



# wwPDB X-ray Structure Validation Summary Report

Feb 8, 2022 – 03:24 am GMT

PDB ID : 7NRZ  
Title : Crystal structure of malate dehydrogenase from Trypanosoma cruzi  
Authors : Sonani, R.R.; Kurpiewska, K.; Lewinski, K.; Dubin, G.  
Deposited on : 2021-03-04  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

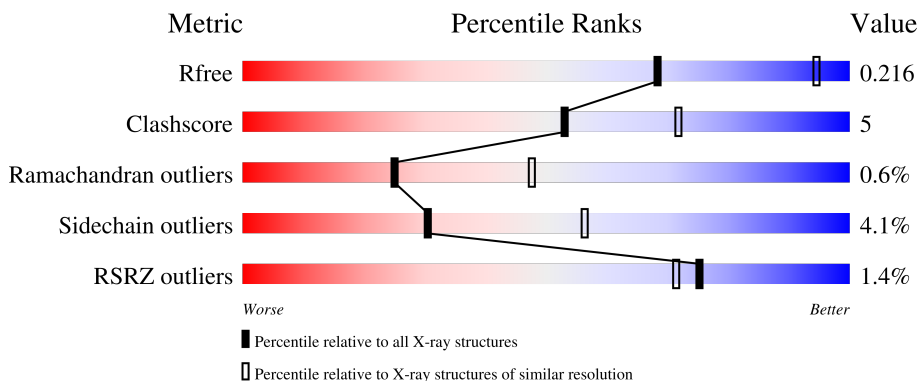
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	 86% 14%
1	B	323	 84% 15%
1	C	323	 85% 15%
1	D	323	 86% 12%
1	E	323	 89% 11%

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Mol	Chain	Length	Quality of chain
1	F	323	 % 88% 12%
1	G	323	 2% 88% 11%
1	H	323	 4% 86% 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
2	EDO	A	414	-	-	-	X
2	EDO	C	407	-	-	-	X
2	EDO	D	411	-	-	-	X
2	EDO	G	1008	-	-	-	X
3	PEG	B	1806	-	-	X	-
5	PG4	D	404	-	-	-	X
6	CL	G	1011	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19867 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	Total 2394	C 1524	N 418	O 439	S 13	0	1	0
1	B	323	Total 2388	C 1521	N 415	O 439	S 13	0	1	0
1	C	323	Total 2384	C 1519	N 413	O 439	S 13	0	0	0
1	D	323	Total 2388	C 1520	N 416	O 440	S 12	0	1	0
1	E	323	Total 2365	C 1508	N 406	O 439	S 12	0	0	0
1	F	323	Total 2384	C 1519	N 413	O 439	S 13	0	0	0
1	G	323	Total 2377	C 1514	N 412	O 439	S 12	0	0	0
1	H	323	Total 2390	C 1522	N 416	O 439	S 13	0	0	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

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

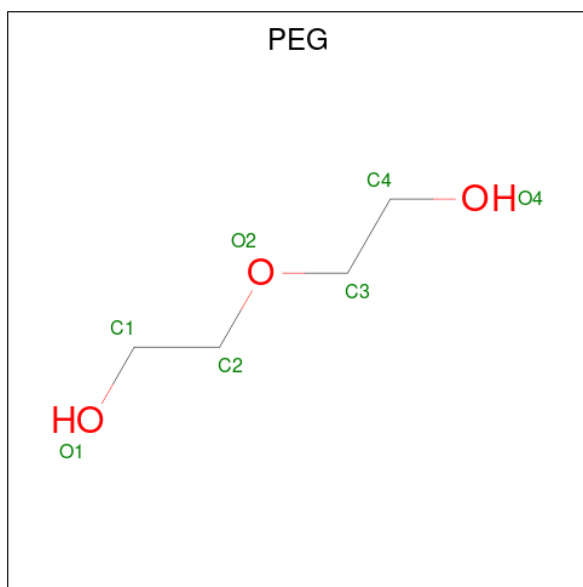
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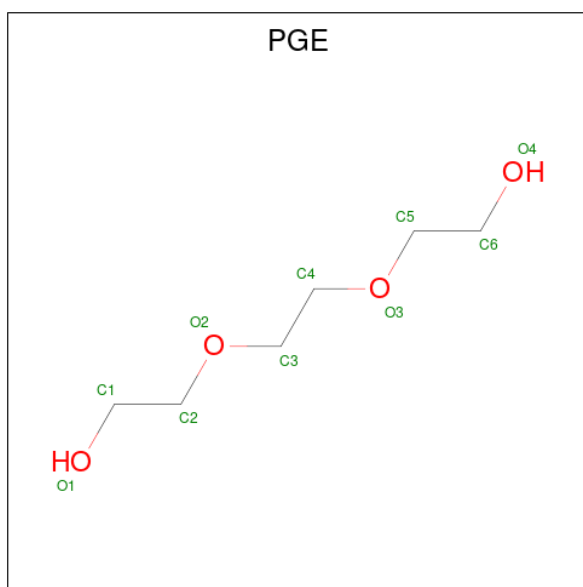
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



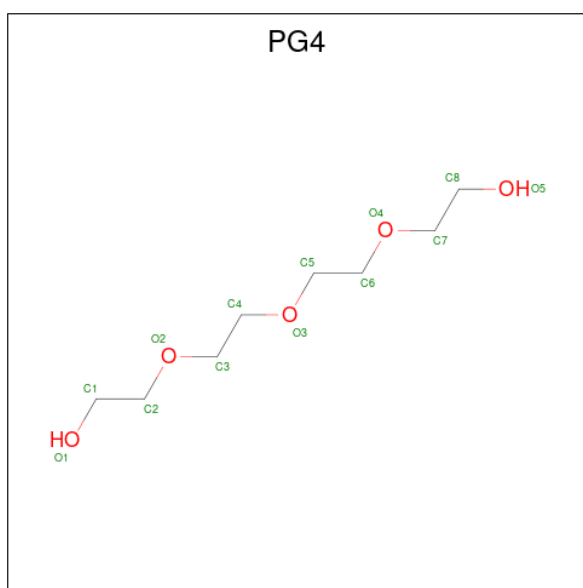
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Cl 1 1	0	0

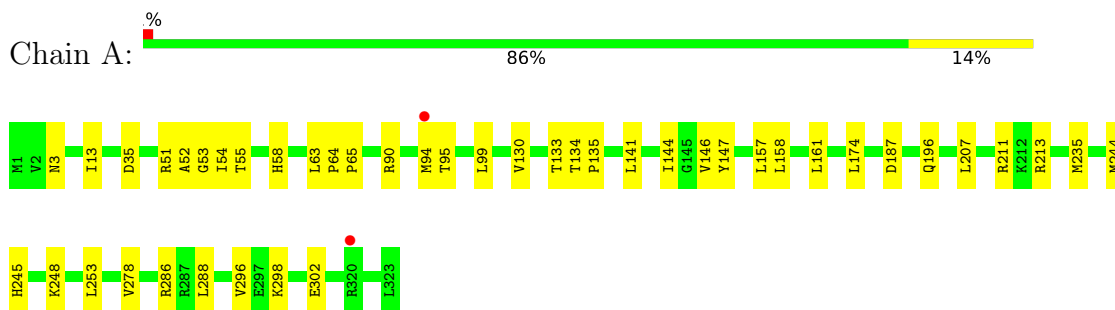
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	56	Total O 56 56	0	0
7	C	59	Total O 59 59	0	0
7	D	57	Total O 57 57	0	0
7	E	44	Total O 44 44	0	0
7	F	45	Total O 45 45	0	0
7	G	42	Total O 42 42	0	0
7	H	34	Total O 34 34	0	0

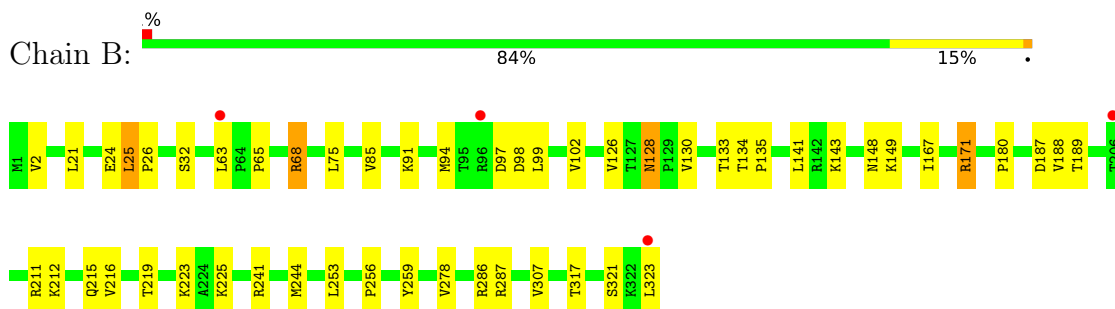
### 3 Residue-property plots [i](#)

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.

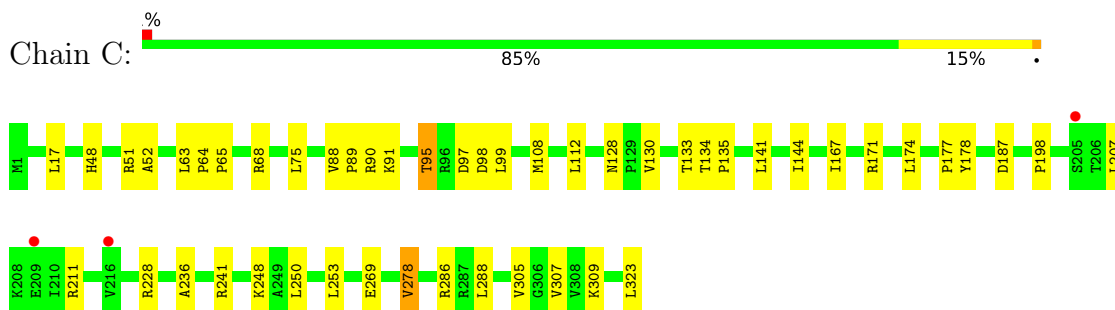
- Molecule 1: Malate dehydrogenase



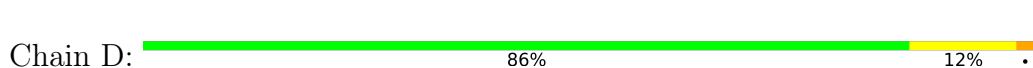
- Molecule 1: Malate dehydrogenase

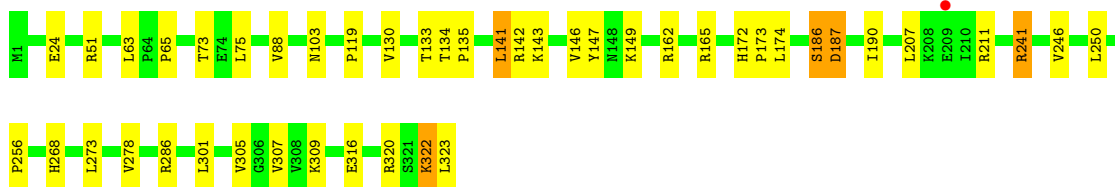


- Molecule 1: Malate dehydrogenase

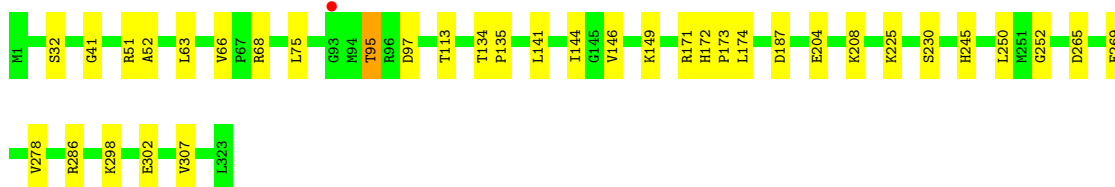
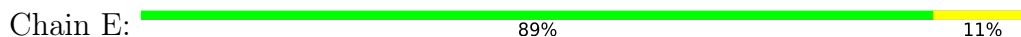


- Molecule 1: Malate dehydrogenase

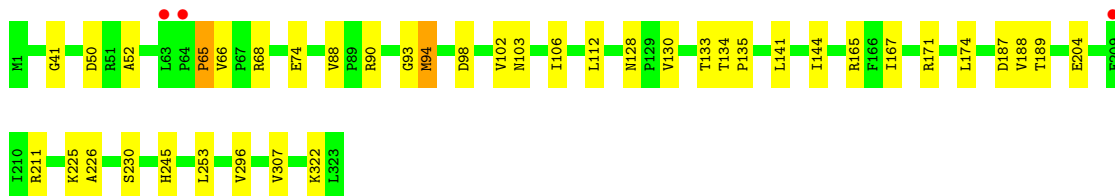
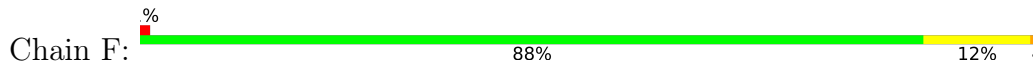




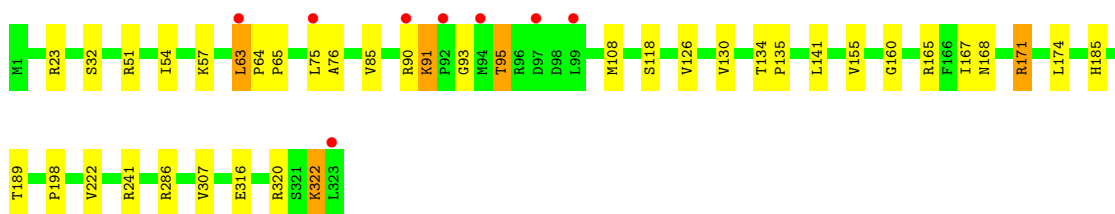
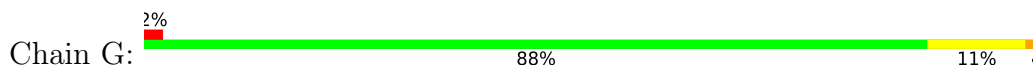
● Molecule 1: Malate dehydrogenase



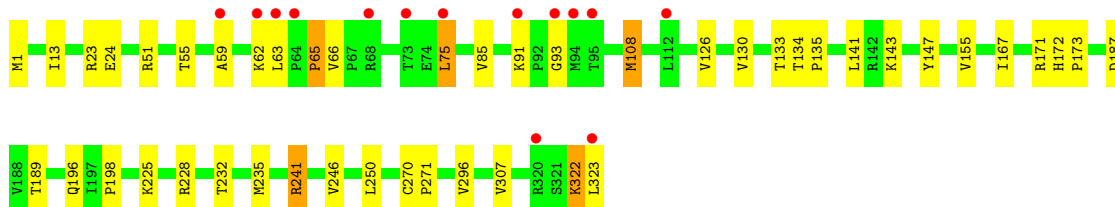
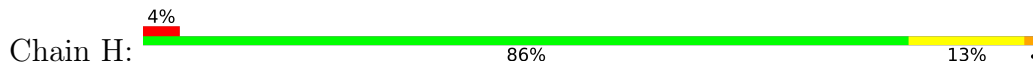
● Molecule 1: Malate dehydrogenase



● Molecule 1: Malate dehydrogenase



● Molecule 1: Malate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.04Å 148.33Å 251.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.32 – 2.60 48.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.32-2.60) 99.0 (48.52-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.203 , 0.216 0.206 , 0.216	Depositor DCC
$R_{free}$ test set	4657 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, PGE, PEG, PG4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	0/2439	0.52	0/3320
1	B	0.35	0/2433	0.58	0/3313
1	C	0.34	0/2426	0.56	0/3303
1	D	0.34	0/2430	0.54	0/3310
1	E	0.36	0/2407	0.58	0/3282
1	F	0.34	0/2426	0.56	0/3303
1	G	0.32	0/2419	0.54	0/3296
1	H	0.30	0/2432	0.52	0/3310
All	All	0.33	0/19412	0.55	0/26437

There are no bond length outliers.

There are no bond angle outliers.

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	A	2394	0	2506	31	0
1	B	2388	0	2495	33	0
1	C	2384	0	2493	24	0
1	D	2388	0	2487	33	0
1	E	2365	0	2453	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2384	0	2493	22	0
1	G	2377	0	2475	26	0
1	H	2390	0	2504	31	0
2	A	60	0	90	9	0
2	B	48	0	72	3	0
2	C	36	0	54	3	0
2	D	44	0	66	3	0
2	E	16	0	24	1	0
2	F	56	0	84	2	0
2	G	40	0	60	2	0
2	H	16	0	24	3	0
3	A	14	0	20	0	0
3	B	7	0	10	5	0
3	C	7	0	10	0	0
3	F	7	0	10	1	0
4	A	20	0	28	5	0
5	D	13	0	18	2	0
5	E	13	0	18	2	0
6	G	1	0	0	2	0
7	A	62	0	0	2	0
7	B	56	0	0	0	0
7	C	59	0	0	0	0
7	D	57	0	0	0	0
7	E	44	0	0	1	0
7	F	45	0	0	1	0
7	G	42	0	0	0	0
7	H	34	0	0	0	0
All	All	19867	0	20494	214	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 5.

The worst 5 of 214 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:H:13:ILE:HD13	1:H:232:THR:HA	1.54	0.88
1:H:143:LYS:HE2	1:H:323:LEU:HD21	1.54	0.87
1:H:13:ILE:CD1	1:H:232:THR:HA	2.07	0.85
1:E:51:ARG:HE	5:E:403:PG4:H51	1.42	0.82
1:C:52:ALA:H	2:C:409:EDO:H11	1.43	0.82



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	322/323 (100%)	314 (98%)	7 (2%)	1 (0%)	41	64
1	B	322/323 (100%)	312 (97%)	9 (3%)	1 (0%)	41	64
1	C	321/323 (99%)	314 (98%)	6 (2%)	1 (0%)	41	64
1	D	322/323 (100%)	312 (97%)	8 (2%)	2 (1%)	25	47
1	E	321/323 (99%)	311 (97%)	9 (3%)	1 (0%)	41	64
1	F	321/323 (99%)	308 (96%)	8 (2%)	5 (2%)	9	19
1	G	321/323 (99%)	309 (96%)	11 (3%)	1 (0%)	41	64
1	H	321/323 (99%)	313 (98%)	5 (2%)	3 (1%)	17	35
All	All	2571/2584 (100%)	2493 (97%)	63 (2%)	15 (1%)	25	47

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASP
1	B	97	ASP
1	C	187	ASP
1	D	268	HIS
1	F	65	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/261 (100%)	257 (98%)	4 (2%)	65	83
1	B	260/261 (100%)	246 (95%)	14 (5%)	22	44
1	C	260/261 (100%)	244 (94%)	16 (6%)	18	37
1	D	259/261 (99%)	247 (95%)	12 (5%)	27	51
1	E	256/261 (98%)	245 (96%)	11 (4%)	29	54
1	F	260/261 (100%)	251 (96%)	9 (4%)	36	62
1	G	258/261 (99%)	249 (96%)	9 (4%)	36	62
1	H	261/261 (100%)	251 (96%)	10 (4%)	33	59
All	All	2075/2088 (99%)	1990 (96%)	85 (4%)	30	56

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	65	PRO
1	G	171	ARG
1	F	74	GLU
1	F	322	LYS
1	H	24	GLU

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

Mol	Chain	Res	Type
1	B	128	ASN
1	D	103	ASN
1	G	101	ASN

### 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 89 ligands modelled in this entry, 1 is monoatomic - leaving 88 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	EDO	G	1005	-	3,3,3	0.10	0	2,2,2	0.27	0
2	EDO	B	1804	-	3,3,3	0.50	0	2,2,2	0.17	0
2	EDO	D	407	-	3,3,3	0.15	0	2,2,2	0.12	0
2	EDO	D	408	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	A	405	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	B	1811	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	C	409	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	G	1003	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	F	813	-	3,3,3	0.16	0	2,2,2	0.17	0
2	EDO	G	1006	-	3,3,3	0.50	0	2,2,2	0.22	0
2	EDO	G	1008	-	3,3,3	0.45	0	2,2,2	0.41	0
2	EDO	A	402	-	3,3,3	0.49	0	2,2,2	0.17	0
2	EDO	A	415	-	3,3,3	0.15	0	2,2,2	0.16	0
2	EDO	H	1104	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	A	416	-	3,3,3	0.06	0	2,2,2	0.38	0
2	EDO	C	408	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	F	808	-	3,3,3	0.45	0	2,2,2	0.25	0
2	EDO	F	814	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	F	804	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	F	806	-	3,3,3	0.45	0	2,2,2	0.38	0
3	PEG	F	807	-	6,6,6	0.49	0	5,5,5	0.21	0
2	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.31	0
2	EDO	G	1002	-	3,3,3	0.47	0	2,2,2	0.23	0
2	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.35	0
5	PG4	E	403	-	12,12,12	0.51	0	11,11,11	0.22	0
2	EDO	F	812	-	3,3,3	0.39	0	2,2,2	0.78	0
2	EDO	A	413	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	F	801	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	H	1102	-	3,3,3	0.21	0	2,2,2	0.21	0
2	EDO	F	815	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	H	1101	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	C	404	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	D	410	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	B	1812	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	C	402	-	3,3,3	0.45	0	2,2,2	0.38	0
5	PG4	D	404	-	12,12,12	0.53	0	11,11,11	0.25	0
3	PEG	A	406	-	6,6,6	0.48	0	5,5,5	0.28	0
2	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	805	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	F	811	-	3,3,3	0.41	0	2,2,2	0.38	0
2	EDO	H	1103	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	D	409	-	3,3,3	0.44	0	2,2,2	0.40	0
2	EDO	D	402	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	A	411	-	3,3,3	0.50	0	2,2,2	0.24	0
3	PEG	A	419	-	6,6,6	0.49	0	5,5,5	0.27	0
2	EDO	F	809	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	C	410	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	F	803	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	B	1805	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	D	405	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	F	810	-	3,3,3	0.42	0	2,2,2	0.51	0
2	EDO	G	1001	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	B	1813	-	3,3,3	0.47	0	2,2,2	0.35	0
3	PEG	B	1806	-	6,6,6	0.48	0	5,5,5	0.30	0
2	EDO	C	403	-	3,3,3	0.18	0	2,2,2	0.18	0
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	G	1010	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	1802	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	B	1801	-	3,3,3	0.49	0	2,2,2	0.32	0
2	EDO	G	1009	-	3,3,3	0.16	0	2,2,2	0.09	0
4	PGE	A	407	-	9,9,9	0.32	0	8,8,8	0.25	0
2	EDO	D	406	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.42	0
3	PEG	C	401	-	6,6,6	0.48	0	5,5,5	0.31	0
2	EDO	C	405	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	B	1808	-	3,3,3	0.48	0	2,2,2	0.19	0
2	EDO	E	404	-	3,3,3	0.49	0	2,2,2	0.23	0
2	EDO	A	412	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	E	402	-	3,3,3	0.52	0	2,2,2	0.08	0
2	EDO	A	401	-	3,3,3	0.49	0	2,2,2	0.15	0
2	EDO	A	414	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	G	1007	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	B	1809	-	3,3,3	0.49	0	2,2,2	0.19	0
2	EDO	C	406	-	3,3,3	0.48	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PGE	A	418	-	9,9,9	0.32	0	8,8,8	0.24	0
2	EDO	B	1803	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	B	1810	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	F	802	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	B	1807	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	A	417	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	D	403	-	3,3,3	0.09	0	2,2,2	0.40	0
2	EDO	E	405	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	D	412	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	D	411	-	3,3,3	0.49	0	2,2,2	0.17	0
2	EDO	D	401	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	E	401	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	G	1004	-	3,3,3	0.46	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	G	1005	-	-	1/1/1/1	-
2	EDO	B	1804	-	-	0/1/1/1	-
2	EDO	D	407	-	-	1/1/1/1	-
2	EDO	D	408	-	-	1/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	B	1811	-	-	1/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
2	EDO	G	1003	-	-	1/1/1/1	-
2	EDO	F	813	-	-	0/1/1/1	-
2	EDO	G	1006	-	-	1/1/1/1	-
2	EDO	G	1008	-	-	1/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	A	415	-	-	1/1/1/1	-
2	EDO	H	1104	-	-	1/1/1/1	-
2	EDO	A	410	-	-	1/1/1/1	-
2	EDO	A	416	-	-	0/1/1/1	-
2	EDO	C	408	-	-	1/1/1/1	-
2	EDO	F	808	-	-	1/1/1/1	-
2	EDO	F	814	-	-	0/1/1/1	-
2	EDO	F	804	-	-	1/1/1/1	-
2	EDO	F	806	-	-	0/1/1/1	-
3	PEG	F	807	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	G	1002	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
5	PG4	E	403	-	-	4/10/10/10	-
2	EDO	F	812	-	-	0/1/1/1	-
2	EDO	A	413	-	-	0/1/1/1	-
2	EDO	F	801	-	-	1/1/1/1	-
2	EDO	H	1102	-	-	1/1/1/1	-
2	EDO	F	815	-	-	0/1/1/1	-
2	EDO	H	1101	-	-	0/1/1/1	-
2	EDO	C	404	-	-	1/1/1/1	-
2	EDO	D	410	-	-	0/1/1/1	-
2	EDO	B	1812	-	-	1/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
5	PG4	D	404	-	-	8/10/10/10	-
3	PEG	A	406	-	-	2/4/4/4	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	F	805	-	-	1/1/1/1	-
2	EDO	F	811	-	-	1/1/1/1	-
2	EDO	H	1103	-	-	1/1/1/1	-
2	EDO	D	409	-	-	1/1/1/1	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
3	PEG	A	419	-	-	1/4/4/4	-
2	EDO	F	809	-	-	0/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	F	803	-	-	1/1/1/1	-
2	EDO	B	1805	-	-	1/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	F	810	-	-	0/1/1/1	-
2	EDO	G	1001	-	-	0/1/1/1	-
2	EDO	B	1813	-	-	1/1/1/1	-
3	PEG	B	1806	-	-	0/4/4/4	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	G	1010	-	-	0/1/1/1	-
2	EDO	B	1802	-	-	0/1/1/1	-
2	EDO	B	1801	-	-	0/1/1/1	-
2	EDO	G	1009	-	-	0/1/1/1	-
4	PGE	A	407	-	-	5/7/7/7	-
2	EDO	D	406	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	409	-	-	0/1/1/1	-
3	PEG	C	401	-	-	2/4/4/4	-
2	EDO	C	405	-	-	1/1/1/1	-
2	EDO	B	1808	-	-	0/1/1/1	-
2	EDO	E	404	-	-	0/1/1/1	-
2	EDO	A	412	-	-	1/1/1/1	-
2	EDO	E	402	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	414	-	-	1/1/1/1	-
2	EDO	G	1007	-	-	0/1/1/1	-
2	EDO	B	1809	-	-	1/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
4	PGE	A	418	-	-	4/7/7/7	-
2	EDO	B	1803	-	-	1/1/1/1	-
2	EDO	B	1810	-	-	0/1/1/1	-
2	EDO	F	802	-	-	0/1/1/1	-
2	EDO	B	1807	-	-	0/1/1/1	-
2	EDO	A	417	-	-	1/1/1/1	-
2	EDO	D	403	-	-	1/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	D	412	-	-	0/1/1/1	-
2	EDO	D	411	-	-	0/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
2	EDO	G	1004	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	418	PGE	C4-C3-O2-C2
5	D	404	PG4	O3-C5-C6-O4
5	D	404	PG4	O2-C3-C4-O3
5	E	403	PG4	C6-C5-O3-C4
4	A	407	PGE	O2-C3-C4-O3

There are no ring outliers.

27 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	EDO	1	0
2	C	409	EDO	2	0
2	F	814	EDO	1	0
3	F	807	PEG	1	0
2	A	404	EDO	2	0
2	G	1002	EDO	1	0
5	E	403	PG4	2	0
2	A	413	EDO	1	0
2	H	1101	EDO	1	0
5	D	404	PG4	2	0
2	F	811	EDO	1	0
2	H	1103	EDO	2	0
2	D	409	EDO	1	0
2	A	411	EDO	1	0
2	D	405	EDO	1	0
3	B	1806	PEG	5	0
4	A	407	PGE	2	0
2	A	409	EDO	1	0
2	A	412	EDO	3	0
2	G	1007	EDO	1	0
2	B	1809	EDO	1	0
2	C	406	EDO	1	0
4	A	418	PGE	3	0
2	B	1810	EDO	1	0
2	B	1807	EDO	1	0
2	D	411	EDO	1	0
2	E	401	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	323/323 (100%)	-0.04	2 (0%) 89 88	30, 48, 74, 99	0
1	B	323/323 (100%)	-0.09	4 (1%) 79 76	33, 48, 75, 116	0
1	C	323/323 (100%)	-0.09	3 (0%) 84 82	32, 50, 78, 121	0
1	D	323/323 (100%)	-0.07	1 (0%) 94 93	34, 54, 79, 113	0
1	E	323/323 (100%)	-0.11	1 (0%) 94 93	40, 54, 85, 130	0
1	F	323/323 (100%)	-0.06	3 (0%) 84 82	36, 54, 83, 125	0
1	G	323/323 (100%)	0.06	8 (2%) 57 51	37, 57, 90, 145	0
1	H	323/323 (100%)	0.13	14 (4%) 35 28	42, 62, 93, 141	0
All	All	2584/2584 (100%)	-0.03	36 (1%) 75 71	30, 54, 85, 145	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	90	ARG	4.3
1	H	63	LEU	4.1
1	F	63	LEU	3.6
1	H	62	LYS	3.6
1	H	93	GLY	3.1

### 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 i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	F	804	4/4	0.56	0.28	85,92,93,93	0
2	EDO	D	411	4/4	0.61	0.42	73,76,79,79	0
2	EDO	D	403	4/4	0.61	0.34	76,80,82,84	0
2	EDO	A	404	4/4	0.65	0.25	65,72,72,75	0
2	EDO	G	1007	4/4	0.69	0.26	71,72,72,74	0
2	EDO	C	407	4/4	0.71	0.63	80,81,83,84	0
2	EDO	B	1813	4/4	0.73	0.17	86,88,89,89	0
2	EDO	G	1008	4/4	0.75	0.48	61,62,62,66	0
3	PEG	A	419	7/7	0.75	0.39	83,86,89,91	0
5	PG4	D	404	13/13	0.75	0.40	72,83,88,89	0
2	EDO	B	1809	4/4	0.77	0.27	67,68,69,69	0
2	EDO	A	416	4/4	0.77	0.36	20,20,20,20	0
4	PGE	A	418	10/10	0.77	0.34	71,79,86,87	0
2	EDO	D	405	4/4	0.77	0.39	68,69,72,72	0
2	EDO	A	414	4/4	0.79	0.53	62,65,65,65	0
2	EDO	F	801	4/4	0.79	0.28	69,72,73,73	0
2	EDO	C	405	4/4	0.80	0.19	66,70,72,77	0
6	CL	G	1011	1/1	0.80	0.19	85,85,85,85	0
2	EDO	D	412	4/4	0.81	0.45	81,85,86,88	0
2	EDO	F	814	4/4	0.81	0.27	59,63,64,66	0
3	PEG	A	406	7/7	0.82	0.28	58,62,73,74	0
2	EDO	D	410	4/4	0.82	0.32	75,76,78,81	0
3	PEG	C	401	7/7	0.82	0.39	74,83,87,91	0
2	EDO	C	408	4/4	0.82	0.42	67,68,69,70	0
2	EDO	A	412	4/4	0.82	0.59	78,79,83,83	0
5	PG4	E	403	13/13	0.82	0.23	60,80,92,93	0
2	EDO	A	413	4/4	0.82	0.20	62,63,66,66	0
2	EDO	A	410	4/4	0.83	0.17	73,76,77,78	0
2	EDO	B	1810	4/4	0.83	0.25	66,68,68,72	0
2	EDO	G	1006	4/4	0.83	0.24	62,66,67,68	0
2	EDO	H	1103	4/4	0.84	0.43	70,70,70,72	0
2	EDO	A	411	4/4	0.84	0.35	50,53,53,55	0
2	EDO	G	1005	4/4	0.85	0.25	70,70,71,71	0
2	EDO	A	403	4/4	0.85	0.21	56,58,59,61	0
2	EDO	B	1811	4/4	0.86	0.30	67,68,69,70	0
4	PGE	A	407	10/10	0.86	0.27	66,74,81,81	0
2	EDO	C	410	4/4	0.86	0.24	58,62,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	401	4/4	0.86	0.24	51,54,55,57	0
2	EDO	F	810	4/4	0.86	0.21	64,68,71,76	0
3	PEG	B	1806	7/7	0.86	0.25	64,71,77,79	0
2	EDO	B	1808	4/4	0.87	0.23	41,43,45,47	0
2	EDO	H	1101	4/4	0.87	0.18	73,73,76,76	0
2	EDO	E	402	4/4	0.88	0.18	49,52,52,54	0
2	EDO	G	1004	4/4	0.88	0.18	68,70,73,74	0
2	EDO	H	1104	4/4	0.88	0.21	54,57,58,59	0
2	EDO	D	407	4/4	0.89	0.46	53,55,59,59	0
2	EDO	A	405	4/4	0.89	0.20	66,68,70,71	0
2	EDO	F	803	4/4	0.90	0.31	78,80,83,84	0
2	EDO	C	404	4/4	0.90	0.25	59,64,65,66	0
3	PEG	F	807	7/7	0.90	0.28	71,83,88,90	0
2	EDO	B	1801	4/4	0.90	0.24	60,62,66,71	0
2	EDO	B	1812	4/4	0.90	0.29	67,73,74,74	0
2	EDO	A	408	4/4	0.90	0.21	49,49,50,50	0
2	EDO	E	404	4/4	0.90	0.19	54,59,59,62	0
2	EDO	D	409	4/4	0.90	0.21	69,70,70,72	0
2	EDO	E	401	4/4	0.91	0.20	60,63,65,65	0
2	EDO	F	812	4/4	0.91	0.14	34,34,34,34	0
2	EDO	B	1804	4/4	0.91	0.17	48,50,51,55	0
2	EDO	F	806	4/4	0.92	0.25	63,67,68,72	0
2	EDO	F	813	4/4	0.92	0.33	20,20,20,20	0
2	EDO	C	406	4/4	0.92	0.22	50,51,56,57	0
2	EDO	F	811	4/4	0.93	0.33	87,88,88,89	0
2	EDO	D	406	4/4	0.93	0.30	58,60,60,61	0
2	EDO	C	403	4/4	0.93	0.29	57,58,58,59	0
2	EDO	H	1102	4/4	0.93	0.22	45,49,50,52	0
2	EDO	D	408	4/4	0.93	0.19	51,56,60,64	0
2	EDO	F	805	4/4	0.93	0.25	56,58,59,60	0
2	EDO	B	1807	4/4	0.93	0.22	58,61,61,64	0
2	EDO	C	402	4/4	0.93	0.22	45,46,47,49	0
2	EDO	G	1009	4/4	0.94	0.28	20,20,20,20	0
2	EDO	G	1010	4/4	0.94	0.28	56,56,57,58	0
2	EDO	A	402	4/4	0.94	0.22	42,43,44,45	0
2	EDO	F	802	4/4	0.94	0.30	51,53,55,57	0
2	EDO	D	401	4/4	0.95	0.17	48,50,53,56	0
2	EDO	F	815	4/4	0.95	0.20	64,65,66,67	0
2	EDO	G	1002	4/4	0.95	0.20	46,47,49,54	0
2	EDO	D	402	4/4	0.95	0.20	51,52,54,58	0
2	EDO	A	415	4/4	0.95	0.13	20,20,20,20	0
2	EDO	B	1803	4/4	0.95	0.17	49,49,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	C	409	4/4	0.95	0.19	60,68,69,70	0
2	EDO	A	409	4/4	0.95	0.21	63,64,65,68	0
2	EDO	G	1001	4/4	0.96	0.16	55,58,60,65	0
2	EDO	B	1805	4/4	0.96	0.18	47,48,49,49	0
2	EDO	G	1003	4/4	0.96	0.21	55,57,60,62	0
2	EDO	F	809	4/4	0.96	0.14	62,62,63,64	0
2	EDO	F	808	4/4	0.97	0.23	62,63,66,67	0
2	EDO	B	1802	4/4	0.97	0.20	37,41,42,43	0
2	EDO	A	417	4/4	0.97	0.13	35,36,38,39	0
2	EDO	E	405	4/4	0.97	0.13	46,46,46,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.