



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 05:31 PM EDT

PDB ID : 3EZW
Title : Crystal Structure of a Hyperactive Escherichia coli Glycerol Kinase Mutant Gly230 → Asp Obtained Using Microfluidic Crystallization Devices
Authors : Anderson, M.J.; DeLaBarre, B.; Dunten, P.; Brunger, A.T.; Quake, S.R.
Deposited on : 2008-10-23
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.23.2
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)	:	2.23.2

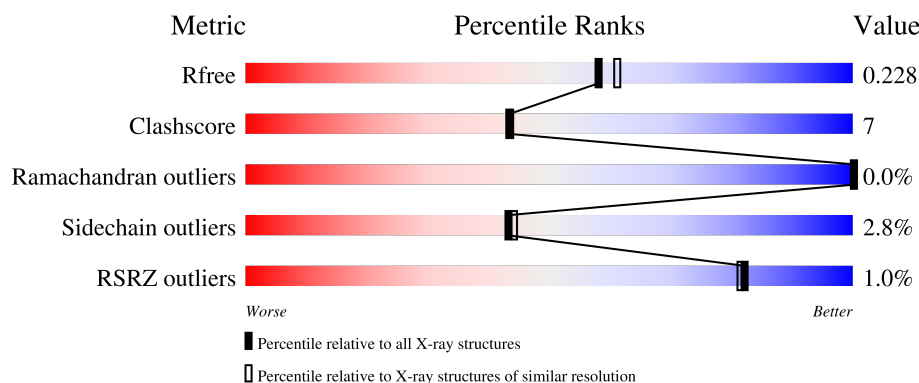
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 78%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 15% • 5% </div> </div>
1	B	526	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 13%, orange 6%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 81% 13% • 6% </div> </div>
1	C	526	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 75%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 75% 17% • 7% </div> </div>
1	D	526	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 20%, green 71%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 71% 20% • 8% </div> </div>
1	E	526	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 76%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 17% • 6% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>79%12%• 6%</div></div>
1	G	526	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>81%12%• 5%</div></div>
1	H	526	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>77%16%• 6%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32916 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	5	0
			3970	2501	698	750	21			
1	B	496	Total	C	N	O	S	0	2	0
			3933	2481	687	746	19			
1	E	492	Total	C	N	O	S	0	2	0
			3908	2464	683	742	19			
1	G	498	Total	C	N	O	S	0	3	0
			3948	2488	689	752	19			
1	C	489	Total	C	N	O	S	0	3	0
			3890	2452	682	735	21			
1	D	482	Total	C	N	O	S	0	1	0
			3818	2409	666	723	20			
1	F	492	Total	C	N	O	S	0	0	0
			3890	2454	680	737	19			
1	H	492	Total	C	N	O	S	0	1	0
			3900	2461	681	739	19			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	ASP	GLY	engineered mutation	UNP P0A6F3
A	501	GLN	-	expression tag	UNP P0A6F3
A	502	LEU	-	expression tag	UNP P0A6F3
A	503	TYR	-	expression tag	UNP P0A6F3
A	504	THR	-	expression tag	UNP P0A6F3
A	505	ARG	-	expression tag	UNP P0A6F3
A	506	ALA	-	expression tag	UNP P0A6F3
A	507	SER	-	expression tag	UNP P0A6F3
A	508	GLN	-	expression tag	UNP P0A6F3
A	509	PRO	-	expression tag	UNP P0A6F3
A	510	GLU	-	expression tag	UNP P0A6F3
A	511	LEU	-	expression tag	UNP P0A6F3
A	512	ALA	-	expression tag	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	513	PRO	-	expression tag	UNP P0A6F3
A	514	GLU	-	expression tag	UNP P0A6F3
A	515	ASP	-	expression tag	UNP P0A6F3
A	516	PRO	-	expression tag	UNP P0A6F3
A	517	GLU	-	expression tag	UNP P0A6F3
A	518	ASP	-	expression tag	UNP P0A6F3
A	519	LEU	-	expression tag	UNP P0A6F3
A	520	GLU	-	expression tag	UNP P0A6F3
A	521	HIS	-	expression tag	UNP P0A6F3
A	522	HIS	-	expression tag	UNP P0A6F3
A	523	HIS	-	expression tag	UNP P0A6F3
A	524	HIS	-	expression tag	UNP P0A6F3
A	525	HIS	-	expression tag	UNP P0A6F3
A	526	HIS	-	expression tag	UNP P0A6F3
B	230	ASP	GLY	engineered mutation	UNP P0A6F3
B	501	GLN	-	expression tag	UNP P0A6F3
B	502	LEU	-	expression tag	UNP P0A6F3
B	503	TYR	-	expression tag	UNP P0A6F3
B	504	THR	-	expression tag	UNP P0A6F3
B	505	ARG	-	expression tag	UNP P0A6F3
B	506	ALA	-	expression tag	UNP P0A6F3
B	507	SER	-	expression tag	UNP P0A6F3
B	508	GLN	-	expression tag	UNP P0A6F3
B	509	PRO	-	expression tag	UNP P0A6F3
B	510	GLU	-	expression tag	UNP P0A6F3
B	511	LEU	-	expression tag	UNP P0A6F3
B	512	ALA	-	expression tag	UNP P0A6F3
B	513	PRO	-	expression tag	UNP P0A6F3
B	514	GLU	-	expression tag	UNP P0A6F3
B	515	ASP	-	expression tag	UNP P0A6F3
B	516	PRO	-	expression tag	UNP P0A6F3
B	517	GLU	-	expression tag	UNP P0A6F3
B	518	ASP	-	expression tag	UNP P0A6F3
B	519	LEU	-	expression tag	UNP P0A6F3
B	520	GLU	-	expression tag	UNP P0A6F3
B	521	HIS	-	expression tag	UNP P0A6F3
B	522	HIS	-	expression tag	UNP P0A6F3
B	523	HIS	-	expression tag	UNP P0A6F3
B	524	HIS	-	expression tag	UNP P0A6F3
B	525	HIS	-	expression tag	UNP P0A6F3
B	526	HIS	-	expression tag	UNP P0A6F3
E	230	ASP	GLY	engineered mutation	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	501	GLN	-	expression tag	UNP P0A6F3
E	502	LEU	-	expression tag	UNP P0A6F3
E	503	TYR	-	expression tag	UNP P0A6F3
E	504	THR	-	expression tag	UNP P0A6F3
E	505	ARG	-	expression tag	UNP P0A6F3
E	506	ALA	-	expression tag	UNP P0A6F3
E	507	SER	-	expression tag	UNP P0A6F3
E	508	GLN	-	expression tag	UNP P0A6F3
E	509	PRO	-	expression tag	UNP P0A6F3
E	510	GLU	-	expression tag	UNP P0A6F3
E	511	LEU	-	expression tag	UNP P0A6F3
E	512	ALA	-	expression tag	UNP P0A6F3
E	513	PRO	-	expression tag	UNP P0A6F3
E	514	GLU	-	expression tag	UNP P0A6F3
E	515	ASP	-	expression tag	UNP P0A6F3
E	516	PRO	-	expression tag	UNP P0A6F3
E	517	GLU	-	expression tag	UNP P0A6F3
E	518	ASP	-	expression tag	UNP P0A6F3
E	519	LEU	-	expression tag	UNP P0A6F3
E	520	GLU	-	expression tag	UNP P0A6F3
E	521	HIS	-	expression tag	UNP P0A6F3
E	522	HIS	-	expression tag	UNP P0A6F3
E	523	HIS	-	expression tag	UNP P0A6F3
E	524	HIS	-	expression tag	UNP P0A6F3
E	525	HIS	-	expression tag	UNP P0A6F3
E	526	HIS	-	expression tag	UNP P0A6F3
G	230	ASP	GLY	engineered mutation	UNP P0A6F3
G	501	GLN	-	expression tag	UNP P0A6F3
G	502	LEU	-	expression tag	UNP P0A6F3
G	503	TYR	-	expression tag	UNP P0A6F3
G	504	THR	-	expression tag	UNP P0A6F3
G	505	ARG	-	expression tag	UNP P0A6F3
G	506	ALA	-	expression tag	UNP P0A6F3
G	507	SER	-	expression tag	UNP P0A6F3
G	508	GLN	-	expression tag	UNP P0A6F3
G	509	PRO	-	expression tag	UNP P0A6F3
G	510	GLU	-	expression tag	UNP P0A6F3
G	511	LEU	-	expression tag	UNP P0A6F3
G	512	ALA	-	expression tag	UNP P0A6F3
G	513	PRO	-	expression tag	UNP P0A6F3
G	514	GLU	-	expression tag	UNP P0A6F3
G	515	ASP	-	expression tag	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	516	PRO	-	expression tag	UNP P0A6F3
G	517	GLU	-	expression tag	UNP P0A6F3
G	518	ASP	-	expression tag	UNP P0A6F3
G	519	LEU	-	expression tag	UNP P0A6F3
G	520	GLU	-	expression tag	UNP P0A6F3
G	521	HIS	-	expression tag	UNP P0A6F3
G	522	HIS	-	expression tag	UNP P0A6F3
G	523	HIS	-	expression tag	UNP P0A6F3
G	524	HIS	-	expression tag	UNP P0A6F3
G	525	HIS	-	expression tag	UNP P0A6F3
G	526	HIS	-	expression tag	UNP P0A6F3
C	230	ASP	GLY	engineered mutation	UNP P0A6F3
C	501	GLN	-	expression tag	UNP P0A6F3
C	502	LEU	-	expression tag	UNP P0A6F3
C	503	TYR	-	expression tag	UNP P0A6F3
C	504	THR	-	expression tag	UNP P0A6F3
C	505	ARG	-	expression tag	UNP P0A6F3
C	506	ALA	-	expression tag	UNP P0A6F3
C	507	SER	-	expression tag	UNP P0A6F3
C	508	GLN	-	expression tag	UNP P0A6F3
C	509	PRO	-	expression tag	UNP P0A6F3
C	510	GLU	-	expression tag	UNP P0A6F3
C	511	LEU	-	expression tag	UNP P0A6F3
C	512	ALA	-	expression tag	UNP P0A6F3
C	513	PRO	-	expression tag	UNP P0A6F3
C	514	GLU	-	expression tag	UNP P0A6F3
C	515	ASP	-	expression tag	UNP P0A6F3
C	516	PRO	-	expression tag	UNP P0A6F3
C	517	GLU	-	expression tag	UNP P0A6F3
C	518	ASP	-	expression tag	UNP P0A6F3
C	519	LEU	-	expression tag	UNP P0A6F3
C	520	GLU	-	expression tag	UNP P0A6F3
C	521	HIS	-	expression tag	UNP P0A6F3
C	522	HIS	-	expression tag	UNP P0A6F3
C	523	HIS	-	expression tag	UNP P0A6F3
C	524	HIS	-	expression tag	UNP P0A6F3
C	525	HIS	-	expression tag	UNP P0A6F3
C	526	HIS	-	expression tag	UNP P0A6F3
D	230	ASP	GLY	engineered mutation	UNP P0A6F3
D	501	GLN	-	expression tag	UNP P0A6F3
D	502	LEU	-	expression tag	UNP P0A6F3
D	503	TYR	-	expression tag	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	504	THR	-	expression tag	UNP P0A6F3
D	505	ARG	-	expression tag	UNP P0A6F3
D	506	ALA	-	expression tag	UNP P0A6F3
D	507	SER	-	expression tag	UNP P0A6F3
D	508	GLN	-	expression tag	UNP P0A6F3
D	509	PRO	-	expression tag	UNP P0A6F3
D	510	GLU	-	expression tag	UNP P0A6F3
D	511	LEU	-	expression tag	UNP P0A6F3
D	512	ALA	-	expression tag	UNP P0A6F3
D	513	PRO	-	expression tag	UNP P0A6F3
D	514	GLU	-	expression tag	UNP P0A6F3
D	515	ASP	-	expression tag	UNP P0A6F3
D	516	PRO	-	expression tag	UNP P0A6F3
D	517	GLU	-	expression tag	UNP P0A6F3
D	518	ASP	-	expression tag	UNP P0A6F3
D	519	LEU	-	expression tag	UNP P0A6F3
D	520	GLU	-	expression tag	UNP P0A6F3
D	521	HIS	-	expression tag	UNP P0A6F3
D	522	HIS	-	expression tag	UNP P0A6F3
D	523	HIS	-	expression tag	UNP P0A6F3
D	524	HIS	-	expression tag	UNP P0A6F3
D	525	HIS	-	expression tag	UNP P0A6F3
D	526	HIS	-	expression tag	UNP P0A6F3
F	230	ASP	GLY	engineered mutation	UNP P0A6F3
F	501	GLN	-	expression tag	UNP P0A6F3
F	502	LEU	-	expression tag	UNP P0A6F3
F	503	TYR	-	expression tag	UNP P0A6F3
F	504	THR	-	expression tag	UNP P0A6F3
F	505	ARG	-	expression tag	UNP P0A6F3
F	506	ALA	-	expression tag	UNP P0A6F3
F	507	SER	-	expression tag	UNP P0A6F3
F	508	GLN	-	expression tag	UNP P0A6F3
F	509	PRO	-	expression tag	UNP P0A6F3
F	510	GLU	-	expression tag	UNP P0A6F3
F	511	LEU	-	expression tag	UNP P0A6F3
F	512	ALA	-	expression tag	UNP P0A6F3
F	513	PRO	-	expression tag	UNP P0A6F3
F	514	GLU	-	expression tag	UNP P0A6F3
F	515	ASP	-	expression tag	UNP P0A6F3
F	516	PRO	-	expression tag	UNP P0A6F3
F	517	GLU	-	expression tag	UNP P0A6F3
F	518	ASP	-	expression tag	UNP P0A6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	519	LEU	-	expression tag	UNP P0A6F3
F	520	GLU	-	expression tag	UNP P0A6F3
F	521	HIS	-	expression tag	UNP P0A6F3
F	522	HIS	-	expression tag	UNP P0A6F3
F	523	HIS	-	expression tag	UNP P0A6F3
F	524	HIS	-	expression tag	UNP P0A6F3
F	525	HIS	-	expression tag	UNP P0A6F3
F	526	HIS	-	expression tag	UNP P0A6F3
H	230	ASP	GLY	engineered mutation	UNP P0A6F3
H	501	GLN	-	expression tag	UNP P0A6F3
H	502	LEU	-	expression tag	UNP P0A6F3
H	503	TYR	-	expression tag	UNP P0A6F3
H	504	THR	-	expression tag	UNP P0A6F3
H	505	ARG	-	expression tag	UNP P0A6F3
H	506	ALA	-	expression tag	UNP P0A6F3
H	507	SER	-	expression tag	UNP P0A6F3
H	508	GLN	-	expression tag	UNP P0A6F3
H	509	PRO	-	expression tag	UNP P0A6F3
H	510	GLU	-	expression tag	UNP P0A6F3
H	511	LEU	-	expression tag	UNP P0A6F3
H	512	ALA	-	expression tag	UNP P0A6F3
H	513	PRO	-	expression tag	UNP P0A6F3
H	514	GLU	-	expression tag	UNP P0A6F3
H	515	ASP	-	expression tag	UNP P0A6F3
H	516	PRO	-	expression tag	UNP P0A6F3
H	517	GLU	-	expression tag	UNP P0A6F3
H	518	ASP	-	expression tag	UNP P0A6F3
H	519	LEU	-	expression tag	UNP P0A6F3
H	520	GLU	-	expression tag	UNP P0A6F3
H	521	HIS	-	expression tag	UNP P0A6F3
H	522	HIS	-	expression tag	UNP P0A6F3
H	523	HIS	-	expression tag	UNP P0A6F3
H	524	HIS	-	expression tag	UNP P0A6F3
H	525	HIS	-	expression tag	UNP P0A6F3
H	526	HIS	-	expression tag	UNP P0A6F3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		

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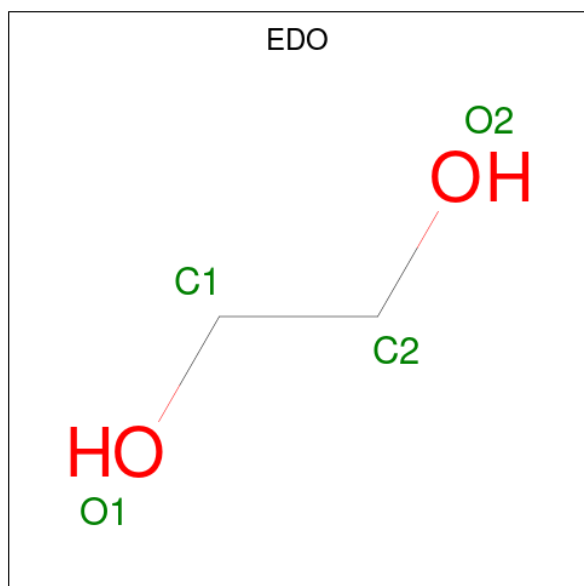
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

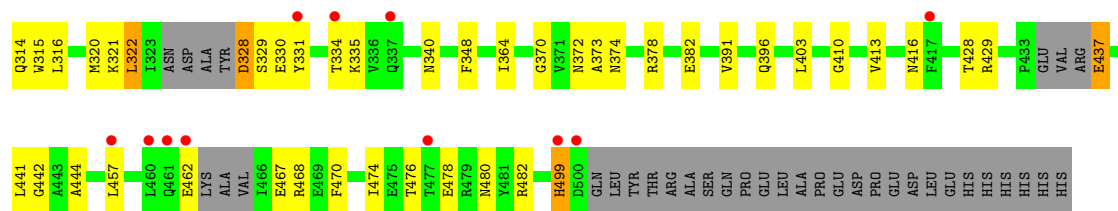
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	214	Total O 214 214	0	0
6	B	237	Total O 237 237	0	0
6	E	209	Total O 209 209	0	0
6	G	218	Total O 218 218	0	0

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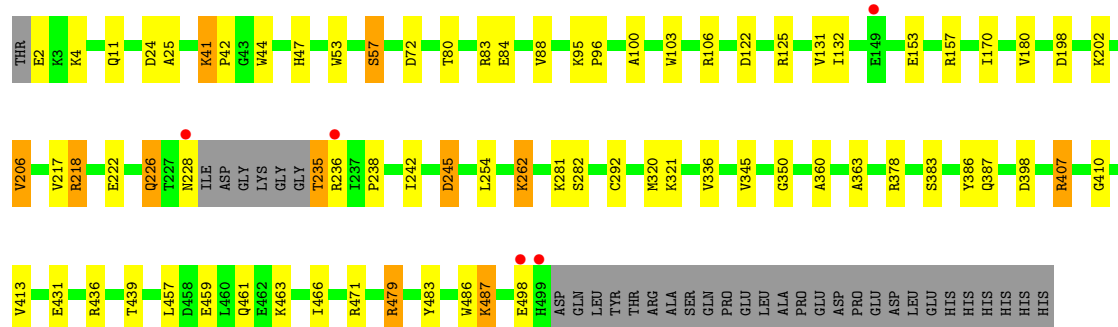
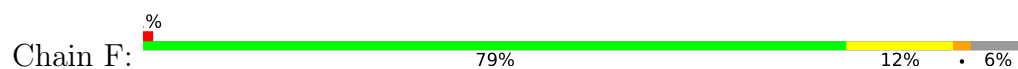
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	157	Total 157	O 157	0	0
6	D	130	Total 130	O 130	0	0
6	F	193	Total 193	O 193	0	0
6	H	168	Total 168	O 168	0	0

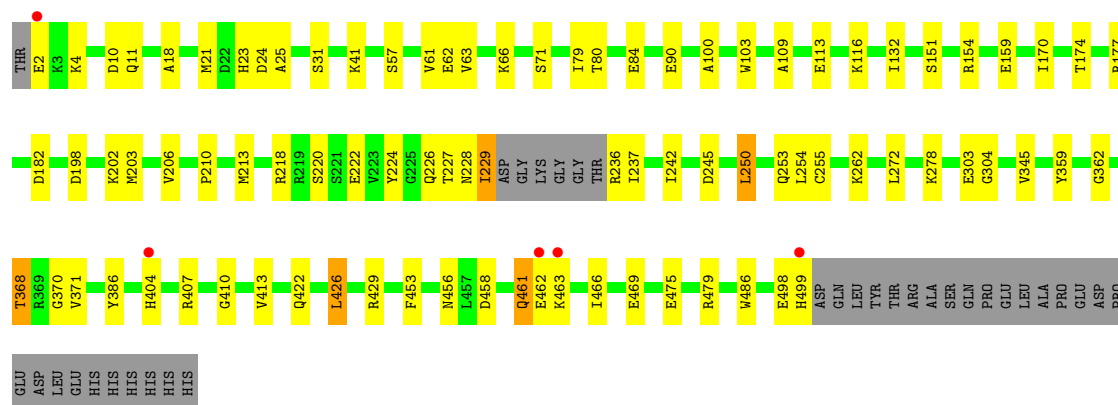
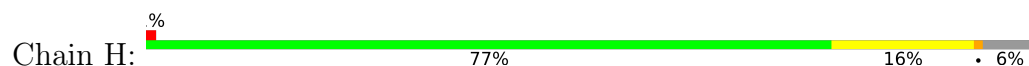




● Molecule 1: Glycerol kinase



● Molecule 1: Glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.12Å 114.26Å 212.62Å 90.00° 91.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 44.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.00) 84.0 (44.23-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0067, CNS	Depositor
R, R_{free}	0.167 , 0.225 0.173 , 0.228	Depositor DCC
R_{free} test set	5036 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32916	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, EDO, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	7/4050 (0.2%)	1.07	14/5488 (0.3%)
1	B	1.17	7/4012 (0.2%)	1.03	8/5439 (0.1%)
1	C	1.14	3/3967 (0.1%)	1.04	10/5374 (0.2%)
1	D	1.06	5/3893 (0.1%)	1.01	4/5272 (0.1%)
1	E	1.15	5/3987 (0.1%)	1.05	8/5405 (0.1%)
1	F	1.07	3/3969 (0.1%)	1.01	12/5381 (0.2%)
1	G	1.14	4/4027 (0.1%)	1.04	9/5458 (0.2%)
1	H	1.04	3/3979 (0.1%)	0.99	6/5394 (0.1%)
All	All	1.12	37/31884 (0.1%)	1.03	71/43211 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	LYS	CE-NZ	8.80	1.71	1.49
1	D	269	CYS	CB-SG	-8.78	1.67	1.82
1	C	314	GLN	CG-CD	7.51	1.68	1.51
1	G	461	GLN	CG-CD	7.02	1.67	1.51
1	B	269	CYS	CB-SG	-6.82	1.70	1.82

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	471	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	D	83	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	E	389	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	281	LYS	CD-CE-NZ	8.10	130.32	111.70
1	C	389	ARG	NE-CZ-NH2	-7.91	116.34	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3970	0	3904	47	0
1	B	3933	0	3870	45	0
1	C	3890	0	3825	63	0
1	D	3818	0	3745	84	0
1	E	3908	0	3837	51	0
1	F	3890	0	3822	45	0
1	G	3948	0	3884	38	0
1	H	3900	0	3831	52	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	C	16	0	24	1	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
5	F	8	0	12	0	0
5	G	16	0	24	0	0
5	H	8	0	12	0	0
6	A	214	0	0	2	0
6	B	237	0	0	2	0
6	C	157	0	0	1	0
6	D	130	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	209	0	0	1	0
6	F	193	0	0	2	0
6	G	218	0	0	2	0
6	H	168	0	0	0	0
All	All	32916	0	30896	419	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 419 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:281:LYS:CE	1:B:281:LYS:NZ	1.71	1.51
1:E:317:ARG:O	1:E:321:LYS:HA	1.31	1.25
1:D:21[A]:MET:CE	1:D:441:LEU:HD23	1.79	1.13
1:D:21[A]:MET:HE1	1:D:441:LEU:CD2	1.90	1.00
1:D:70:SER:CB	1:D:72:ASP:OD1	2.10	0.99

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	A	501/526 (95%)	487 (97%)	14 (3%)	0	100	100
1	B	494/526 (94%)	485 (98%)	9 (2%)	0	100	100
1	C	486/526 (92%)	475 (98%)	11 (2%)	0	100	100
1	D	473/526 (90%)	460 (97%)	13 (3%)	0	100	100
1	E	490/526 (93%)	475 (97%)	15 (3%)	0	100	100
1	F	488/526 (93%)	482 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	499/526 (95%)	485 (97%)	13 (3%)	1 (0%)	47	44
1	H	489/526 (93%)	479 (98%)	10 (2%)	0	100	100
All	All	3920/4208 (93%)	3828 (98%)	91 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	222	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/436 (95%)	405 (98%)	10 (2%)	49	51
1	B	412/436 (94%)	406 (98%)	6 (2%)	65	69
1	C	408/436 (94%)	398 (98%)	10 (2%)	47	49
1	D	400/436 (92%)	386 (96%)	14 (4%)	36	35
1	E	409/436 (94%)	396 (97%)	13 (3%)	39	38
1	F	407/436 (93%)	395 (97%)	12 (3%)	42	43
1	G	413/436 (95%)	401 (97%)	12 (3%)	42	43
1	H	408/436 (94%)	393 (96%)	15 (4%)	34	32
All	All	3272/3488 (94%)	3180 (97%)	92 (3%)	43	44

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	299	ASN
1	F	228	ASN
1	D	328	ASP
1	F	4	LYS
1	F	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	340	ASN
1	F	228	ASN
1	D	499	HIS
1	F	461	GLN
1	E	461	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 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	G	2643	-	5,5,5	0.65	0	5,5,5	0.67	0
5	EDO	C	2651	-	3,3,3	0.56	0	2,2,2	0.36	0
5	EDO	G	2645	-	3,3,3	0.40	0	2,2,2	0.16	0
5	EDO	D	2643	-	3,3,3	0.67	0	2,2,2	0.37	0
2	GOL	H	2644	-	5,5,5	0.49	0	5,5,5	0.40	0
5	EDO	C	2652	-	3,3,3	0.26	0	2,2,2	0.47	0
5	EDO	C	2654	-	3,3,3	0.31	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	2653	-	3,3,3	0.32	0	2,2,2	0.69	0
5	EDO	H	2647	-	3,3,3	0.58	0	2,2,2	0.51	0
2	GOL	A	2647	-	5,5,5	0.35	0	5,5,5	1.27	0
5	EDO	E	2643	-	3,3,3	0.54	0	2,2,2	0.73	0
2	GOL	E	2641	-	5,5,5	0.70	0	5,5,5	0.77	0
5	EDO	A	2650	-	3,3,3	0.43	0	2,2,2	0.14	0
5	EDO	G	2647	-	3,3,3	0.32	0	2,2,2	0.59	0
2	GOL	C	2649	-	5,5,5	0.72	0	5,5,5	0.47	0
5	EDO	D	2642	-	3,3,3	0.53	0	2,2,2	0.73	0
5	EDO	F	2645	-	3,3,3	0.60	0	2,2,2	0.32	0
5	EDO	B	2651	-	3,3,3	0.68	0	2,2,2	0.62	0
5	EDO	F	2644	-	3,3,3	0.31	0	2,2,2	1.04	0
5	EDO	A	2651	-	3,3,3	0.57	0	2,2,2	0.72	0
5	EDO	G	2646	-	3,3,3	0.34	0	2,2,2	0.63	0
2	GOL	D	2640	-	5,5,5	0.50	0	5,5,5	0.65	0
5	EDO	H	2646	-	3,3,3	0.39	0	2,2,2	0.44	0
2	GOL	B	2648	-	5,5,5	0.32	0	5,5,5	0.88	0
5	EDO	B	2650	-	3,3,3	0.39	0	2,2,2	0.15	0
5	EDO	G	2648	-	3,3,3	0.52	0	2,2,2	0.48	0
2	GOL	F	2642	-	5,5,5	0.53	0	5,5,5	0.60	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	GOL	G	2643	-	-	0/4/4/4	-
5	EDO	C	2651	-	-	0/1/1/1	-
5	EDO	G	2645	-	-	0/1/1/1	-
5	EDO	D	2643	-	-	0/1/1/1	-
2	GOL	H	2644	-	-	0/4/4/4	-
5	EDO	C	2652	-	-	1/1/1/1	-
5	EDO	C	2654	-	-	0/1/1/1	-
5	EDO	C	2653	-	-	0/1/1/1	-
5	EDO	H	2647	-	-	0/1/1/1	-
2	GOL	A	2647	-	-	0/4/4/4	-
5	EDO	E	2643	-	-	0/1/1/1	-
2	GOL	E	2641	-	-	0/4/4/4	-
5	EDO	A	2650	-	-	0/1/1/1	-
5	EDO	G	2647	-	-	0/1/1/1	-
2	GOL	C	2649	-	-	0/4/4/4	-
5	EDO	D	2642	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	F	2645	-	-	1/1/1/1	-
5	EDO	B	2651	-	-	0/1/1/1	-
5	EDO	F	2644	-	-	1/1/1/1	-
5	EDO	A	2651	-	-	0/1/1/1	-
5	EDO	G	2646	-	-	0/1/1/1	-
2	GOL	D	2640	-	-	0/4/4/4	-
5	EDO	H	2646	-	-	0/1/1/1	-
2	GOL	B	2648	-	-	0/4/4/4	-
5	EDO	B	2650	-	-	0/1/1/1	-
5	EDO	G	2648	-	-	1/1/1/1	-
2	GOL	F	2642	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2642	EDO	O1-C1-C2-O2
5	G	2648	EDO	O1-C1-C2-O2
5	C	2652	EDO	O1-C1-C2-O2
5	F	2644	EDO	O1-C1-C2-O2
5	F	2645	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2653	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, 95th 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	A	498/526 (94%)	-0.37	3 (0%) 89 88	17, 24, 44, 57	0
1	B	496/526 (94%)	-0.36	1 (0%) 95 94	17, 24, 42, 57	0
1	C	489/526 (92%)	-0.31	4 (0%) 86 85	17, 28, 47, 71	0
1	D	482/526 (91%)	-0.18	12 (2%) 57 56	19, 31, 56, 71	0
1	E	492/526 (93%)	-0.39	5 (1%) 82 81	16, 25, 45, 61	0
1	F	492/526 (93%)	-0.32	5 (1%) 82 81	19, 28, 45, 66	0
1	G	498/526 (94%)	-0.41	3 (0%) 89 88	17, 26, 42, 56	0
1	H	492/526 (93%)	-0.30	5 (1%) 82 81	21, 30, 48, 66	0
All	All	3939/4208 (93%)	-0.33	38 (0%) 82 81	16, 27, 47, 71	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	500	ASP	5.7
1	C	499	HIS	5.2
1	D	499	HIS	4.5
1	D	331	TYR	4.3
1	B	1	THR	4.1

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

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, 95th 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 ²)	Q<0.9
4	MG	A	2649	1/1	0.87	0.11	52,52,52,52	0
5	EDO	G	2648	4/4	0.95	0.10	29,38,40,45	0
5	EDO	C	2653	4/4	0.95	0.15	33,35,40,44	0
5	EDO	D	2642	4/4	0.95	0.12	33,35,35,35	0
5	EDO	H	2647	4/4	0.95	0.11	28,33,33,35	0
5	EDO	C	2651	4/4	0.96	0.10	24,31,32,33	0
5	EDO	A	2651	4/4	0.96	0.12	22,24,25,26	0
5	EDO	B	2651	4/4	0.96	0.10	26,27,28,28	0
5	EDO	D	2643	4/4	0.96	0.15	27,31,33,37	0
3	CL	E	2642	1/1	0.96	0.07	34,34,34,34	0
5	EDO	B	2650	4/4	0.97	0.11	28,28,28,30	0
2	GOL	D	2640	6/6	0.97	0.09	18,22,26,31	0
5	EDO	F	2645	4/4	0.97	0.10	24,27,31,33	0
5	EDO	G	2647	4/4	0.97	0.14	30,31,31,33	0
5	EDO	E	2643	4/4	0.98	0.13	23,27,27,28	0
5	EDO	G	2646	4/4	0.98	0.15	31,33,33,34	0
2	GOL	H	2644	6/6	0.98	0.13	21,22,26,30	0
2	GOL	B	2648	6/6	0.98	0.09	16,17,22,28	0
3	CL	D	2641	1/1	0.98	0.06	37,37,37,37	0
5	EDO	C	2652	4/4	0.98	0.12	34,35,36,37	0
2	GOL	E	2641	6/6	0.98	0.09	16,20,22,22	0
5	EDO	C	2654	4/4	0.98	0.08	24,25,29,31	0
5	EDO	A	2650	4/4	0.98	0.09	33,34,34,35	0
2	GOL	G	2643	6/6	0.98	0.11	19,20,20,21	0
2	GOL	A	2647	6/6	0.98	0.13	14,17,24,27	0
5	EDO	H	2646	4/4	0.98	0.14	25,26,29,32	0
2	GOL	F	2642	6/6	0.98	0.12	20,25,27,29	0
3	CL	H	2645	1/1	0.99	0.05	39,39,39,39	0
5	EDO	G	2645	4/4	0.99	0.08	22,23,24,29	0
3	CL	B	2649	1/1	0.99	0.07	33,33,33,33	0
2	GOL	C	2649	6/6	0.99	0.09	18,19,25,28	0
5	EDO	F	2644	4/4	0.99	0.07	24,25,28,29	0
3	CL	C	2650	1/1	0.99	0.07	32,32,32,32	0
3	CL	A	2648	1/1	0.99	0.08	23,23,23,23	0
3	CL	F	2643	1/1	0.99	0.08	35,35,35,35	0
3	CL	G	2644	1/1	1.00	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.