP 008795
В	4	VAL	-	expression tag	UNP 008795
В	5	LEU	-	expression tag	UNP 008795
В	6	LEU	-	expression tag	UNP 008795
В	7	MET	-	expression tag	UNP 008795
В	8	GLY	-	expression tag	UNP 008795
В	9	CYS	-	expression tag	UNP 008795
В	10	VAL	-	expression tag	UNP 008795
В	11	ALA	-	expression tag	UNP 008795
В	12	GLU	-	expression tag	UNP 008795
В	13	THR	-	expression tag	UNP 008795
В	14	GLY	-	expression tag	UNP 008795
D	-16	MET	-	initiating methionine	UNP 008795
D	-15	GLY	-	expression tag	UNP 008795
D	-14	ILE	-	expression tag	UNP 008795
D	-13	LEU	-	expression tag	UNP 008795



Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP 008795
D	-11	SER	-	expression tag	UNP 008795
D	-10	PRO	-	expression tag	UNP 008795
D	-9	GLY	-	expression tag	UNP 008795
D	-8	MET	-	expression tag	UNP 008795
D	-7	PRO	-	expression tag	UNP 008795
D	-6	ALA	-	expression tag	UNP 008795
D	-5	LEU	-	expression tag	UNP 008795
D	-4	LEU	-	expression tag	UNP 008795
D	-3	SER	-	expression tag	UNP 008795
D	-2	LEU	-	expression tag	UNP 008795
D	-1	VAL	-	expression tag	UNP 008795
D	0	SER	-	expression tag	UNP 008795
D	1	LEU	-	expression tag	UNP 008795
D	2	LEU	-	expression tag	UNP 008795
D	3	SER	-	expression tag	UNP 008795
D	4	VAL	-	expression tag	UNP 008795
D	5	LEU	-	expression tag	UNP 008795
D	6	LEU	-	expression tag	UNP 008795
D	7	MET	-	expression tag	UNP 008795
D	8	GLY	-	expression tag	UNP 008795
D	9	CYS	-	expression tag	UNP 008795
D	10	VAL	-	expression tag	UNP 008795
D	11	ALA	-	expression tag	UNP 008795
D	12	GLU	-	expression tag	UNP 008795
D	13	THR	-	expression tag	UNP 008795
D	14	GLY	-	expression tag	UNP 008795

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	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
5	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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



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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
6	А	1	Total 7	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	O 3	0	0

• Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total         C         O           13         8         5	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
8	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	2	Total Ca 2 2	0	0
9	D	2	Total Ca 2 2	0	0

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	Е	61	Total O 61 61	0	0
10	F	45	$\begin{array}{cc} \text{Total} & \text{O} \\ 45 & 45 \end{array}$	0	0
10	А	249	Total         O           249         249	0	0
10	В	25	TotalO2525	0	0
10	G	24	TotalO2424	0	0
10	Н	31	Total O 31 31	0	0
10	С	223	Total         O           223         223	0	0
10	D	22	TotalO2222	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: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1





• Molecule 3:	Neutral alpha-glucosidase AB 'I	Typsin-cleaved Fragment $#3$	· · · · · · · · · · · · · · · · · · ·
Chain A:	89%	8% •	
1370 1387 1423 1424 1432 1432 1432	V447 R469 Y460 D490 D496 D496 R464 R464 R500 V501 V501 V501 V501 V501 V501 V501 V	R588 W542 W562 W562 F568 F568 F568 F568 F568 F568 F568 F569 F560 F600 F600 F601 F600 F611	L622
6634 6635 V635 635 633 633 633 633 644 1650	L658 F665 F665 F01 L701 R706 F732 Q754 Q754 Q754 D772 H777	F195 F196 F196 F196 F195 F12 F12 F12 F12 F12 F12 F12 F12 F12 F12	ALA TRP SER HIS PRO GLN
PHE GLU GLU GLU GLU			
• Molecule 3:	Neutral alpha-glucosidase AB T	Trypsin-cleaved Fragment #3	5
Chain C:	90%	8%	- -
1370 ● 1374 1387 1428 1428 1428	D435 M442 M442 D446 V447 V447 V447 V486 D496 R540 K540 K540 K560	P574 P574 M578 M578 L579 L579 L579 L579 L578 A624 A635 R624 A635 R624 A635 R636 C639	L665 F665 F665
L701 R706 L711 Q714 D721	Hr 85 (7) 94 (7) 94 (7) 94 (7) 94 (7) 94 (7) 94 (7) 94 (7) 96 (7) 96 (7) 96 (7) 96 (7) 96 (7) 96 (7) 96 (7) 96 (7) 96 (7) 94 (7) 96 (7) 94 (7) 96 (7)	R886 L905 L905 M910 M910 B911 E912 SER A1A A1A A1A A1A A1A A1A A1A A1A A1A A1	GLU LEU
• Molecule 4:	Glucosidase 2 subunit beta		
Chain B:	5% 61%	• 37%	-
MET GLY ILE LEU PRO SER SER GLY MET PRO	LEU LEU SER LEU LEU LEU VAL LEU VAL LEU LEU LEU LEU LEU CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	LYN LYN ARG ARG ARG ARD ARU VAL SER ASR HIS HIS HIS HIS HIS F33 534 453 534 138 534	C39 L40 D41 G42 A44 A44
T45 C77 T78 N79 T80 C81 Y82 Y82 Y88	C100 V111 C112 C112 C116 R117		
• Molecule 4:	Glucosidase 2 subunit beta		
Chain D:	58%	•• 37%	-
MET GLY ILE ILE PRO SER PRO GLY MET PRO	ALA LEU LEU SER SER LEU VAL LEU LEU LEU LEU LEU VAL CYS GLU VAL CYS GLU VAL CYS GLU VAL CYS GLU VAL	LYNS LYNS ARG ARG ARG ARA ARA ARA ARA ASR ASR ASR ASR ASR ASR	C39 L40 D41 G42 T43 A44
145 146 050 061 C70 H76	C/7 T/78 178 180 681 783 783 784 184 184 184 184 184 115 8117		





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	102.97Å 102.97Å 240.60Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	47.33 - 2.29	Depositor
Resolution (A)	49.87 - 2.29	EDS
% Data completeness	99.8 (47.33-2.29)	Depositor
(in resolution range)	96.3(49.87-2.29)	EDS
R <sub>merge</sub>	0.12	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.73 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
B B.	0.180 , $0.206$	Depositor
It, It <sub>free</sub>	0.180 , $0.206$	DCC
$R_{free}$ test set	2019 reflections $(1.57%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.3	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.34 , $46.3$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.32$	Xtriage
	0.004 for -h,-k,l	
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
	0.020 for -k,-h,-l	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms $(Å^2)$	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: PEG, PG4, EDO, SO4, CA

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		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Е	0.25	0/1211	0.49	0/1643	
1	G	0.24	0/1203	0.52	2/1636~(0.1%)	
2	F	0.25	0/856	0.48	0/1171	
2	Н	0.25	0/863	0.47	0/1181	
3	А	0.26	0/5039	0.46	0/6865	
3	С	0.26	0/5029	0.46	0/6852	
4	В	0.26	0/614	0.51	0/840	
4	D	0.26	0/606	0.51	0/831	
All	All	0.25	0/15421	0.47	2/21019~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	35	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	G	97	ASP	CB-CG-OD2	5.24	123.02	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	Е	1189	0	1215	15	1



7	L9E
(]	L9E

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1183	0	1172	17	1
2	F	828	0	765	11	0
2	Н	835	0	777	11	0
3	А	4858	0	4624	37	0
3	С	4848	0	4615	26	0
4	В	603	0	493	1	0
4	D	595	0	482	3	0
5	А	36	0	52	10	0
5	В	4	0	6	0	0
5	С	32	0	48	3	0
5	Е	12	0	18	0	0
5	F	4	0	6	1	0
5	G	4	0	6	1	0
6	А	21	0	30	1	0
7	А	13	0	18	0	0
8	А	10	0	0	1	0
8	С	5	0	0	0	0
9	В	2	0	0	0	0
9	D	2	0	0	0	0
10	А	249	0	0	6	0
10	В	25	0	0	0	0
10	С	223	0	0	7	0
10	D	22	0	0	1	0
10	Е	61	0	0	5	0
10	F	45	0	0	1	0
10	G	24	0	0	6	0
10	Н	31	0	0	1	0
All	All	15764	0	14327	110	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.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:A:1006:EDO:O1	10:A:1101:HOH:O	1.92	0.87
3:A:796:GLU:OE1	10:A:1102:HOH:O	1.93	0.86
3:C:721:ASP:OD1	10:C:1101:HOH:O	1.98	0.82
1:G:110:ARG:NH2	10:G:304:HOH:O	2.16	0.79
1:E:60:TYR:OH	10:E:301:HOH:O	2.02	0.78
1:G:60:TYR:OH	10:G:301:HOH:O	2.01	0.77



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:C:1007:EDO:O1	10:C:1102:HOH:O	2.02	0.76	
3:A:795:GLU:OE1	10:A:1103:HOH:O	2.05	0.74	
2:H:291:LYS:NZ	2:H:312:ASN:OD1	2.21	0.74	
3:A:739:GLN:HG2	5:A:1007:EDO:H22	1.71	0.73	
3:A:772:ASP:OD1	10:A:1104:HOH:O	2.08	0.72	
4:D:76:HIS:O	10:D:701:HOH:O	2.07	0.72	
1:E:167:LEU:O	10:E:302:HOH:O	2.09	0.71	
1:G:72:ASP:O	10:G:302:HOH:O	2.09	0.70	
2:H:269:ASP:OD2	10:H:401:HOH:O	2.09	0.69	
1:G:142:VAL:O	10:G:303:HOH:O	2.11	0.68	
3:C:496:ASP:OD2	10:C:1103:HOH:O	2.11	0.68	
2:F:278:VAL:HG22	5:F:401:EDO:H21	1.76	0.67	
1:E:159:ASP:OD2	10:E:304:HOH:O	2.14	0.66	
3:A:538:ARG:HG2	5:A:1010:EDO:H11	1.79	0.64	
1:E:148:LYS:NZ	1:E:163:ASP:O	2.28	0.64	
3:C:540:ARG:HH12	5:C:1007:EDO:H11	1.61	0.64	
3:A:572:ASN:HD22	3:A:572:ASN:H	1.46	0.63	
3:C:426:ARG:NE	10:C:1104:HOH:O	2.18	0.62	
5:G:201:EDO:H22	2:H:257:ASP:HB2	1.83	0.61	
1:G:112:ARG:NH2	1:G:179:GLU:O	2.35	0.60	
2:F:250:GLU:OE1	2:F:259:LYS:NZ	2.35	0.58	
3:C:477[A]:HIS:HE1	10:C:1105:HOH:O	1.86	0.58	
3:C:793:GLY:HA3	3:C:796:GLU:HG3	1.85	0.58	
1:E:35:ARG:NH2	2:F:307:PHE:O	2.33	0.57	
3:C:423:TRP:O	3:C:701:LEU:HA	2.05	0.56	
3:A:542:TRP:CE2	5:A:1011:EDO:H21	2.40	0.56	
1:E:129:SER:HB2	10:E:312:HOH:O	2.05	0.56	
1:G:61:ARG:NE	1:G:81:GLU:OE1	2.36	0.56	
1:E:112:ARG:NH2	1:E:179:GLU:O	2.38	0.55	
3:A:929:THR:HG23	3:A:932:SER:HB2	1.87	0.55	
4:B:82:TYR:HB2	4:B:116:CYS:HB3	1.87	0.55	
1:E:133[B]:ARG:HD3	1:E:138:VAL:HG22	1.87	0.55	
3:A:423:TRP:O	3:A:701:LEU:HA	2.06	0.55	
3:A:607[B]:ASP:OD1	3:A:611:GLN:NE2	2.42	0.53	
2:H:298:PRO:HG2	2:H:344:TRP:HE3	1.74	0.52	
2:H:298:PRO:HG2	2:H:344:TRP:CE3	2.45	0.52	
3:C:794:GLN:HA	3:C:810:PRO:HD3	1.92	0.50	
4:D:46:ILE:HG13	4:D:50:GLN:HB2	1.92	0.50	
3:A:572:ASN:HD22	3:A:572:ASN:N	2.10	0.49	
3:C:435:ASP:OD2	10:C:1105:HOH:O	2.20	0.49	
1:G:74:LEU:HD13	1:G:140:LEU:HD11	1.94	0.49	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:113:TYR:OH	10:G:305:HOH:O	2.19	0.49
3:A:447:VAL:HG11	3:A:486:VAL:HG23	1.94	0.49
1:G:67:LEU:HD11	1:G:74:LEU:HD11	1.94	0.49
1:E:158:LEU:HB2	1:E:170:VAL:HB	1.94	0.49
8:A:1015:SO4:O3	3:C:426:ARG:NH1	2.46	0.49
1:E:171:ASN:HA	2:F:269:ASP:OD1	2.13	0.48
2:H:318:TYR:CE2	3:C:639:GLY:HA3	2.49	0.48
3:C:447:VAL:HG11	3:C:486:VAL:HG23	1.96	0.48
3:A:644:GLU:OE1	10:A:1105:HOH:O	2.20	0.48
3:C:442:ASN:OD1	5:C:1006:EDO:H11	2.14	0.47
3:A:501:VAL:O	3:A:505:LEU:HG	2.13	0.47
3:A:849:PRO:HB2	3:A:912:GLU:HB3	1.97	0.47
2:F:297:GLU:OE2	10:F:501:HOH:O	2.20	0.47
2:H:336:PHE:HB3	3:C:387:PHE:HB2	1.96	0.47
3:C:849:PRO:HB2	3:C:912:GLU:HB3	1.96	0.47
2:F:278:VAL:HG23	2:F:290:LEU:HB2	1.97	0.47
1:G:134:ASP:OD1	1:G:137:SER:N	2.48	0.47
1:G:147:TYR:OH	2:H:331:ARG:NH2	2.48	0.46
3:A:732:PHE:CD1	5:A:1006:EDO:H21	2.50	0.46
1:E:67:LEU:HD21	1:E:74:LEU:HD11	1.98	0.46
3:A:459:ARG:NH1	3:A:494:LYS:HE2	2.31	0.46
3:A:858:PRO:HA	5:A:1003:EDO:H12	1.98	0.46
3:A:567:GLU:N	3:A:568:PRO:HA	2.31	0.45
1:E:113:TYR:CZ	3:A:593:ILE:HG22	2.51	0.45
3:A:767:GLN:HG3	3:A:777:HIS:ND1	2.32	0.45
1:G:51:ARG:CZ	2:H:298:PRO:HD3	2.46	0.45
2:F:320:SER:O	3:A:627:PHE:HA	2.18	0.44
3:A:534:PHE:HB3	3:A:600:TYR:HB3	1.99	0.44
2:H:276:GLU:O	2:H:289:ARG:NH2	2.44	0.44
3:C:567:GLU:N	3:C:568:PRO:HA	2.32	0.44
3:C:910:TRP:CE3	3:C:954:GLY:HA2	2.53	0.44
3:C:706:ARG:O	10:C:1106:HOH:O	2.21	0.43
3:A:460:TYR:CE2	3:A:490:ASP:HB2	2.54	0.43
3:A:754:GLN:HB3	10:A:1122:HOH:O	2.19	0.43
3:A:960:ASP:HB3	5:A:1001:EDO:H12	2.01	0.43
3:C:512:VAL:HG11	3:C:578:MET:SD	2.59	0.43
3:A:520:TYR:HE2	3:A:579:LEU:HD12	1.82	0.43
3:A:732:PHE:CE1	5:A:1006:EDO:H21	2.54	0.43
3:C:574:PRO:HG3	3:C:579:LEU:HD23	2.00	0.43
3:A:633:PHE:CE1	5:A:1008:EDO:H21	2.54	0.43
3:C:535:THR:HG21	3:C:593:ILE:HD13	2.01	0.43



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
3:C:865:GLU:OE2	3:C:886:ARG:NH2	2.52	0.43	
3:A:633:PHE:HE1	5:A:1008:EDO:H21	1.84	0.42	
2:F:318:TYR:CE2	3:A:639:GLY:HA3	2.54	0.42	
4:D:61:GLY:HA2	4:D:70:CYS:SG	2.59	0.42	
1:G:72:ASP:O	1:G:92:GLN:HG2	2.20	0.42	
2:F:336:PHE:HB3	3:A:387:PHE:HB2	2.00	0.42	
1:G:66:THR:HG21	1:G:77:HIS:HB2	2.01	0.42	
1:E:148:LYS:HZ2	1:E:148:LYS:HB2	1.84	0.42	
3:A:432:LEU:HD22	3:A:477[A]:HIS:ND1	2.34	0.41	
1:G:154:GLN:HA	1:G:155:PRO:HA	1.95	0.41	
2:F:311:LEU:HD22	3:A:650:ILE:HD13	2.03	0.41	
3:C:486:VAL:HG22	3:C:560:TYR:HB2	2.03	0.41	
3:A:460:TYR:CZ	3:A:490:ASP:HB2	2.55	0.41	
2:H:350:ASN:ND2	3:C:374:ASP:OD2	2.54	0.41	
1:G:142:VAL:HB	10:G:303:HOH:O	2.20	0.41	
3:C:883:LEU:HG	3:C:905:LEU:HB3	2.03	0.41	
1:E:35:ARG:HG2	2:F:315:MET:SD	2.62	0.41	
3:A:572:ASN:H	3:A:572:ASN:ND2	2.16	0.41	
1:G:158:LEU:HB2	1:G:170:VAL:HB	2.04	0.40	
3:C:679:PRO:HB3	3:C:711:LEU:HD23	2.01	0.40	
1:E:133[B]:ARG:HD2	10:E:306:HOH:O	2.21	0.40	
3:A:902:LYS:HD2	6:A:1005:PEG:O4	2.22	0.40	

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)	
1:E:72:ASP:OD1	1:G:110:ARG:NH1[3_565]	2.18	0.02	

#### 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	Ε	149/184~(81%)	143~(96%)	6 (4%)	0	100 100
1	G	151/184~(82%)	147~(97%)	4 (3%)	0	100 100
2	F	103/107~(96%)	97~(94%)	6~(6%)	0	100 100
2	Н	105/107~(98%)	99~(94%)	6~(6%)	0	100 100
3	А	601/609~(99%)	590~(98%)	11 (2%)	0	100 100
3	С	601/609~(99%)	589~(98%)	12 (2%)	0	100 100
4	В	83/134~(62%)	82~(99%)	1 (1%)	0	100 100
4	D	82/134~(61%)	79~(96%)	3 (4%)	0	100 100
All	All	1875/2068~(91%)	1826 (97%)	49 (3%)	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	Ε	134/163~(82%)	128~(96%)	6 (4%)	27 39
1	G	126/163~(77%)	123~(98%)	3~(2%)	49 66
2	F	87/92~(95%)	86~(99%)	1 (1%)	73 86
2	Н	88/92~(96%)	88 (100%)	0	100 100
3	А	521/529~(98%)	511 (98%)	10 (2%)	57 73
3	С	519/529~(98%)	509~(98%)	10 (2%)	57 73
4	В	67/116~(58%)	66~(98%)	1 (2%)	65 79
4	D	67/116~(58%)	65~(97%)	2(3%)	41 57
All	All	1609/1800 (89%)	1576 (98%)	33 (2%)	55 70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	33	VAL
1	Е	35	ARG
	<u> </u>	7	



Mol	Chain	Res	Type
1	Е	67	LEU
1	Е	129	SER
1	Е	133[A]	ARG
1	Е	133[B]	ARG
2	F	251	THR
3	А	370	THR
3	А	424	ASN
3	А	446	ASP
3	А	500	ARG
3	А	572	ASN
3	А	637	TRP
3	А	665	PHE
3	А	706	ARG
3	А	728	SER
3	А	929	THR
4	В	78	THR
1	G	144	GLU
1	G	161	LEU
1	G	173	ARG
3	С	370	THR
3	С	424	ASN
3	C	426	ARG
3	С	446	ASP
3	С	637	TRP
3	С	665	PHE
3	С	805	GLN
3	C	806	LYS
3	С	808	HIS
3	С	863	GLN
4	D	38	THR
4	D	46	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	572	ASN
3	С	563	ASN
3	С	808	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	В	ond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
5	EDO	С	1003	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	G	201	-	3,3,3	0.41	0	2,2,2	0.41	0
5	EDO	A	1013	-	3,3,3	0.56	0	2,2,2	0.27	0
5	EDO	Е	201	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	1006	-	3,3,3	0.44	0	$2,\!2,\!2$	0.31	0
5	EDO	А	1007	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	А	1011	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	С	1005	-	3,3,3	0.48	0	2,2,2	0.32	0
5	EDO	А	1010	-	3,3,3	0.45	0	2,2,2	0.40	0
7	PG4	А	1009	-	12,12,12	0.53	0	11,11,11	0.20	0
5	EDO	А	1001	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	С	1004	-	3,3,3	0.46	0	2,2,2	0.40	0
6	PEG	А	1005	-	6,6,6	0.48	0	$5,\!5,\!5$	0.49	0
5	EDO	Е	202	-	3,3,3	0.42	0	2,2,2	0.42	0
5	EDO	С	1007	-	3,3,3	0.43	0	2,2,2	0.45	0
5	EDO	С	1002	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	С	1008	-	3,3,3	0.58	0	2,2,2	0.25	0
6	PEG	A	1004	-	6,6,6	0.50	0	$5,\!5,\!5$	0.33	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les		
IVIOI	туре	Unam	nes	nes	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
8	SO4	А	1014	-	$4,\!4,\!4$	0.13	0	$6,\!6,\!6$	0.12	0		
5	EDO	А	1003	3	3,3,3	0.48	0	2,2,2	0.33	0		
5	EDO	А	1008	-	3, 3, 3	0.53	0	$2,\!2,\!2$	0.18	0		
5	EDO	А	1012	3	3,3,3	0.46	0	2,2,2	0.44	0		
5	EDO	F	401	-	3,3,3	0.45	0	2,2,2	0.37	0		
8	SO4	С	1009	-	4,4,4	0.13	0	$6,\!6,\!6$	0.11	0		
6	PEG	А	1002	-	$6,\!6,\!6$	0.48	0	$5,\!5,\!5$	0.26	0		
5	EDO	С	1001	-	3,3,3	0.51	0	2,2,2	0.30	0		
5	EDO	Е	203	-	3,3,3	0.40	0	$2,\!2,\!2$	0.44	0		
5	EDO	В	603	-	3,3,3	0.44	0	$2,\!2,\!2$	0.47	0		
8	SO4	А	1015	-	4,4,4	0.13	0	$6,\!6,\!6$	0.11	0		
5	EDO	С	1006	-	3,3,3	0.42	0	2,2,2	0.49	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
5	EDO	С	1003	-	-	1/1/1/1	-
5	EDO	G	201	-	-	1/1/1/1	-
5	EDO	А	1013	-	-	0/1/1/1	-
5	EDO	Е	201	-	-	1/1/1/1	-
5	EDO	А	1006	-	-	1/1/1/1	-
5	EDO	А	1007	-	-	1/1/1/1	-
5	EDO	А	1011	-	-	1/1/1/1	-
5	EDO	С	1005	-	-	0/1/1/1	-
5	EDO	А	1010	-	-	0/1/1/1	-
7	PG4	А	1009	-	-	5/10/10/10	-
5	EDO	А	1001	-	-	1/1/1/1	-
5	EDO	С	1004	-	-	0/1/1/1	-
6	PEG	А	1005	-	-	3/4/4/4	-
5	EDO	Е	202	-	-	0/1/1/1	-
5	EDO	С	1007	-	-	0/1/1/1	-
5	EDO	С	1002	-	-	1/1/1/1	-
5	EDO	С	1008	-	-	0/1/1/1	-
6	PEG	А	1004	-	-	1/4/4/4	-
5	EDO	А	1003	3	-	1/1/1/1	-
5	EDO	A	1008	-	-	0/1/1/1	-
5	EDO	А	1012	3	-	1/1/1/1	-
5	EDO	F	401	-	-	1/1/1/1	-
6	PEG	A	1002	-	-	3/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	С	1001	-	-	1/1/1/1	-
5	EDO	Е	203	-	-	1/1/1/1	-
5	EDO	В	603	-	-	0/1/1/1	-
5	EDO	С	1006	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	1004	PEG	O2-C3-C4-O4
5	Е	201	EDO	O1-C1-C2-O2
5	А	1001	EDO	O1-C1-C2-O2
5	А	1003	EDO	O1-C1-C2-O2
5	С	1001	EDO	O1-C1-C2-O2
5	С	1003	EDO	O1-C1-C2-O2
6	А	1002	PEG	O2-C3-C4-O4
7	А	1009	PG4	O3-C5-C6-O4
5	Е	203	EDO	O1-C1-C2-O2
5	А	1011	EDO	O1-C1-C2-O2
5	А	1012	EDO	O1-C1-C2-O2
5	G	201	EDO	O1-C1-C2-O2
5	F	401	EDO	O1-C1-C2-O2
7	А	1009	PG4	O2-C3-C4-O3
7	А	1009	PG4	O1-C1-C2-O2
6	А	1005	PEG	C1-C2-O2-C3
5	А	1007	EDO	O1-C1-C2-O2
5	С	1002	EDO	O1-C1-C2-O2
6	А	1005	PEG	O1-C1-C2-O2
6	А	1005	PEG	C4-C3-O2-C2
7	А	1009	PG4	C1-C2-O2-C3
6	А	1002	PEG	O1-C1-C2-O2
7	A	1009	PG4	C4-C3-O2-C2
5	A	1006	EDO	01-C1-C2-O2
5	С	1006	EDO	O1-C1-C2-O2
6	A	1002	PEG	C1-C2-O2-C3

There are no ring outliers.

13 monomers are involved in 17 short contacts:



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Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
5	G	201	EDO	1	0
5	А	1006	EDO	3	0
5	А	1007	EDO	1	0
5	А	1011	EDO	1	0
5	А	1010	EDO	1	0
5	А	1001	EDO	1	0
6	А	1005	PEG	1	0
5	С	1007	EDO	2	0
5	А	1003	EDO	1	0
5	А	1008	EDO	2	0
5	F	401	EDO	1	0
8	А	1015	SO4	1	0
5	С	1006	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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	Е	150/184 (81%)	-0.16	2 (1%) 77 81	37, 51, 75, 106	0
1	G	153/184~(83%)	1.37	56 (36%) 0 0	45, 75, 98, 113	0
2	F	105/107~(98%)	0.01	5 (4%) 30 37	33, 41, 76, 97	0
2	Н	107/107~(100%)	0.15	0 100 100	37, 54, 74, 104	0
3	А	597/609~(98%)	-0.15	9 (1%) 73 79	30, 40, 59, 80	0
3	С	597/609~(98%)	-0.04	11 (1%) 68 74	31, 43, 63, 102	0
4	В	85/134~(63%)	0.72	20 (23%) 0 1	38, 58, 106, 144	0
4	D	84/134~(62%)	0.67	14 (16%) 1 2	36, 59, 105, 119	0
All	All	1878/2068~(90%)	0.11	117 (6%) 20 26	30, 46, 83, 144	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
4	D	81	GLY	8.4	
4	D	82	TYR	7.0	
4	D	80	THR	6.8	
4	В	82	TYR	6.7	
2	F	247	ALA	5.8	
1	G	130	VAL	5.1	
1	G	67	LEU	4.8	
4	D	44	ALA	4.7	
1	G	143	ALA	4.5	
1	G	136	ASN	4.4	
1	G	165	SER	4.3	
1	G	128	LEU	4.3	
4	В	117	ARG	4.2	
1	G	141	THR	4.2	
1	G	129	SER	4.2	
1	G 135 ASP		4.2		



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Mol	Chain	Res	Type	RSRZ			
2	F	246	GLY	4.1			
1	G	69	LEU	4.1			
1	G	85	VAL	4.0			
1	G	137	SER	3.9			
1	G	66	THR	3.8			
1	G	138	VAL	3.7			
1	G	60	TYR	3.7			
1	G	64	LEU	3.7			
4	D	85	LEU	3.6			
1	G	140	LEU	3.6			
1	G	126	ALA	3.6			
4	D	78	THR	3.5			
1	G	163	ASP	3.4			
2	F	251	THR	3.4			
1	G	61	ARG	3.3			
1	G	156	PHE	3.3			
1	G	132	GLY	3.3			
4	В	41	ASP	3.3			
1	Е	34	ASP	3.2			
2	F	248	TRP	3.2			
1	G	63	LEU	3.2			
3	С	370	THR	3.1			
4	В	77	CYS	3.1			
4	D	37	PHE	3.1			
1	G	76	VAL	3.1			
4	В	116	CYS	3.1			
1	G	149	ILE	3.1			
4	В	44	ALA	3.1			
4	D	45	THR	3.0			
1	G	142	VAL	3.0			
3	С	622	LEU	3.0			
1	G	65	ASP	3.0			
1	G	161	LEU	2.9			
1	G	150	ILE	2.9			
3	С	714	GLN	2.9			
4	В	100	CYS	2.9			
1	G	185	ARG	2.8			
4	D	77	CYS	2.7			
3	А	622	LEU	2.7			
1	G	68	GLN	2.7			
3	С	785	HIS	2.6			
4	D	43	THR	2.6			



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Mol	Chain	Res	Type	RSRZ
3	С	621	VAL	2.6
3	С	636	VAL	2.6
1	G	74	LEU	2.6
1	G	131	SER	2.6
4	В	111	VAL	2.6
1	G	151	LEU	2.6
4	В	86	TYR	2.6
1	G	78	LEU	2.6
4	В	40	LEU	2.6
3	С	635	ALA	2.5
1	G	133	ARG	2.5
3	А	636	VAL	2.5
4	В	39	CYS	2.5
1	G	147	TYR	2.5
1	G	160	LEU	2.5
1	G	97	ASP	2.5
4	D	84	PRO	2.5
4	D	116	CYS	2.5
1	G	166	LEU	2.5
4	В	34	SER	2.4
1	G	81	GLU	2.4
1	G	153	ALA	2.4
3	А	562	TRP	2.4
3	А	665	PHE	2.4
3	С	625	ALA	2.4
4	В	112	CYS	2.4
4	В	45	THR	2.4
3	С	623	SER	2.4
1	G	62	ALA	2.4
4	В	38	THR	2.3
4	В	43	THR	2.3
3	А	658	LEU	2.3
4	D	40	LEU	2.3
1	G	91	LEU	2.2
1	G	183	ALA	2.2
1	G	184	PRO	2.2
1	G	146	PRO	2.2
1	G	155	PRO	2.2
1	G	33	VAL	2.2
4	В	37	PHE	2.2
4	D	41	ASP	2.2
1	G	73	ALA	2.2



Mol	Chain	Res	Type	RSRZ
4	В	115	THR	2.2
1	G	87	LEU	2.2
3	А	635	ALA	2.1
1	G	72	ASP	2.1
3	А	517	GLY	2.1
3	С	819	LEU	2.1
3	А	694	PHE	2.1
1	G	89	LEU	2.1
4	В	78	THR	2.1
3	С	663	LEU	2.1
1	G	127	ARG	2.0
4	В	80	THR	2.0
3	А	637	TRP	2.0
1	G	144	GLU	2.0
2	F	254	THR	2.0
1	E	70	GLY	2.0
1	G	134	ASP	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 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	С	1001	4/4	0.77	0.32	59,62,63,68	0
7	PG4	А	1009	13/13	0.77	0.41	56,72,85,88	0
5	EDO	С	1007	4/4	0.81	0.36	57,63,63,64	0
6	PEG	А	1004	7/7	0.82	0.27	43,62,71,74	0
5	EDO	С	1002	4/4	0.82	0.21	54,55,64,65	0
6	PEG	А	1005	7/7	0.83	0.16	50,66,76,80	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
5	EDO	А	1010	4/4	0.84	0.19	57,59,63,68	0
6	PEG	А	1002	7/7	0.86	0.14	58,63,71,76	0
5	EDO	А	1006	4/4	0.86	0.19	47,55,58,67	0
5	EDO	G	201	4/4	0.87	0.22	62,65,67,71	0
5	EDO	А	1008	4/4	0.88	0.19	50,60,65,73	0
5	EDO	А	1012	4/4	0.88	0.40	52,52,62,72	0
5	EDO	С	1006	4/4	0.89	0.24	54,56,58,71	0
5	EDO	В	603	4/4	0.90	0.27	59,60,60,61	0
8	SO4	А	1014	5/5	0.91	0.15	79,80,83,109	0
5	EDO	С	1005	4/4	0.92	0.10	51,55,57,60	0
5	EDO	Е	202	4/4	0.92	0.16	49,55,62,62	0
8	SO4	А	1015	5/5	0.92	0.25	78,90,99,100	0
5	EDO	А	1001	4/4	0.93	0.09	51,51,58,58	0
5	EDO	А	1003	4/4	0.93	0.32	61,69,74,85	0
5	EDO	Е	201	4/4	0.93	0.09	57,57,62,71	0
5	EDO	А	1007	4/4	0.93	0.10	54,56,63,65	0
5	EDO	С	1004	4/4	0.94	0.15	49,50,52,70	0
5	EDO	F	401	4/4	0.94	0.19	49,52,57,63	0
5	EDO	А	1011	4/4	0.95	0.28	$50,\!54,\!55,\!64$	0
5	EDO	С	1003	4/4	0.96	0.19	53,54,60,64	0
5	EDO	С	1008	4/4	0.96	0.34	38,48,53,58	0
5	EDO	Е	203	4/4	0.97	0.18	41,42,53,67	0
5	EDO	А	1013	4/4	0.97	0.38	44,46,47,54	0
8	SO4	С	1009	5/5	0.97	0.30	64,66,85,99	0
9	CA	D	601	1/1	0.98	0.04	48,48,48,48	0
9	CA	В	602	1/1	0.99	0.06	41,41,41,41	0
9	CA	В	601	1/1	0.99	0.06	49,49,49,49	0
9	CA	D	602	1/1	0.99	0.08	40,40,40,40	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

