



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 01:05 AM GMT

PDB ID : 3EC7
Title : Crystal Structure of Putative Dehydrogenase from Salmonella typhimurium LT2
Authors : Kim, Y.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-08-29
Resolution : 2.15 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

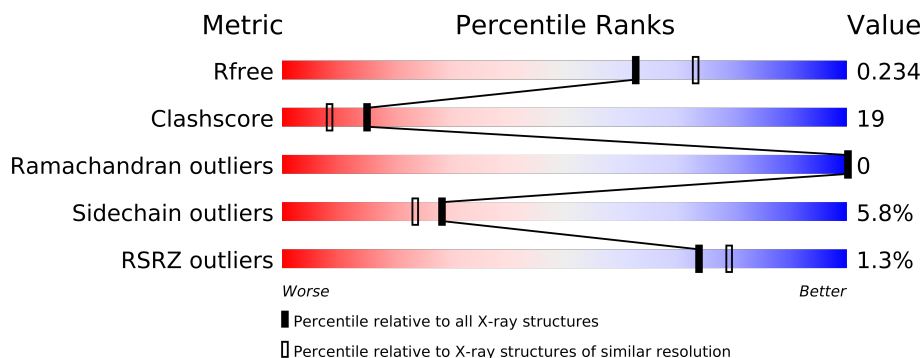
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.15 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}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	
1	C	357	
1	D	357	
1	E	357	
1	F	357	
1	G	357	
1	H	357	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EPE	B	401	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	ACY	A	403	-	X
5	EDO	E	403	-	X
5	EDO	G	402	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23658 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Putative Dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	Se	0	4	0
			2648	1676	445	513	6	8			
1	B	335	Total	C	N	O	S	Se	0	2	0
			2628	1665	443	506	6	8			
1	C	335	Total	C	N	O	S	Se	0	1	0
			2620	1661	442	504	6	7			
1	D	336	Total	C	N	O	S	Se	0	4	0
			2650	1680	446	510	6	8			
1	E	336	Total	C	N	O	S	Se	0	3	0
			2643	1674	446	510	6	7			
1	F	335	Total	C	N	O	S	Se	0	3	0
			2645	1676	446	508	6	9			
1	G	335	Total	C	N	O	S	Se	0	1	0
			2619	1660	441	504	6	8			
1	H	336	Total	C	N	O	S	Se	0	2	0
			2634	1668	443	510	6	7			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	expression tag	UNP Q8ZK57
A	-19	GLY	-	expression tag	UNP Q8ZK57
A	-18	SER	-	expression tag	UNP Q8ZK57
A	-17	SER	-	expression tag	UNP Q8ZK57
A	-16	HIS	-	expression tag	UNP Q8ZK57
A	-15	HIS	-	expression tag	UNP Q8ZK57
A	-14	HIS	-	expression tag	UNP Q8ZK57
A	-13	HIS	-	expression tag	UNP Q8ZK57
A	-12	HIS	-	expression tag	UNP Q8ZK57
A	-11	HIS	-	expression tag	UNP Q8ZK57
A	-10	SER	-	expression tag	UNP Q8ZK57
A	-9	SER	-	expression tag	UNP Q8ZK57
A	-8	GLY	-	expression tag	UNP Q8ZK57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP Q8ZK57
A	-6	GLU	-	expression tag	UNP Q8ZK57
A	-5	ASN	-	expression tag	UNP Q8ZK57
A	-4	LEU	-	expression tag	UNP Q8ZK57
A	-3	TYR	-	expression tag	UNP Q8ZK57
A	-2	PHE	-	expression tag	UNP Q8ZK57
A	-1	GLN	-	expression tag	UNP Q8ZK57
A	0	GLY	-	expression tag	UNP Q8ZK57
B	-20	MSE	-	expression tag	UNP Q8ZK57
B	-19	GLY	-	expression tag	UNP Q8ZK57
B	-18	SER	-	expression tag	UNP Q8ZK57
B	-17	SER	-	expression tag	UNP Q8ZK57
B	-16	HIS	-	expression tag	UNP Q8ZK57
B	-15	HIS	-	expression tag	UNP Q8ZK57
B	-14	HIS	-	expression tag	UNP Q8ZK57
B	-13	HIS	-	expression tag	UNP Q8ZK57
B	-12	HIS	-	expression tag	UNP Q8ZK57
B	-11	HIS	-	expression tag	UNP Q8ZK57
B	-10	SER	-	expression tag	UNP Q8ZK57
B	-9	SER	-	expression tag	UNP Q8ZK57
B	-8	GLY	-	expression tag	UNP Q8ZK57
B	-7	ARG	-	expression tag	UNP Q8ZK57
B	-6	GLU	-	expression tag	UNP Q8ZK57
B	-5	ASN	-	expression tag	UNP Q8ZK57
B	-4	LEU	-	expression tag	UNP Q8ZK57
B	-3	TYR	-	expression tag	UNP Q8ZK57
B	-2	PHE	-	expression tag	UNP Q8ZK57
B	-1	GLN	-	expression tag	UNP Q8ZK57
B	0	GLY	-	expression tag	UNP Q8ZK57
C	-20	MSE	-	expression tag	UNP Q8ZK57
C	-19	GLY	-	expression tag	UNP Q8ZK57
C	-18	SER	-	expression tag	UNP Q8ZK57
C	-17	SER	-	expression tag	UNP Q8ZK57
C	-16	HIS	-	expression tag	UNP Q8ZK57
C	-15	HIS	-	expression tag	UNP Q8ZK57
C	-14	HIS	-	expression tag	UNP Q8ZK57
C	-13	HIS	-	expression tag	UNP Q8ZK57
C	-12	HIS	-	expression tag	UNP Q8ZK57
C	-11	HIS	-	expression tag	UNP Q8ZK57
C	-10	SER	-	expression tag	UNP Q8ZK57
C	-9	SER	-	expression tag	UNP Q8ZK57
C	-8	GLY	-	expression tag	UNP Q8ZK57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ARG	-	expression tag	UNP Q8ZK57
C	-6	GLU	-	expression tag	UNP Q8ZK57
C	-5	ASN	-	expression tag	UNP Q8ZK57
C	-4	LEU	-	expression tag	UNP Q8ZK57
C	-3	TYR	-	expression tag	UNP Q8ZK57
C	-2	PHE	-	expression tag	UNP Q8ZK57
C	-1	GLN	-	expression tag	UNP Q8ZK57
C	0	GLY	-	expression tag	UNP Q8ZK57
D	-20	MSE	-	expression tag	UNP Q8ZK57
D	-19	GLY	-	expression tag	UNP Q8ZK57
D	-18	SER	-	expression tag	UNP Q8ZK57
D	-17	SER	-	expression tag	UNP Q8ZK57
D	-16	HIS	-	expression tag	UNP Q8ZK57
D	-15	HIS	-	expression tag	UNP Q8ZK57
D	-14	HIS	-	expression tag	UNP Q8ZK57
D	-13	HIS	-	expression tag	UNP Q8ZK57
D	-12	HIS	-	expression tag	UNP Q8ZK57
D	-11	HIS	-	expression tag	UNP Q8ZK57
D	-10	SER	-	expression tag	UNP Q8ZK57
D	-9	SER	-	expression tag	UNP Q8ZK57
D	-8	GLY	-	expression tag	UNP Q8ZK57
D	-7	ARG	-	expression tag	UNP Q8ZK57
D	-6	GLU	-	expression tag	UNP Q8ZK57
D	-5	ASN	-	expression tag	UNP Q8ZK57
D	-4	LEU	-	expression tag	UNP Q8ZK57
D	-3	TYR	-	expression tag	UNP Q8ZK57
D	-2	PHE	-	expression tag	UNP Q8ZK57
D	-1	GLN	-	expression tag	UNP Q8ZK57
D	0	GLY	-	expression tag	UNP Q8ZK57
E	-20	MSE	-	expression tag	UNP Q8ZK57
E	-19	GLY	-	expression tag	UNP Q8ZK57
E	-18	SER	-	expression tag	UNP Q8ZK57
E	-17	SER	-	expression tag	UNP Q8ZK57
E	-16	HIS	-	expression tag	UNP Q8ZK57
E	-15	HIS	-	expression tag	UNP Q8ZK57
E	-14	HIS	-	expression tag	UNP Q8ZK57
E	-13	HIS	-	expression tag	UNP Q8ZK57
E	-12	HIS	-	expression tag	UNP Q8ZK57
E	-11	HIS	-	expression tag	UNP Q8ZK57
E	-10	SER	-	expression tag	UNP Q8ZK57
E	-9	SER	-	expression tag	UNP Q8ZK57
E	-8	GLY	-	expression tag	UNP Q8ZK57

Continued on next page...

Continued from previous page...

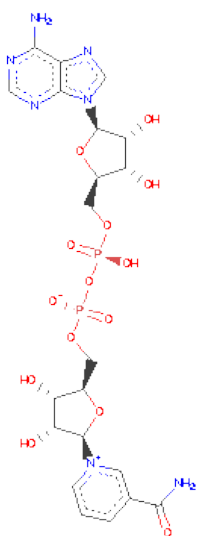
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ARG	-	expression tag	UNP Q8ZK57
E	-6	GLU	-	expression tag	UNP Q8ZK57
E	-5	ASN	-	expression tag	UNP Q8ZK57
E	-4	LEU	-	expression tag	UNP Q8ZK57
E	-3	TYR	-	expression tag	UNP Q8ZK57
E	-2	PHE	-	expression tag	UNP Q8ZK57
E	-1	GLN	-	expression tag	UNP Q8ZK57
E	0	GLY	-	expression tag	UNP Q8ZK57
F	-20	MSE	-	expression tag	UNP Q8ZK57
F	-19	GLY	-	expression tag	UNP Q8ZK57
F	-18	SER	-	expression tag	UNP Q8ZK57
F	-17	SER	-	expression tag	UNP Q8ZK57
F	-16	HIS	-	expression tag	UNP Q8ZK57
F	-15	HIS	-	expression tag	UNP Q8ZK57
F	-14	HIS	-	expression tag	UNP Q8ZK57
F	-13	HIS	-	expression tag	UNP Q8ZK57
F	-12	HIS	-	expression tag	UNP Q8ZK57
F	-11	HIS	-	expression tag	UNP Q8ZK57
F	-10	SER	-	expression tag	UNP Q8ZK57
F	-9	SER	-	expression tag	UNP Q8ZK57
F	-8	GLY	-	expression tag	UNP Q8ZK57
F	-7	ARG	-	expression tag	UNP Q8ZK57
F	-6	GLU	-	expression tag	UNP Q8ZK57
F	-5	ASN	-	expression tag	UNP Q8ZK57
F	-4	LEU	-	expression tag	UNP Q8ZK57
F	-3	TYR	-	expression tag	UNP Q8ZK57
F	-2	PHE	-	expression tag	UNP Q8ZK57
F	-1	GLN	-	expression tag	UNP Q8ZK57
F	0	GLY	-	expression tag	UNP Q8ZK57
G	-20	MSE	-	expression tag	UNP Q8ZK57
G	-19	GLY	-	expression tag	UNP Q8ZK57
G	-18	SER	-	expression tag	UNP Q8ZK57
G	-17	SER	-	expression tag	UNP Q8ZK57
G	-16	HIS	-	expression tag	UNP Q8ZK57
G	-15	HIS	-	expression tag	UNP Q8ZK57
G	-14	HIS	-	expression tag	UNP Q8ZK57
G	-13	HIS	-	expression tag	UNP Q8ZK57
G	-12	HIS	-	expression tag	UNP Q8ZK57
G	-11	HIS	-	expression tag	UNP Q8ZK57
G	-10	SER	-	expression tag	UNP Q8ZK57
G	-9	SER	-	expression tag	UNP Q8ZK57
G	-8	GLY	-	expression tag	UNP Q8ZK57

Continued on next page...

Continued from previous page...

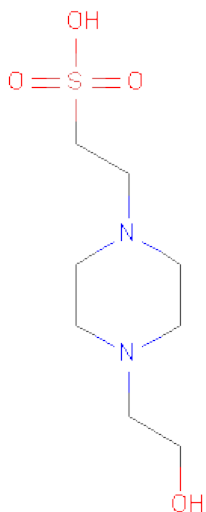
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ARG	-	expression tag	UNP Q8ZK57
G	-6	GLU	-	expression tag	UNP Q8ZK57
G	-5	ASN	-	expression tag	UNP Q8ZK57
G	-4	LEU	-	expression tag	UNP Q8ZK57
G	-3	TYR	-	expression tag	UNP Q8ZK57
G	-2	PHE	-	expression tag	UNP Q8ZK57
G	-1	GLN	-	expression tag	UNP Q8ZK57
G	0	GLY	-	expression tag	UNP Q8ZK57
H	-20	MSE	-	expression tag	UNP Q8ZK57
H	-19	GLY	-	expression tag	UNP Q8ZK57
H	-18	SER	-	expression tag	UNP Q8ZK57
H	-17	SER	-	expression tag	UNP Q8ZK57
H	-16	HIS	-	expression tag	UNP Q8ZK57
H	-15	HIS	-	expression tag	UNP Q8ZK57
H	-14	HIS	-	expression tag	UNP Q8ZK57
H	-13	HIS	-	expression tag	UNP Q8ZK57
H	-12	HIS	-	expression tag	UNP Q8ZK57
H	-11	HIS	-	expression tag	UNP Q8ZK57
H	-10	SER	-	expression tag	UNP Q8ZK57
H	-9	SER	-	expression tag	UNP Q8ZK57
H	-8	GLY	-	expression tag	UNP Q8ZK57
H	-7	ARG	-	expression tag	UNP Q8ZK57
H	-6	GLU	-	expression tag	UNP Q8ZK57
H	-5	ASN	-	expression tag	UNP Q8ZK57
H	-4	LEU	-	expression tag	UNP Q8ZK57
H	-3	TYR	-	expression tag	UNP Q8ZK57
H	-2	PHE	-	expression tag	UNP Q8ZK57
H	-1	GLN	-	expression tag	UNP Q8ZK57
H	0	GLY	-	expression tag	UNP Q8ZK57

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



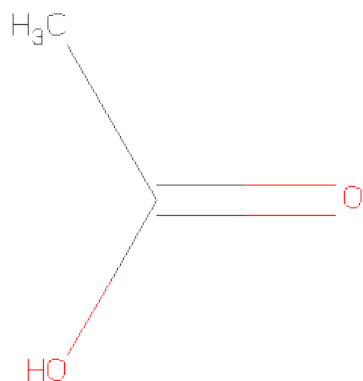
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



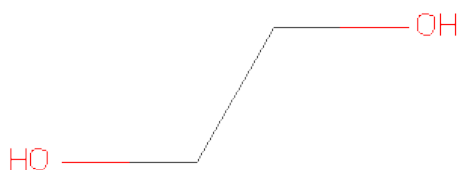
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		

- Molecule 7 is water.

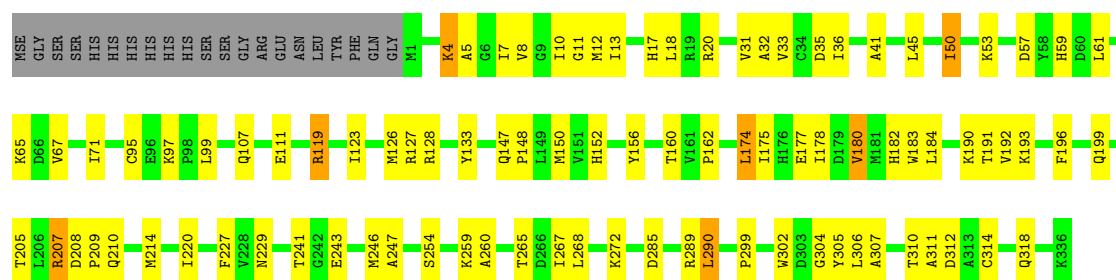
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	321	Total	O	0	0
			321	321		
7	B	264	Total	O	0	0
			264	264		
7	C	226	Total	O	0	0
			226	226		
7	D	260	Total	O	0	0
			260	260		
7	E	282	Total	O	0	0
			282	282		
7	F	231	Total	O	0	0
			231	231		
7	G	219	Total	O	0	0
			219	219		
7	H	266	Total	O	0	0
			266	266		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

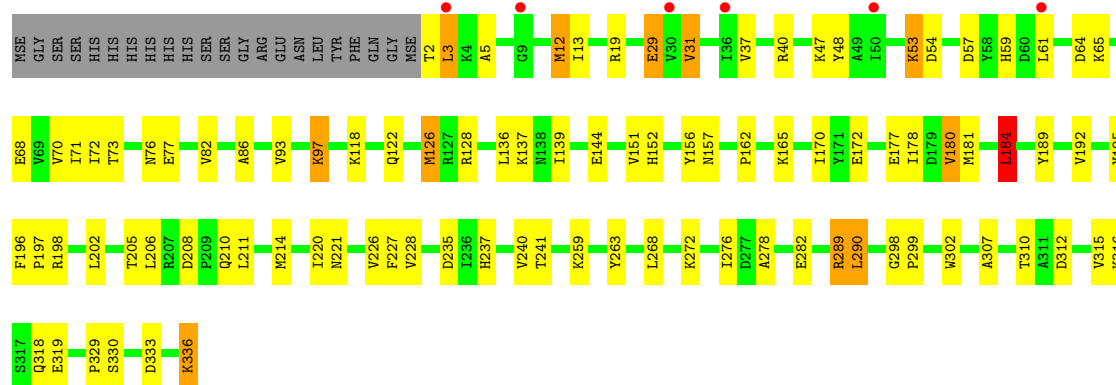
• Molecule 1: Putative Dehydrogenase

Chain A: 



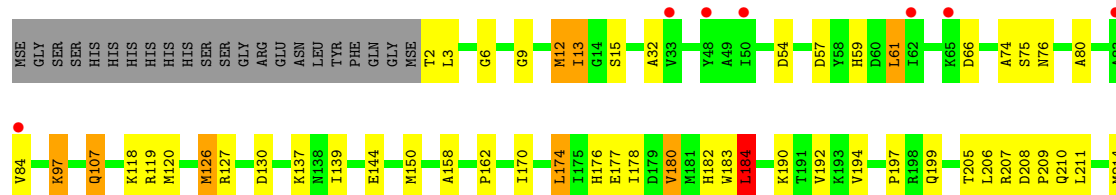
• Molecule 1: Putative Dehydrogenase

Chain B: 



• Molecule 1: Putative Dehydrogenase

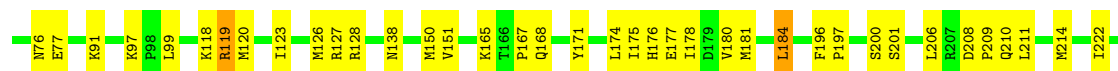
Chain C: 





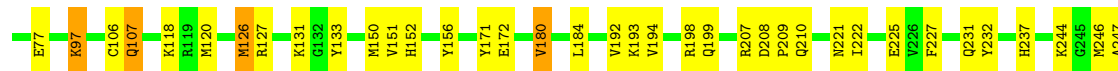
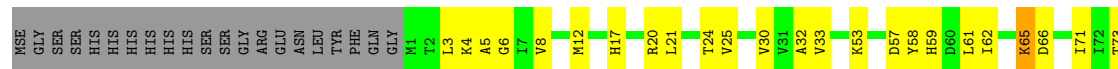
• Molecule 1: Putative Dehydrogenase

Chain D:



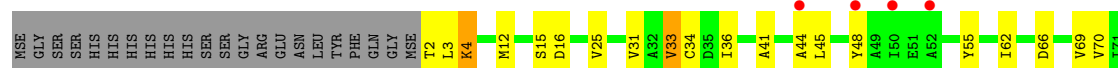
• Molecule 1: Putative Dehydrogenase

Chain E:



• Molecule 1: Putative Dehydrogenase

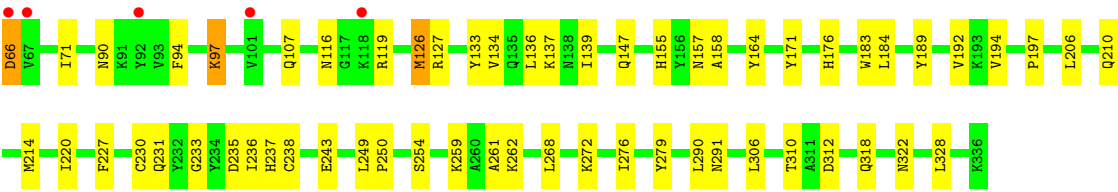
Chain F:



• Molecule 1: Putative Dehydrogenase

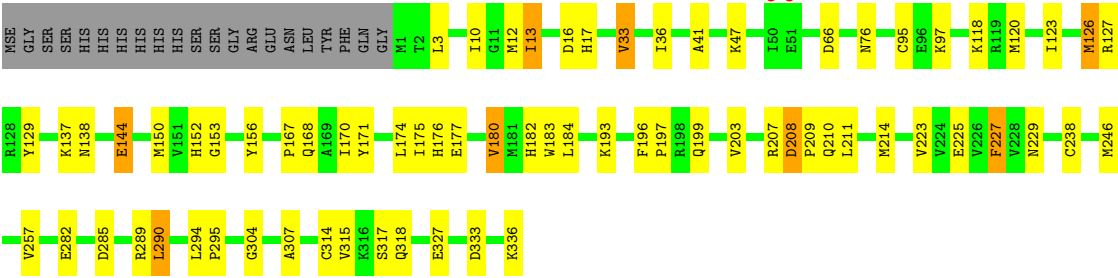
Chain G:





● Molecule 1: Putative Dehydrogenase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.00Å 98.98Å 105.79Å 88.05° 81.78° 89.92°	Depositor
Resolution (Å)	47.00 – 2.15 47.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.00-2.15) 97.9 (47.00-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.176 , 0.231 0.183 , 0.234	Depositor DCC
R_{free} test set	8685 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.813	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
Estimated twinning fraction	0.105 for -h,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 173780 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23658	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, K, EPE, EDO, NAD

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	0.85	1/2692 (0.0%)	0.81	0/3647
1	B	0.79	0/2672	0.76	2/3620 (0.1%)
1	C	0.74	0/2664	0.76	2/3609 (0.1%)
1	D	0.78	0/2694	0.78	2/3649 (0.1%)
1	E	0.81	0/2687	0.76	0/3640
1	F	0.75	0/2689	0.74	1/3642 (0.0%)
1	G	0.72	1/2663 (0.0%)	0.73	0/3608
1	H	0.78	0/2678	0.76	1/3629 (0.0%)
All	All	0.78	2/21439 (0.0%)	0.76	8/29044 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	TYR	CD1-CE1	7.29	1.50	1.39
1	G	261	ALA	CA-CB	5.54	1.64	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	208	ASP	CB-CG-OD1	7.63	125.17	118.30
1	C	208	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	208	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	184	LEU	CB-CG-CD1	6.07	121.32	111.00
1	B	208	ASP	CB-CG-OD1	5.95	123.66	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2648	0	2605	118	0
1	B	2628	0	2593	113	0
1	C	2620	0	2590	109	0
1	D	2650	0	2618	114	0
1	E	2643	0	2607	94	0
1	F	2645	0	2615	116	0
1	G	2619	0	2586	93	0
1	H	2634	0	2593	71	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	4	0
2	D	44	0	26	2	0
2	E	44	0	26	0	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	1	0
3	A	15	0	18	1	0
3	B	15	0	17	2	0
3	C	15	0	17	2	0
3	D	15	0	17	0	0
3	E	15	0	17	1	0
3	F	15	0	18	0	0
3	G	15	0	18	4	0
3	H	15	0	18	0	0
4	A	8	0	6	1	0
5	D	4	0	6	3	0
5	E	8	0	12	3	0
5	G	4	0	6	3	0
5	H	4	0	6	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
7	A	321	0	0	65	0
7	B	264	0	0	54	0
7	C	226	0	0	56	1
7	D	260	0	0	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	282	0	0	58	1
7	F	231	0	0	69	0
7	G	219	0	0	64	0
7	H	266	0	0	41	0
All	All	23658	0	21191	813	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 813 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:151:VAL:HG11	1:D:181:MSE:CE	1.40	1.47
1:C:246:MSE:HG2	7:C:585:HOH:O	1.23	1.32
1:H:210:GLN:HA	7:H:665:HOH:O	1.16	1.31
1:C:176:HIS:HB2	7:C:617:HOH:O	1.28	1.30
1:B:210:GLN:HA	7:B:645:HOH:O	1.32	1.30

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	Distance(Å)	Clash(Å)
7:C:607:HOH:O	7:E:703:HOH:O[1_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	338/357 (95%)	328 (97%)	10 (3%)	0	100	100
1	B	335/357 (94%)	322 (96%)	13 (4%)	0	100	100
1	C	334/357 (94%)	322 (96%)	12 (4%)	0	100	100
1	D	338/357 (95%)	326 (96%)	12 (4%)	0	100	100
1	E	337/357 (94%)	325 (96%)	12 (4%)	0	100	100
1	F	337/357 (94%)	321 (95%)	16 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	334/357 (94%)	319 (96%)	15 (4%)	0	100	100
1	H	336/357 (94%)	324 (96%)	12 (4%)	0	100	100
All	All	2689/2856 (94%)	2587 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/290 (98%)	271 (95%)	13 (5%)	37	34
1	B	282/290 (97%)	256 (91%)	26 (9%)	13	8
1	C	281/290 (97%)	262 (93%)	19 (7%)	22	17
1	D	284/290 (98%)	266 (94%)	18 (6%)	25	20
1	E	283/290 (98%)	270 (95%)	13 (5%)	37	34
1	F	284/290 (98%)	267 (94%)	17 (6%)	27	22
1	G	281/290 (97%)	269 (96%)	12 (4%)	40	38
1	H	282/290 (97%)	269 (95%)	13 (5%)	37	34
All	All	2261/2320 (98%)	2130 (94%)	131 (6%)	28	23

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4	LYS
1	D	290	LEU
1	H	36	ILE
1	D	36	ILE
1	D	126	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	322	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	76	ASN
1	H	88	ASN
1	D	76	ASN
1	D	231	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	NAD	A	400	-	48,48,48	1.35	4 (8%)	73,73,73	2.20	15 (20%)
3	EPE	A	401	-	15,15,15	0.94	1 (6%)	20,20,20	2.41	5 (25%)
4	ACY	A	402	-	3,3,3	0.66	0	3,3,3	0.80	0
4	ACY	A	403	-	3,3,3	0.66	0	3,3,3	0.74	0
2	NAD	B	400	-	48,48,48	1.49	5 (10%)	73,73,73	1.81	8 (10%)
3	EPE	B	401	-	15,15,15	1.12	1 (6%)	20,20,20	1.99	6 (30%)
2	NAD	C	400	-	48,48,48	1.36	3 (6%)	73,73,73	1.71	8 (10%)
3	EPE	C	401	-	15,15,15	1.04	1 (6%)	20,20,20	2.56	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	400	-	48,48,48	1.46	3 (6%)	73,73,73	1.76	10 (13%)
3	EPE	D	401	-	15,15,15	0.94	1 (6%)	20,20,20	2.18	6 (30%)
5	EDO	D	402	-	3,3,3	0.35	0	2,2,2	0.85	0
2	NAD	E	400	-	48,48,48	1.50	4 (8%)	73,73,73	1.94	7 (9%)
3	EPE	E	401	-	15,15,15	0.98	1 (6%)	20,20,20	4.06	11 (55%)
5	EDO	E	402	-	3,3,3	0.54	0	2,2,2	0.83	0
5	EDO	E	403	-	3,3,3	0.34	0	2,2,2	1.06	0
2	NAD	F	400	-	48,48,48	1.47	5 (10%)	73,73,73	1.72	7 (9%)
3	EPE	F	401	-	15,15,15	1.09	1 (6%)	20,20,20	1.86	5 (25%)
2	NAD	G	400	-	48,48,48	1.37	3 (6%)	73,73,73	1.84	10 (13%)
3	EPE	G	401	-	15,15,15	1.03	1 (6%)	20,20,20	2.30	9 (45%)
5	EDO	G	402	-	3,3,3	0.57	0	2,2,2	0.43	0
2	NAD	H	400	-	48,48,48	1.40	3 (6%)	73,73,73	1.80	13 (17%)
3	EPE	H	401	-	15,15,15	1.07	1 (6%)	20,20,20	2.19	6 (30%)
5	EDO	H	402	-	3,3,3	0.53	0	2,2,2	0.93	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	NAD	A	400	-	-	0/30/62/62	0/3/5/5
3	EPE	A	401	-	-	0/9/19/19	0/1/1/1
4	ACY	A	402	-	-	0/0/0/0	0/0/0/0
4	ACY	A	403	-	-	0/0/0/0	0/0/0/0
2	NAD	B	400	-	-	0/30/62/62	0/3/5/5
3	EPE	B	401	-	-	0/9/19/19	0/1/1/1
2	NAD	C	400	-	-	0/30/62/62	0/3/5/5
3	EPE	C	401	-	-	0/9/19/19	0/1/1/1
2	NAD	D	400	-	-	0/30/62/62	0/3/5/5
3	EPE	D	401	-	-	0/9/19/19	0/1/1/1
5	EDO	D	402	-	-	0/1/1/1	0/0/0/0
2	NAD	E	400	-	-	0/30/62/62	0/3/5/5
3	EPE	E	401	-	-	0/9/19/19	0/1/1/1
5	EDO	E	402	-	-	0/1/1/1	0/0/0/0
5	EDO	E	403	-	-	0/1/1/1	0/0/0/0
2	NAD	F	400	-	-	0/30/62/62	0/3/5/5
3	EPE	F	401	-	-	0/9/19/19	0/1/1/1
2	NAD	G	400	-	-	0/30/62/62	0/3/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	G	401	-	-	0/9/19/19	0/1/1/1
5	EDO	G	402	-	-	0/1/1/1	0/0/0/0
2	NAD	H	400	-	-	0/30/62/62	0/3/5/5
3	EPE	H	401	-	-	0/9/19/19	0/1/1/1
5	EDO	H	402	-	-	0/1/1/1	0/0/0/0

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	NAD	O7N-C7N	7.49	1.41	1.24
2	B	400	NAD	O7N-C7N	7.44	1.41	1.24
2	D	400	NAD	O7N-C7N	7.25	1.41	1.24
2	H	400	NAD	O7N-C7N	7.15	1.40	1.24
2	F	400	NAD	O7N-C7N	7.15	1.40	1.24

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAD	N3A-C2A-N1A	-12.23	118.48	128.71
2	E	400	NAD	N3A-C2A-N1A	-12.01	118.67	128.71
2	B	400	NAD	N3A-C2A-N1A	-11.59	119.02	128.71
2	G	400	NAD	N3A-C2A-N1A	-11.33	119.23	128.71
3	E	401	EPE	O3S-S-C10	11.06	119.94	105.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	336/357 (94%)	-0.20	0 100 100	11, 19, 30, 37	0
1	B	335/357 (93%)	-0.06	6 (1%) 65 71	12, 21, 34, 40	0
1	C	335/357 (93%)	0.05	7 (2%) 60 65	11, 23, 37, 43	0
1	D	336/357 (94%)	-0.13	1 (0%) 91 95	10, 21, 34, 42	0
1	E	336/357 (94%)	-0.17	0 100 100	12, 21, 31, 37	0
1	F	335/357 (93%)	0.04	7 (2%) 60 65	11, 24, 37, 47	0
1	G	335/357 (93%)	0.10	12 (3%) 41 44	11, 23, 37, 47	0
1	H	336/357 (94%)	-0.14	2 (0%) 86 90	11, 20, 33, 43	0
All	All	2684/2856 (93%)	-0.06	35 (1%) 74 79	10, 21, 35, 47	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	ILE	4.2
1	C	65	LYS	4.2
1	F	44	ALA	3.8
1	C	62	ILE	3.7
1	C	33	VAL	3.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACY	A	403	4/4	0.20	9.17	36,36,36,36	0
3	EPE	B	401	15/15	0.13	3.13	37,40,52,53	0
5	EDO	E	403	4/4	0.15	2.67	50,52,53,53	0
5	EDO	G	402	4/4	0.14	2.29	39,41,41,44	0
4	ACY	A	402	4/4	0.14	1.75	53,53,53,53	0
6	K	D	403	1/1	0.15	1.42	73,73,73,73	0
5	EDO	E	402	4/4	0.14	1.08	21,23,29,32	0
3	EPE	F	401	15/15	0.12	1.01	38,41,47,50	0
3	EPE	H	401	15/15	0.13	0.96	37,39,45,48	0
6	K	H	403	1/1	0.12	0.81	65,65,65,65	0
3	EPE	A	401	15/15	0.12	0.77	32,35,38,41	0
2	NAD	F	400	44/44	0.11	-0.17	30,43,53,56	0
3	EPE	C	401	15/15	0.10	-0.27	43,45,48,49	0
2	NAD	B	400	44/44	0.11	-0.36	33,44,53,55	0
3	EPE	G	401	15/15	0.10	-0.45	40,42,50,51	0
2	NAD	C	400	44/44	0.10	-0.51	37,46,54,54	0
3	EPE	D	401	15/15	0.10	-0.53	33,36,41,44	0
2	NAD	A	400	44/44	0.10	-0.63	25,31,34,38	0
2	NAD	H	400	44/44	0.10	-0.73	32,38,44,46	0
2	NAD	D	400	44/44	0.10	-0.74	30,39,46,48	0
2	NAD	G	400	44/44	0.11	-0.80	35,44,51,54	0
2	NAD	E	400	44/44	0.10	-0.84	24,37,44,45	0
3	EPE	E	401	15/15	0.10	-1.33	26,30,37,38	0
5	EDO	H	402	4/4	0.09	-1.36	20,24,25,34	0
5	EDO	D	402	4/4	0.10	-1.42	29,29,33,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.