



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2017 – 11:10 AM EDT

PDB ID : 5VG6
Title : Crystal structure of D-isomer specific 2-hydroxyacid dehydrogenase from Xanthobacter autotrophicus Py2 in complex with NADPH and MES.
Authors : Lipowska, J.; Shabalin, I.G.; Kutner, J.; Gasiorowska, O.A.; Almo, S.C.; Minor, W.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : unknown
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

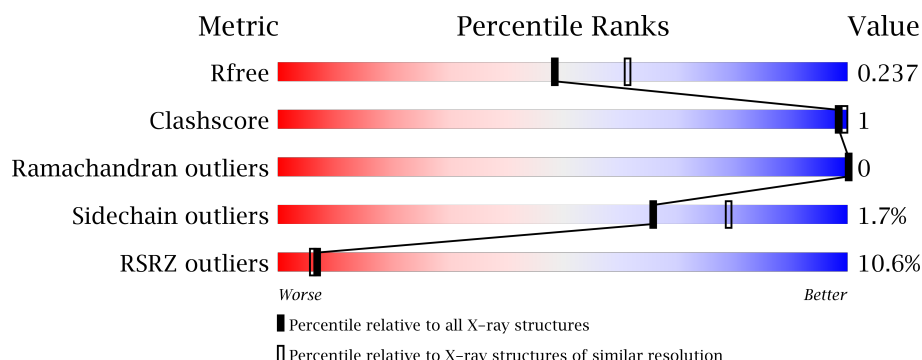
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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	341	<div> <div>87%</div> <div>5% 8%</div> </div>
1	B	341	<div>6%</div> <div>91% 8%</div>
1	C	341	<div>2%</div> <div>90% 8%</div>
1	D	341	<div>27%</div> <div>86% 10%</div>
1	E	341	<div>4%</div> <div>90% 8%</div>

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Mol	Chain	Length	Quality of chain
1	F	341	
1	G	341	
1	H	341	
1	I	341	
1	J	341	

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
3	MES	B	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25838 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 D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	3	0
			2415	1537	445	425	8			
1	B	315	Total	C	N	O	S	0	0	0
			2387	1521	435	423	8			
1	C	315	Total	C	N	O	S	0	1	0
			2400	1530	433	429	8			
1	D	308	Total	C	N	O	S	0	0	0
			2274	1453	409	404	8			
1	E	314	Total	C	N	O	S	0	1	0
			2385	1520	432	425	8			
1	F	312	Total	C	N	O	S	0	0	0
			2284	1461	411	404	8			
1	G	242	Total	C	N	O	S	0	0	0
			1796	1142	323	323	8			
1	H	242	Total	C	N	O	S	0	0	0
			1789	1134	324	323	8			
1	I	315	Total	C	N	O	S	0	3	0
			2412	1537	437	430	8			
1	J	315	Total	C	N	O	S	0	3	0
			2428	1544	447	429	8			

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A7IIH0
A	-20	HIS	-	expression tag	UNP A7IIH0
A	-19	HIS	-	expression tag	UNP A7IIH0
A	-18	HIS	-	expression tag	UNP A7IIH0
A	-17	HIS	-	expression tag	UNP A7IIH0
A	-16	HIS	-	expression tag	UNP A7IIH0
A	-15	HIS	-	expression tag	UNP A7IIH0
A	-14	SER	-	expression tag	UNP A7IIH0
A	-13	SER	-	expression tag	UNP A7IIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	expression tag	UNP A7IIH0
A	-11	VAL	-	expression tag	UNP A7IIH0
A	-10	ASP	-	expression tag	UNP A7IIH0
A	-9	LEU	-	expression tag	UNP A7IIH0
A	-8	GLY	-	expression tag	UNP A7IIH0
A	-7	THR	-	expression tag	UNP A7IIH0
A	-6	GLU	-	expression tag	UNP A7IIH0
A	-5	ASN	-	expression tag	UNP A7IIH0
A	-4	LEU	-	expression tag	UNP A7IIH0
A	-3	TYR	-	expression tag	UNP A7IIH0
A	-2	PHE	-	expression tag	UNP A7IIH0
A	-1	GLN	-	expression tag	UNP A7IIH0
A	0	SER	-	expression tag	UNP A7IIH0
B	-21	MET	-	initiating methionine	UNP A7IIH0
B	-20	HIS	-	expression tag	UNP A7IIH0
B	-19	HIS	-	expression tag	UNP A7IIH0
B	-18	HIS	-	expression tag	UNP A7IIH0
B	-17	HIS	-	expression tag	UNP A7IIH0
B	-16	HIS	-	expression tag	UNP A7IIH0
B	-15	HIS	-	expression tag	UNP A7IIH0
B	-14	SER	-	expression tag	UNP A7IIH0
B	-13	SER	-	expression tag	UNP A7IIH0
B	-12	GLY	-	expression tag	UNP A7IIH0
B	-11	VAL	-	expression tag	UNP A7IIH0
B	-10	ASP	-	expression tag	UNP A7IIH0
B	-9	LEU	-	expression tag	UNP A7IIH0
B	-8	GLY	-	expression tag	UNP A7IIH0
B	-7	THR	-	expression tag	UNP A7IIH0
B	-6	GLU	-	expression tag	UNP A7IIH0
B	-5	ASN	-	expression tag	UNP A7IIH0
B	-4	LEU	-	expression tag	UNP A7IIH0
B	-3	TYR	-	expression tag	UNP A7IIH0
B	-2	PHE	-	expression tag	UNP A7IIH0
B	-1	GLN	-	expression tag	UNP A7IIH0
B	0	SER	-	expression tag	UNP A7IIH0
C	-21	MET	-	initiating methionine	UNP A7IIH0
C	-20	HIS	-	expression tag	UNP A7IIH0
C	-19	HIS	-	expression tag	UNP A7IIH0
C	-18	HIS	-	expression tag	UNP A7IIH0
C	-17	HIS	-	expression tag	UNP A7IIH0
C	-16	HIS	-	expression tag	UNP A7IIH0
C	-15	HIS	-	expression tag	UNP A7IIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	SER	-	expression tag	UNP A7IIH0
C	-13	SER	-	expression tag	UNP A7IIH0
C	-12	GLY	-	expression tag	UNP A7IIH0
C	-11	VAL	-	expression tag	UNP A7IIH0
C	-10	ASP	-	expression tag	UNP A7IIH0
C	-9	LEU	-	expression tag	UNP A7IIH0
C	-8	GLY	-	expression tag	UNP A7IIH0
C	-7	THR	-	expression tag	UNP A7IIH0
C	-6	GLU	-	expression tag	UNP A7IIH0
C	-5	ASN	-	expression tag	UNP A7IIH0
C	-4	LEU	-	expression tag	UNP A7IIH0
C	-3	TYR	-	expression tag	UNP A7IIH0
C	-2	PHE	-	expression tag	UNP A7IIH0
C	-1	GLN	-	expression tag	UNP A7IIH0
C	0	SER	-	expression tag	UNP A7IIH0
D	-21	MET	-	initiating methionine	UNP A7IIH0
D	-20	HIS	-	expression tag	UNP A7IIH0
D	-19	HIS	-	expression tag	UNP A7IIH0
D	-18	HIS	-	expression tag	UNP A7IIH0
D	-17	HIS	-	expression tag	UNP A7IIH0
D	-16	HIS	-	expression tag	UNP A7IIH0
D	-15	HIS	-	expression tag	UNP A7IIH0
D	-14	SER	-	expression tag	UNP A7IIH0
D	-13	SER	-	expression tag	UNP A7IIH0
D	-12	GLY	-	expression tag	UNP A7IIH0
D	-11	VAL	-	expression tag	UNP A7IIH0
D	-10	ASP	-	expression tag	UNP A7IIH0
D	-9	LEU	-	expression tag	UNP A7IIH0
D	-8	GLY	-	expression tag	UNP A7IIH0
D	-7	THR	-	expression tag	UNP A7IIH0
D	-6	GLU	-	expression tag	UNP A7IIH0
D	-5	ASN	-	expression tag	UNP A7IIH0
D	-4	LEU	-	expression tag	UNP A7IIH0
D	-3	TYR	-	expression tag	UNP A7IIH0
D	-2	PHE	-	expression tag	UNP A7IIH0
D	-1	GLN	-	expression tag	UNP A7IIH0
D	0	SER	-	expression tag	UNP A7IIH0
E	-21	MET	-	initiating methionine	UNP A7IIH0
E	-20	HIS	-	expression tag	UNP A7IIH0
E	-19	HIS	-	expression tag	UNP A7IIH0
E	-18	HIS	-	expression tag	UNP A7IIH0
E	-17	HIS	-	expression tag	UNP A7IIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP A7IIH0
E	-15	HIS	-	expression tag	UNP A7IIH0
E	-14	SER	-	expression tag	UNP A7IIH0
E	-13	SER	-	expression tag	UNP A7IIH0
E	-12	GLY	-	expression tag	UNP A7IIH0
E	-11	VAL	-	expression tag	UNP A7IIH0
E	-10	ASP	-	expression tag	UNP A7IIH0
E	-9	LEU	-	expression tag	UNP A7IIH0
E	-8	GLY	-	expression tag	UNP A7IIH0
E	-7	THR	-	expression tag	UNP A7IIH0
E	-6	GLU	-	expression tag	UNP A7IIH0
E	-5	ASN	-	expression tag	UNP A7IIH0
E	-4	LEU	-	expression tag	UNP A7IIH0
E	-3	TYR	-	expression tag	UNP A7IIH0
E	-2	PHE	-	expression tag	UNP A7IIH0
E	-1	GLN	-	expression tag	UNP A7IIH0
E	0	SER	-	expression tag	UNP A7IIH0
F	-21	MET	-	initiating methionine	UNP A7IIH0
F	-20	HIS	-	expression tag	UNP A7IIH0
F	-19	HIS	-	expression tag	UNP A7IIH0
F	-18	HIS	-	expression tag	UNP A7IIH0
F	-17	HIS	-	expression tag	UNP A7IIH0
F	-16	HIS	-	expression tag	UNP A7IIH0
F	-15	HIS	-	expression tag	UNP A7IIH0
F	-14	SER	-	expression tag	UNP A7IIH0
F	-13	SER	-	expression tag	UNP A7IIH0
F	-12	GLY	-	expression tag	UNP A7IIH0
F	-11	VAL	-	expression tag	UNP A7IIH0
F	-10	ASP	-	expression tag	UNP A7IIH0
F	-9	LEU	-	expression tag	UNP A7IIH0
F	-8	GLY	-	expression tag	UNP A7IIH0
F	-7	THR	-	expression tag	UNP A7IIH0
F	-6	GLU	-	expression tag	UNP A7IIH0
F	-5	ASN	-	expression tag	UNP A7IIH0
F	-4	LEU	-	expression tag	UNP A7IIH0
F	-3	TYR	-	expression tag	UNP A7IIH0
F	-2	PHE	-	expression tag	UNP A7IIH0
F	-1	GLN	-	expression tag	UNP A7IIH0
F	0	SER	-	expression tag	UNP A7IIH0
G	-21	MET	-	initiating methionine	UNP A7IIH0
G	-20	HIS	-	expression tag	UNP A7IIH0
G	-19	HIS	-	expression tag	UNP A7IIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	HIS	-	expression tag	UNP A7IIH0
G	-17	HIS	-	expression tag	UNP A7IIH0
G	-16	HIS	-	expression tag	UNP A7IIH0
G	-15	HIS	-	expression tag	UNP A7IIH0
G	-14	SER	-	expression tag	UNP A7IIH0
G	-13	SER	-	expression tag	UNP A7IIH0
G	-12	GLY	-	expression tag	UNP A7IIH0
G	-11	VAL	-	expression tag	UNP A7IIH0
G	-10	ASP	-	expression tag	UNP A7IIH0
G	-9	LEU	-	expression tag	UNP A7IIH0
G	-8	GLY	-	expression tag	UNP A7IIH0
G	-7	THR	-	expression tag	UNP A7IIH0
G	-6	GLU	-	expression tag	UNP A7IIH0
G	-5	ASN	-	expression tag	UNP A7IIH0
G	-4	LEU	-	expression tag	UNP A7IIH0
G	-3	TYR	-	expression tag	UNP A7IIH0
G	-2	PHE	-	expression tag	UNP A7IIH0
G	-1	GLN	-	expression tag	UNP A7IIH0
G	0	SER	-	expression tag	UNP A7IIH0
H	-21	MET	-	initiating methionine	UNP A7IIH0
H	-20	HIS	-	expression tag	UNP A7IIH0
H	-19	HIS	-	expression tag	UNP A7IIH0
H	-18	HIS	-	expression tag	UNP A7IIH0
H	-17	HIS	-	expression tag	UNP A7IIH0
H	-16	HIS	-	expression tag	UNP A7IIH0
H	-15	HIS	-	expression tag	UNP A7IIH0
H	-14	SER	-	expression tag	UNP A7IIH0
H	-13	SER	-	expression tag	UNP A7IIH0
H	-12	GLY	-	expression tag	UNP A7IIH0
H	-11	VAL	-	expression tag	UNP A7IIH0
H	-10	ASP	-	expression tag	UNP A7IIH0
H	-9	LEU	-	expression tag	UNP A7IIH0
H	-8	GLY	-	expression tag	UNP A7IIH0
H	-7	THR	-	expression tag	UNP A7IIH0
H	-6	GLU	-	expression tag	UNP A7IIH0
H	-5	ASN	-	expression tag	UNP A7IIH0
H	-4	LEU	-	expression tag	UNP A7IIH0
H	-3	TYR	-	expression tag	UNP A7IIH0
H	-2	PHE	-	expression tag	UNP A7IIH0
H	-1	GLN	-	expression tag	UNP A7IIH0
H	0	SER	-	expression tag	UNP A7IIH0
I	-21	MET	-	initiating methionine	UNP A7IIH0

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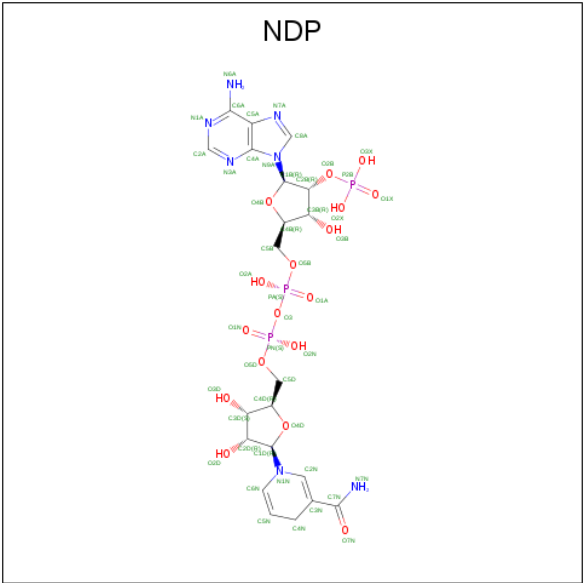
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I	-19	HIS	-	expression tag	UNP A7IIH0
I	-18	HIS	-	expression tag	UNP A7IIH0
I	-17	HIS	-	expression tag	UNP A7IIH0
I	-16	HIS	-	expression tag	UNP A7IIH0
I	-15	HIS	-	expression tag	UNP A7IIH0
I	-14	SER	-	expression tag	UNP A7IIH0
I	-13	SER	-	expression tag	UNP A7IIH0
I	-12	GLY	-	expression tag	UNP A7IIH0
I	-11	VAL	-	expression tag	UNP A7IIH0
I	-10	ASP	-	expression tag	UNP A7IIH0
I	-9	LEU	-	expression tag	UNP A7IIH0
I	-8	GLY	-	expression tag	UNP A7IIH0
I	-7	THR	-	expression tag	UNP A7IIH0
I	-6	GLU	-	expression tag	UNP A7IIH0
I	-5	ASN	-	expression tag	UNP A7IIH0
I	-4	LEU	-	expression tag	UNP A7IIH0
I	-3	TYR	-	expression tag	UNP A7IIH0
I	-2	PHE	-	expression tag	UNP A7IIH0
I	-1	GLN	-	expression tag	UNP A7IIH0
I	0	SER	-	expression tag	UNP A7IIH0
J	-21	MET	-	initiating methionine	UNP A7IIH0
J	-20	HIS	-	expression tag	UNP A7IIH0
J	-19	HIS	-	expression tag	UNP A7IIH0
J	-18	HIS	-	expression tag	UNP A7IIH0
J	-17	HIS	-	expression tag	UNP A7IIH0
J	-16	HIS	-	expression tag	UNP A7IIH0
J	-15	HIS	-	expression tag	UNP A7IIH0
J	-14	SER	-	expression tag	UNP A7IIH0
J	-13	SER	-	expression tag	UNP A7IIH0
J	-12	GLY	-	expression tag	UNP A7IIH0
J	-11	VAL	-	expression tag	UNP A7IIH0
J	-10	ASP	-	expression tag	UNP A7IIH0
J	-9	LEU	-	expression tag	UNP A7IIH0
J	-8	GLY	-	expression tag	UNP A7IIH0
J	-7	THR	-	expression tag	UNP A7IIH0
J	-6	GLU	-	expression tag	UNP A7IIH0
J	-5	ASN	-	expression tag	UNP A7IIH0
J	-4	LEU	-	expression tag	UNP A7IIH0
J	-3	TYR	-	expression tag	UNP A7IIH0
J	-2	PHE	-	expression tag	UNP A7IIH0
J	-1	GLN	-	expression tag	UNP A7IIH0

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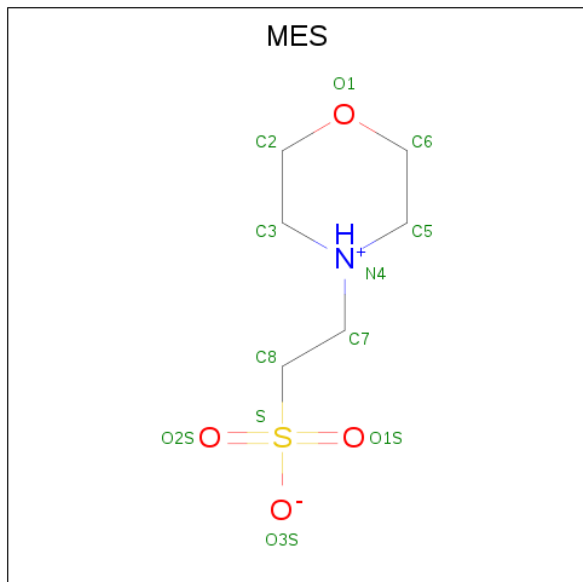
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	expression tag	UNP A7IIH0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	456	Total	O	0	0
			456	456		

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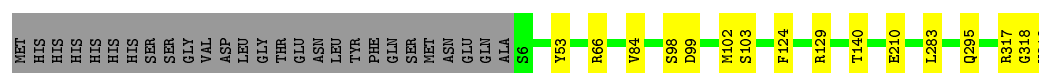
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	301	Total 301	O 301	0	0
4	C	420	Total 420	O 420	0	0
4	D	86	Total 86	O 86	0	0
4	E	304	Total 304	O 304	0	0
4	F	86	Total 86	O 86	0	0
4	G	75	Total 75	O 75	0	0
4	H	77	Total 77	O 77	0	0
4	I	422	Total 422	O 422	0	0
4	J	453	Total 453	O 453	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

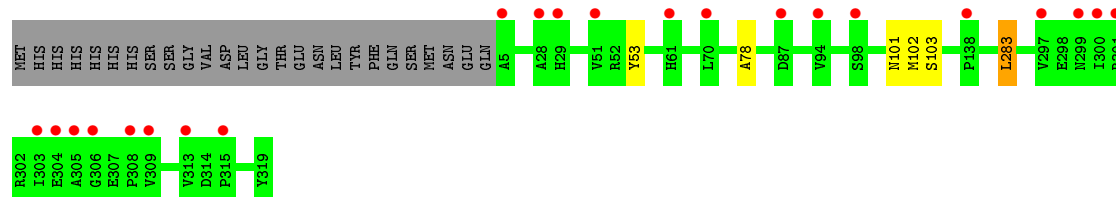
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

Chain A: 




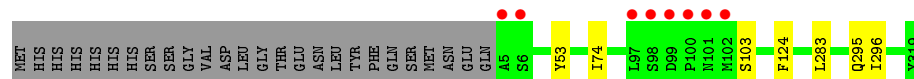
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

Chain B: 




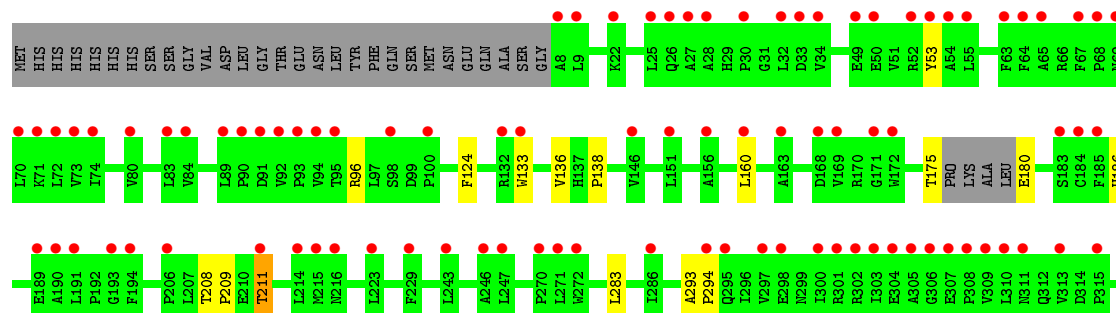
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

Chain C: 

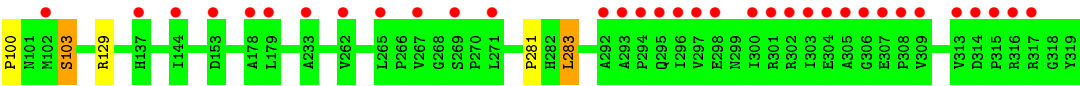


- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

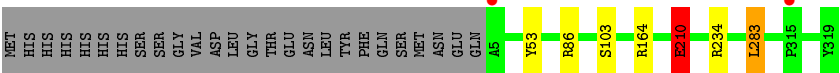
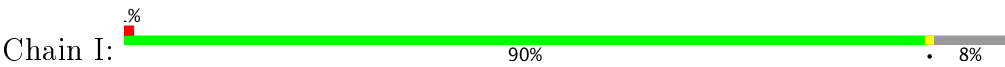
Chain D: 



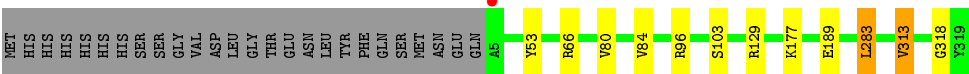
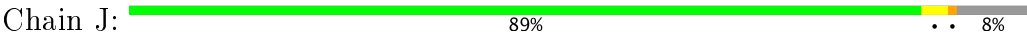
ALA	GLY	ASP	GLY	HIS	VAL	GLU	GLY	ASP	PRO	GLU	GLU	VAL	ARG	TYR	ALA	ALA	LEU	VAL	TRP	LYS	PRO	PRO	HIS	GLY	PHE	PHE	ALA	ALA	ARG	PHE	PRO	ASN	LEU	LEU	LYS	VAL	ILE	ASN	LEU	GLY	A78	G79	V80	L83	V84	A85	R86	D87	D88	L89	F90	F90	D91	V92	F93	V94	T95	R96	L97	S98	P99
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● Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding



● Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	132.51Å 311.04Å 98.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 44.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.20) 99.8 (44.43-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.233 0.203 , 0.237	Depositor DCC
R_{free} test set	10343 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25838	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.96 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6117e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, MES

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	0.53	0/2489	0.72	2/3391 (0.1%)
1	B	0.44	0/2447	0.68	0/3338
1	C	0.49	0/2463	0.69	0/3360
1	D	0.43	0/2331	0.68	0/3187
1	E	0.43	0/2448	0.69	1/3341 (0.0%)
1	F	0.42	0/2341	0.68	1/3205 (0.0%)
1	G	0.42	0/1838	0.71	2/2512 (0.1%)
1	H	0.45	0/1831	0.71	3/2502 (0.1%)
1	I	0.47	0/2485	0.72	4/3388 (0.1%)
1	J	0.54	0/2497	0.73	2/3402 (0.1%)
All	All	0.47	0/23170	0.70	15/31626 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	210[A]	GLU	CA-CB-CG	7.03	128.87	113.40
1	I	210[B]	GLU	CA-CB-CG	7.03	128.87	113.40
1	G	129	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	H	129	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	H	99	ASP	CB-CG-OD1	-6.18	112.73	118.30

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	2415	0	2428	7	0
1	B	2387	0	2375	3	0
1	C	2400	0	2397	2	0
1	D	2274	0	2198	9	0
1	E	2385	0	2372	2	0
1	F	2284	0	2215	6	0
1	G	1796	0	1773	1	0
1	H	1789	0	1743	3	0
1	I	2412	0	2414	3	0
1	J	2428	0	2442	5	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
2	E	48	0	26	0	0
2	F	48	0	26	1	0
2	G	48	0	26	0	0
2	H	48	0	26	0	0
2	I	48	0	26	0	0
2	J	48	0	26	0	0
3	A	24	0	26	0	0
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	0	0
3	E	12	0	13	0	0
3	F	12	0	13	0	0
3	I	12	0	13	0	0
3	J	12	0	13	0	0
4	A	456	0	0	1	0
4	B	301	0	0	0	0
4	C	420	0	0	0	0
4	D	86	0	0	0	0
4	E	304	0	0	0	0
4	F	86	0	0	0	0
4	G	75	0	0	0	0
4	H	77	0	0	0	0
4	I	422	0	0	1	0
4	J	453	0	0	2	0
All	All	25838	0	22734	34	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 1.

The worst 5 of 34 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:D:208:THR:OG1	1:D:211:THR:HG23	1.66	0.93
1:A:99:ASP:H	1:A:102:MET:HE3	1.53	0.73
1:D:175:THR:O	1:D:186:HIS:ND1	2.23	0.72
1:I:210[B]:GLU:OE1	4:I:501:HOH:O	2.10	0.69
1:B:78:ALA:HB2	1:B:102:MET:HE3	1.74	0.69

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	315/341 (92%)	309 (98%)	6 (2%)	0	100	100
1	B	313/341 (92%)	306 (98%)	7 (2%)	0	100	100
1	C	314/341 (92%)	307 (98%)	7 (2%)	0	100	100
1	D	304/341 (89%)	297 (98%)	7 (2%)	0	100	100
1	E	313/341 (92%)	306 (98%)	7 (2%)	0	100	100
1	F	310/341 (91%)	303 (98%)	7 (2%)	0	100	100
1	G	240/341 (70%)	235 (98%)	5 (2%)	0	100	100
1	H	240/341 (70%)	236 (98%)	4 (2%)	0	100	100
1	I	316/341 (93%)	310 (98%)	6 (2%)	0	100	100
1	J	316/341 (93%)	310 (98%)	6 (2%)	0	100	100
All	All	2981/3410 (87%)	2919 (98%)	62 (2%)	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	248/270 (92%)	243 (98%)	5 (2%)	60	74
1	B	240/270 (89%)	236 (98%)	4 (2%)	66	79
1	C	245/270 (91%)	241 (98%)	4 (2%)	68	81
1	D	218/270 (81%)	215 (99%)	3 (1%)	71	84
1	E	242/270 (90%)	238 (98%)	4 (2%)	66	79
1	F	217/270 (80%)	212 (98%)	5 (2%)	56	69
1	G	179/270 (66%)	176 (98%)	3 (2%)	66	79
1	H	175/270 (65%)	173 (99%)	2 (1%)	78	88
1	I	247/270 (92%)	242 (98%)	5 (2%)	60	74
1	J	249/270 (92%)	244 (98%)	5 (2%)	60	74
All	All	2260/2700 (84%)	2220 (98%)	40 (2%)	66	77

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	103	SER
1	F	207	LEU
1	J	103	SER
1	F	53	TYR
1	F	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	I	295	GLN
1	I	311	ASN
1	J	295	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

19 ligands are modelled in this entry.

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	NDP	A	401	-	43,52,52	0.61	0	49,80,80	0.62	0
3	MES	A	402	-	12,12,12	1.97	1 (8%)	14,16,16	2.12	4 (28%)
3	MES	A	403	-	12,12,12	2.23	1 (8%)	14,16,16	1.67	4 (28%)
2	NDP	B	401	-	43,52,52	0.47	0	49,80,80	0.59	0
3	MES	B	402	-	12,12,12	1.97	1 (8%)	14,16,16	2.21	3 (21%)
2	NDP	C	401	-	43,52,52	0.57	0	49,80,80	0.69	0
3	MES	C	402	-	12,12,12	1.94	1 (8%)	14,16,16	2.45	3 (21%)
2	NDP	D	401	-	43,52,52	0.49	0	49,80,80	0.53	0
3	MES	D	402	-	12,12,12	2.01	1 (8%)	14,16,16	2.11	2 (14%)
2	NDP	E	401	-	43,52,52	0.44	0	49,80,80	0.67	1 (2%)
3	MES	E	402	-	12,12,12	2.03	1 (8%)	14,16,16	2.55	1 (7%)
2	NDP	F	401	-	43,52,52	0.46	0	49,80,80	0.55	0
3	MES	F	402	-	12,12,12	2.09	1 (8%)	14,16,16	1.88	2 (14%)
2	NDP	G	401	-	43,52,52	0.49	0	49,80,80	0.61	1 (2%)
2	NDP	H	401	-	43,52,52	0.44	0	49,80,80	0.65	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	I	401	-	43,52,52	0.57	0	49,80,80	0.63	0
3	MES	I	402	-	12,12,12	1.98	1 (8%)	14,16,16	2.50	4 (28%)
2	NDP	J	401	-	43,52,52	0.62	0	49,80,80	0.72	0
3	MES	J	402	-	12,12,12	1.86	1 (8%)	14,16,16	2.99	4 (28%)

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	NDP	A	401	-	-	0/30/77/77	0/5/5/5
3	MES	A	402	-	-	0/6/14/14	0/1/1/1
3	MES	A	403	-	-	0/6/14/14	0/1/1/1
2	NDP	B	401	-	-	0/30/77/77	0/5/5/5
3	MES	B	402	-	-	0/6/14/14	0/1/1/1
2	NDP	C	401	-	-	0/30/77/77	0/5/5/5
3	MES	C	402	-	-	0/6/14/14	0/1/1/1
2	NDP	D	401	-	-	0/30/77/77	0/5/5/5
3	MES	D	402	-	-	0/6/14/14	0/1/1/1
2	NDP	E	401	-	-	0/30/77/77	0/5/5/5
3	MES	E	402	-	-	0/6/14/14	0/1/1/1
2	NDP	F	401	-	-	0/30/77/77	0/5/5/5
3	MES	F	402	-	-	0/6/14/14	0/1/1/1
2	NDP	G	401	-	-	0/30/77/77	0/5/5/5
2	NDP	H	401	-	-	0/30/77/77	0/5/5/5
2	NDP	I	401	-	-	0/30/77/77	0/5/5/5
3	MES	I	402	-	-	0/6/14/14	0/1/1/1
2	NDP	J	401	-	-	0/30/77/77	0/5/5/5
3	MES	J	402	-	-	0/6/14/14	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	MES	C8-S	-7.46	1.66	1.77
3	F	402	MES	C8-S	-6.93	1.67	1.77
3	E	402	MES	C8-S	-6.64	1.67	1.77
3	D	402	MES	C8-S	-6.51	1.67	1.77
3	B	402	MES	C8-S	-6.50	1.67	1.77

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	J	402	MES	O2S-S-O1S	-4.16	99.43	113.86
3	A	402	MES	O3S-S-O1S	-2.92	104.69	111.37
3	I	402	MES	O2S-S-C8	-2.58	104.58	106.79
3	B	402	MES	O3S-S-O1S	-2.55	105.51	111.37
3	A	403	MES	O1-C2-C3	-2.33	106.61	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NDP	1	0
2	F	401	NDP	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 ⓘ

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	314/341 (92%)	-0.31	0 100 100	21, 31, 50, 73	0
1	B	315/341 (92%)	0.24	22 (6%) 17 16	24, 46, 104, 137	0
1	C	315/341 (92%)	-0.17	8 (2%) 58 55	22, 31, 57, 125	0
1	D	308/341 (90%)	1.46	92 (29%) 1 0	41, 103, 150, 179	0
1	E	314/341 (92%)	0.05	15 (4%) 31 30	24, 44, 94, 118	0
1	F	312/341 (91%)	1.19	79 (25%) 1 1	40, 88, 129, 160	0
1	G	242/341 (70%)	0.92	50 (20%) 1 1	43, 69, 134, 153	0
1	H	242/341 (70%)	0.97	49 (20%) 1 1	43, 75, 138, 191	0
1	I	315/341 (92%)	-0.25	2 (0%) 89 88	20, 32, 52, 98	0
1	J	315/341 (92%)	-0.29	1 (0%) 93 93	22, 32, 52, 88	0
All	All	2992/3410 (87%)	0.35	318 (10%) 7 6	20, 47, 126, 191	0

The worst 5 of 318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	308	PRO	10.9
1	D	309	VAL	8.6
1	D	156	ALA	8.2
1	F	303	ILE	8.1
1	G	305	ALA	8.1

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MES	B	402	12/12	0.83	0.23	4.75	61,89,100,111	0
3	MES	F	402	12/12	0.86	0.20	1.34	54,97,113,113	0
3	MES	A	403	12/12	0.88	0.20	0.99	43,73,96,108	0
3	MES	E	402	12/12	0.92	0.17	0.70	53,72,91,99	0
3	MES	C	402	12/12	0.88	0.18	0.17	43,59,72,73	0
3	MES	A	402	12/12	0.95	0.14	0.05	32,43,64,65	0
3	MES	I	402	12/12	0.95	0.14	-0.15	33,51,60,69	0
3	MES	D	402	12/12	0.87	0.15	-0.17	61,93,109,135	0
2	NDP	F	401	48/48	0.87	0.18	-0.25	40,79,107,120	0
3	MES	J	402	12/12	0.94	0.13	-0.50	28,43,55,62	0
2	NDP	B	401	48/48	0.94	0.11	-0.55	29,39,49,55	0
2	NDP	G	401	48/48	0.93	0.14	-0.61	44,63,90,101	0
2	NDP	D	401	48/48	0.88	0.15	-0.64	48,84,121,139	0
2	NDP	C	401	48/48	0.98	0.11	-0.68	18,25,29,32	0
2	NDP	J	401	48/48	0.97	0.11	-0.80	17,27,37,40	0
2	NDP	I	401	48/48	0.97	0.11	-0.90	19,26,32,36	0
2	NDP	A	401	48/48	0.97	0.10	-0.93	20,27,35,44	0
2	NDP	H	401	48/48	0.92	0.13	-0.97	44,72,92,105	0
2	NDP	E	401	48/48	0.97	0.08	-1.27	27,36,43,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.