



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

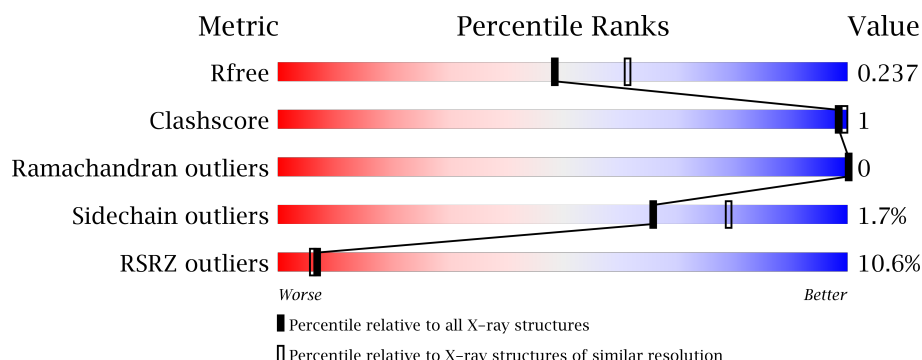
1 Overall quality at a glance

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> <div>6%</div> <div>91% 8%</div> </div>
1	C	341	<div> <div>2%</div> <div>90% 8%</div> </div>
1	D	341	<div> <div>27%</div> <div>86% 10%</div> </div>
1	E	341	<div> <div>4%</div> <div>90% 8%</div> </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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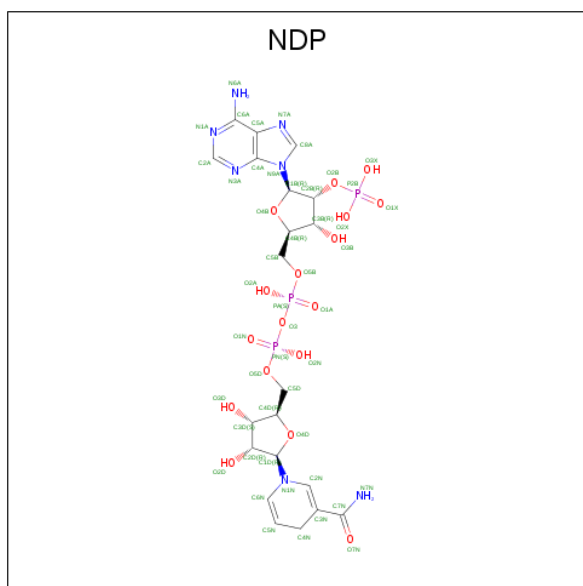
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I	-19	HIS	-	expression tag	UNP A7IIH0
I	-18	HIS	-	expression tag	UNP A7IIH0
I	-17	HIS	-	expression tag	UNP A7IIH0
I	-16	HIS	-	expression tag	UNP A7IIH0
I	-15	HIS	-	expression tag	UNP A7IIH0
I	-14	SER	-	expression tag	UNP A7IIH0
I	-13	SER	-	expression 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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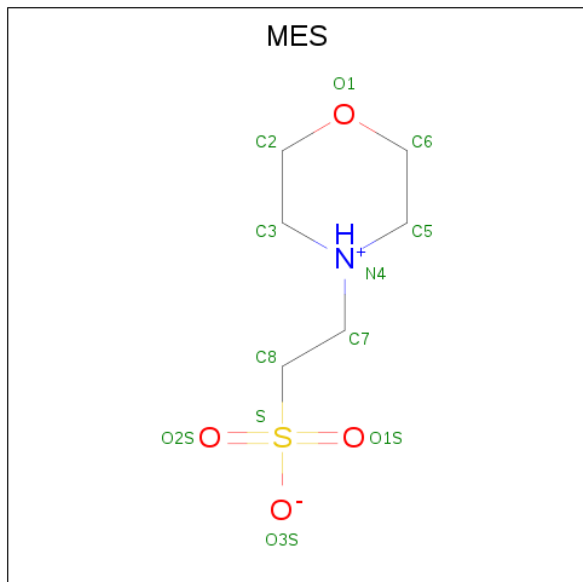
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	expression tag	UNP A7IIH0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

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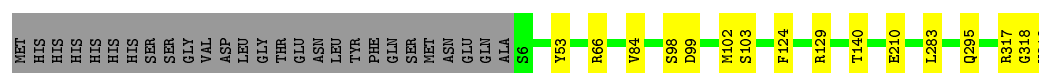
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	301	Total 301	O 301	0	0
4	C	420	Total 420	O 420	0	0
4	D	86	Total 86	O 86	0	0
4	E	304	Total 304	O 304	0	0
4	F	86	Total 86	O 86	0	0
4	G	75	Total 75	O 75	0	0
4	H	77	Total 77	O 77	0	0
4	I	422	Total 422	O 422	0	0
4	J	453	Total 453	O 453	0	0

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.

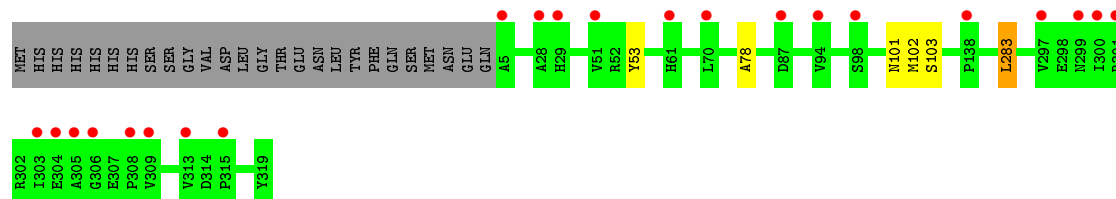
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

Chain A: 




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

Chain B: 




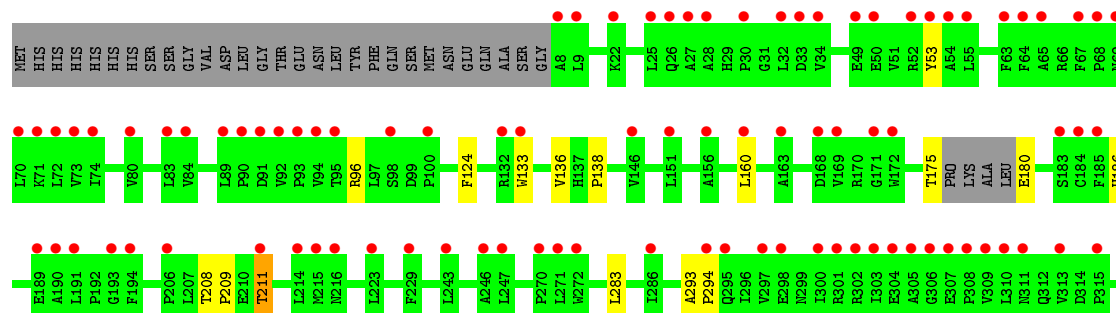
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding

Chain C: 



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

Chain D: 



Y319

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

Chain E: 

MET HIS HIS HIS HIS HIS SER SER VAL ASP LEU LEU THR GLN ASN LEU TYR PHE GLN SER MET MET ASN GLN ALA S6 G31 Y53 F64 L33 V64 F93 P100 N101 M102 S103 F124 R164 E189 L283 L288 V297 R301 E304

A305 G306 E307 F308 Y319

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

Chain F: 

MET HIS HIS HIS HIS HIS SER SER VAL ASP LEU LEU THR GLN ASN LEU TYR PHE GLN SER MET MET ASN GLN ALA S6 G31 Y53 F64 L33 V64 F93 P100 N101 M102 S103 F124 R164 E189 L283 L288 V297 R301 E304

V92 P93 Y94 R96 S98 D99 R129 E130 G131 R132 W133 A141 R145 V146 G147 A156 G159 A163 D168 V169 H172 S173 R174 T175 P176 K177 D83 V34 P48 V182 S183 C184 F185 E189 L191 S198 L205 P206 L207 T208 P209 G213 A217

E218 R219 F229 A245 R248 L283 A293 L296 V297 E298 N299 R301 R302 R303 A304 A305 G306 E307 F308 V309 L310 N311 Q312 V313 D314 F315 G318 Y319

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

Chain G: 

MET HIS HIS HIS HIS HIS SER SER VAL ASP LEU LEU THR GLN ASN LEU TYR PHE GLN SER MET MET ASN GLN ALA S6 G31 Y53 F64 L33 V64 F93 P100 N101 M102 S103 F124 R164 E189 L283 L288 V297 R301 E304

ALA GLY ASP HIS VAL GLY ASP PRO GLU GLU VAL ARG TYR ALA LEU VAL TRP LYS PRO HIS GLY PHE PHE ALA ARG PHE PRO ASN LEU VAL LYS LEU VAL TYR SER ILE ALA ASP ILE GLN ASP TRP ASP LYS SER ALA LEU GLN ALA HIS PRO GLY LEU ASP VAL ARG L97 S98 D99

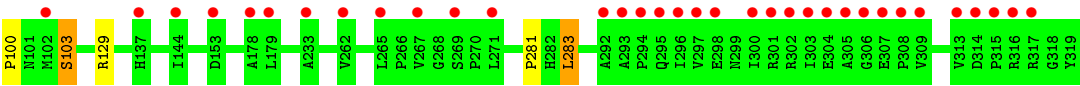
S103 R129 I144 D153 A178 L188 P192 P264 V267 G268 A273 P281 H282 L283 T288 R289 R290 T291 A292 A293 T296 V297 E298 N299 I300 N301 R302 I303 A304 A305 G306 E307 F308 V309 L310 N311 Q312 V313 D314 F315 G318 Y319

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

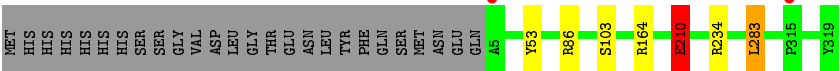
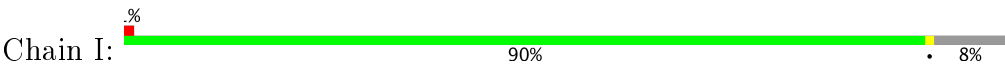
Chain H: 

MET HIS HIS HIS HIS HIS SER SER VAL ASP LEU LEU THR GLN ASN LEU TYR PHE GLN SER MET MET ASN GLN ALA S6 G31 Y53 F64 L33 V64 F93 P100 N101 M102 S103 F124 R164 E189 L283 L288 V297 R301 E304

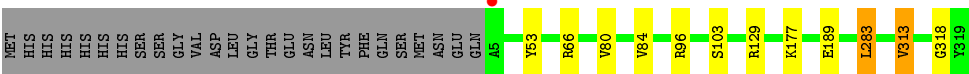
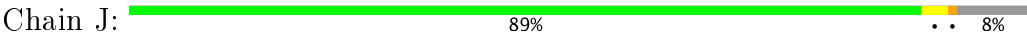
ALA GLY ASP HIS VAL GLY ASP PRO GLU GLU VAL ARG TYR ALA LEU VAL TRP LYS PRO HIS GLY PHE PHE ALA ARG PHE PRO ASN LEU VAL LYS LEU VAL TYR SER ILE ALA ASP ILE GLN ASP TRP ASP LYS SER ALA LEU GLN ALA HIS PRO GLY LEU ASP VAL ARG L97 S98 D99



● 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.

All (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
1	H	129	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	G	129	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	J	96	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	129	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	F	129	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	66	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	E	189	GLU	CA-CB-CG	5.26	124.97	113.40
1	I	234	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	J	129	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	86	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:96:ARG:NH2	2:D:401:NDP:O1A	2.35	0.59
1:F:207:LEU:HD23	1:F:208:THR:N	2.17	0.59
1:E:164:ARG:NH1	1:I:164:ARG:NH1	2.50	0.58
1:A:99:ASP:H	1:A:102:MET:CE	2.16	0.57
1:B:78:ALA:HB2	1:B:102:MET:CE	2.33	0.57
1:D:208:THR:HB	1:D:209:PRO:HD2	1.88	0.54
1:A:295:GLN:NE2	4:A:503:HOH:O	2.42	0.53
1:A:84:VAL:HG21	1:A:318:GLY:HA2	1.91	0.52
1:F:133:TRP:CH2	1:G:281:PRO:HA	2.47	0.50
1:F:207:LEU:C	1:F:207:LEU:CD2	2.80	0.50
1:A:98:SER:N	1:A:102:MET:HE1	2.27	0.49
1:D:124:PHE:CZ	1:H:283:LEU:HD21	2.49	0.47
1:J:84:VAL:HG21	1:J:318:GLY:HA2	1.97	0.47
1:F:207:LEU:C	1:F:207:LEU:HD23	2.36	0.46
1:D:136:VAL:O	1:D:138:PRO:HD3	2.16	0.45
1:F:145:ARG:HD2	1:F:168:ASP:OD2	2.17	0.44
1:E:124:PHE:CZ	1:I:283:LEU:HD21	2.53	0.44
1:B:283:LEU:HD21	1:C:124:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ARG:NH2	2:F:401:NDP:O1A	2.52	0.43
1:D:293:ALA:N	1:D:294:PRO:HD2	2.34	0.42
1:D:160:LEU:HD21	1:D:180:GLU:CB	2.48	0.42
1:J:80:VAL:HG11	1:J:313:VAL:HG21	2.01	0.42
1:A:317:ARG:HG2	1:A:319:TYR:CE1	2.55	0.42
1:J:177:LYS:NZ	4:J:515:HOH:O	2.53	0.42
1:D:133:TRP:CH2	1:H:281:PRO:HA	2.55	0.41
1:J:66:ARG:NH2	4:J:518:HOH:O	2.53	0.41
1:C:74:ILE:HD13	1:C:296:ILE:HG23	2.02	0.40
1:A:124:PHE:CZ	1:J:283:LEU:HD21	2.56	0.40
1:H:100:PRO:HA	1:H:103:SER:HB2	2.04	0.40

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

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	TYR
1	A	103	SER
1	A	140	THR
1	A	210	GLU
1	A	283	LEU
1	B	53	TYR
1	B	101	ASN
1	B	103	SER
1	B	283	LEU
1	C	53	TYR
1	C	103	SER
1	C	283	LEU
1	C	295	GLN
1	D	53	TYR

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Mol	Chain	Res	Type
1	D	211	THR
1	D	283	LEU
1	E	53	TYR
1	E	101	ASN
1	E	103	SER
1	E	283	LEU
1	F	53	TYR
1	F	145	ARG
1	F	207	LEU
1	F	219	ARG
1	F	283	LEU
1	G	103	SER
1	G	283	LEU
1	G	317	ARG
1	H	103	SER
1	H	283	LEU
1	I	53	TYR
1	I	103	SER
1	I	210[A]	GLU
1	I	210[B]	GLU
1	I	283	LEU
1	J	53	TYR
1	J	103	SER
1	J	189	GLU
1	J	283	LEU
1	J	313	VAL

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%)
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

All (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
3	I	402	MES	C8-S	-6.33	1.68	1.77
3	A	402	MES	C8-S	-6.31	1.68	1.77
3	C	402	MES	C8-S	-6.20	1.68	1.77
3	J	402	MES	C8-S	-5.83	1.68	1.77

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	I	402	MES	O3S-S-O1S	-2.24	106.23	111.37
2	H	401	NDP	O5D-PN-O1N	2.09	117.69	109.25
2	E	401	NDP	O5D-PN-O1N	2.12	117.82	109.25
2	G	401	NDP	O5D-PN-O1N	2.13	117.83	109.25
3	J	402	MES	C7-N4-C5	2.21	116.93	111.26
3	A	403	MES	O1S-S-C8	2.22	108.70	106.79
3	B	402	MES	O1S-S-C8	2.64	109.06	106.79
3	A	403	MES	O2S-S-C8	2.78	109.18	106.79
3	A	402	MES	C2-C3-N4	2.95	114.24	110.11
3	D	402	MES	O2S-S-C8	3.16	109.50	106.79
3	A	403	MES	O3S-S-C8	3.35	110.18	106.06
3	I	402	MES	C2-C3-N4	3.52	115.04	110.11
3	C	402	MES	C2-C3-N4	3.69	115.28	110.11
3	A	402	MES	O1S-S-C8	3.76	110.02	106.79
3	C	402	MES	O2S-S-C8	4.10	110.32	106.79
3	F	402	MES	O2S-S-C8	4.20	110.40	106.79
3	F	402	MES	O3S-S-C8	4.49	111.57	106.06
3	A	402	MES	O3S-S-C8	4.90	112.08	106.06
3	J	402	MES	O1S-S-C8	5.97	111.92	106.79
3	C	402	MES	O3S-S-C8	5.99	113.43	106.06
3	D	402	MES	O1S-S-C8	6.34	112.24	106.79
3	B	402	MES	O3S-S-C8	6.53	114.09	106.06
3	J	402	MES	O2S-S-C8	7.40	113.14	106.79
3	I	402	MES	O3S-S-C8	7.52	115.30	106.06
3	E	402	MES	O1S-S-C8	8.75	114.31	106.79

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 ⓘ

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	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

All (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
1	D	72	LEU	7.8
1	F	300	ILE	7.3
1	F	310	LEU	7.2
1	G	85	ALA	7.0
1	H	83	LEU	6.9
1	D	93	PRO	6.8
1	G	308	PRO	6.7
1	F	309	VAL	6.7

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Mol	Chain	Res	Type	RSRZ
1	G	94	VAL	6.7
1	G	300	ILE	6.6
1	G	293	ALA	6.5
1	H	306	GLY	6.5
1	D	90	PRO	6.5
1	D	53	TYR	6.3
1	G	93	PRO	6.3
1	G	309	VAL	6.2
1	G	297	VAL	6.2
1	D	171	GLY	6.2
1	D	310	LEU	6.1
1	F	315	PRO	6.0
1	G	92	VAL	5.9
1	H	94	VAL	5.9
1	F	296	ILE	5.8
1	H	93	PRO	5.8
1	G	288	ILE	5.7
1	D	151	LEU	5.7
1	F	94	VAL	5.6
1	E	305	ALA	5.6
1	D	300	ILE	5.5
1	D	297	VAL	5.4
1	F	53	TYR	5.4
1	C	5	ALA	5.4
1	F	172	TRP	5.3
1	D	172	TRP	5.3
1	F	179	LEU	5.2
1	D	193	GLY	5.2
1	F	91	ASP	5.2
1	G	315	PRO	5.2
1	H	300	ILE	5.2
1	G	83	LEU	5.2
1	D	95	THR	5.1
1	H	92	VAL	5.1
1	F	51	VAL	5.1
1	F	54	ALA	5.0
1	F	297	VAL	5.0
1	H	89	LEU	5.0
1	F	163	ALA	5.0
1	D	247	LEU	5.0
1	G	303	ILE	4.9
1	D	64	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	71	LYS	4.9
1	F	67	PHE	4.8
1	F	92	VAL	4.8
1	D	189	GLU	4.8
1	D	303	ILE	4.7
1	D	194	PHE	4.7
1	B	28	ALA	4.7
1	D	305	ALA	4.7
1	F	205	LEU	4.7
1	D	74	ILE	4.7
1	H	295	GLN	4.6
1	F	313	VAL	4.5
1	D	89	LEU	4.5
1	H	262	VAL	4.4
1	D	8	ALA	4.4
1	H	305	ALA	4.4
1	H	309	VAL	4.4
1	F	130	GLU	4.4
1	G	301	ARG	4.4
1	D	298	GLU	4.4
1	H	293	ALA	4.4
1	D	185	PHE	4.4
1	G	90	PRO	4.3
1	H	315	PRO	4.3
1	F	178	ALA	4.3
1	F	131	GLY	4.3
1	G	318	GLY	4.3
1	D	94	VAL	4.3
1	D	304	GLU	4.3
1	G	97	LEU	4.3
1	F	95	THR	4.3
1	H	303	ILE	4.3
1	D	84	VAL	4.3
1	G	88	ASP	4.2
1	D	286	ILE	4.2
1	D	70	LEU	4.1
1	D	69	ASN	4.1
1	G	268	GLY	4.1
1	H	87	ASP	4.1
1	G	267	VAL	4.0
1	D	163	ALA	4.0
1	F	34	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	313	VAL	4.0
1	D	301	ARG	4.0
1	B	61	HIS	4.0
1	D	308	PRO	3.9
1	D	92	VAL	3.9
1	C	102	MET	3.9
1	F	305	ALA	3.9
1	C	101	ASN	3.8
1	G	89	LEU	3.8
1	F	159	ALA	3.8
1	D	91	ASP	3.8
1	D	306	GLY	3.8
1	B	306	GLY	3.7
1	D	211	THR	3.7
1	H	84	VAL	3.7
1	H	292	ALA	3.7
1	G	87	ASP	3.7
1	F	93	PRO	3.7
1	H	297	VAL	3.7
1	H	298	GLU	3.6
1	H	233	ALA	3.6
1	D	54	ALA	3.6
1	D	243	LEU	3.6
1	F	189	GLU	3.6
1	D	319	TYR	3.6
1	D	100	PRO	3.6
1	F	308	PRO	3.6
1	F	72	LEU	3.6
1	B	303	ILE	3.5
1	H	304	GLU	3.5
1	D	270	PRO	3.5
1	F	90	PRO	3.5
1	G	264	PRO	3.5
1	F	8	ALA	3.5
1	I	5	ALA	3.5
1	H	267	VAL	3.5
1	F	31	GLY	3.4
1	H	316	ARG	3.4
1	D	183	SER	3.4
1	D	214	LEU	3.4
1	F	306	GLY	3.4
1	D	223	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	32	LEU	3.4
1	G	91	ASP	3.3
1	H	88	ASP	3.3
1	F	70	LEU	3.3
1	F	209	PRO	3.3
1	H	317	ARG	3.3
1	F	82	ALA	3.3
1	H	265	LEU	3.3
1	E	308	PRO	3.3
1	G	298	GLU	3.3
1	C	97	LEU	3.3
1	H	97	LEU	3.3
1	G	86	ARG	3.3
1	B	29	HIS	3.2
1	C	98	SER	3.2
1	B	304	GLU	3.2
1	B	315	PRO	3.2
1	D	313	VAL	3.2
1	E	84	VAL	3.2
1	H	301	ARG	3.2
1	H	296	ILE	3.2
1	B	305	ALA	3.2
1	D	295	GLN	3.2
1	F	302	ARG	3.2
1	B	309	VAL	3.1
1	G	289	PRO	3.1
1	E	301	ARG	3.1
1	H	90	PRO	3.1
1	D	83	LEU	3.1
1	D	68	PRO	3.1
1	D	190	ALA	3.1
1	G	188	LEU	3.1
1	H	102	MET	3.1
1	D	146	VAL	3.1
1	F	191	LEU	3.0
1	D	302	ARG	3.0
1	F	169	VAL	3.0
1	F	301	ARG	3.0
1	D	184	CYS	3.0
1	H	307	GLU	3.0
1	F	141	ALA	3.0
1	D	307	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	307	GLU	3.0
1	D	34	VAL	3.0
1	D	169	VAL	3.0
1	H	80	VAL	3.0
1	D	160	LEU	2.9
1	G	273	ALA	2.9
1	F	28	ALA	2.9
1	F	182	VAL	2.9
1	D	55	LEU	2.9
1	D	246	ALA	2.9
1	F	299	ASN	2.8
1	C	6	SER	2.8
1	F	68	PRO	2.8
1	E	31	GLY	2.8
1	G	296	ILE	2.8
1	D	50	GLU	2.8
1	F	307	GLU	2.8
1	D	133	TRP	2.8
1	H	178	ALA	2.8
1	H	95	THR	2.8
1	D	27	ALA	2.7
1	D	33	ASP	2.7
1	D	65	ALA	2.7
1	D	49	GLU	2.7
1	F	311	ASN	2.7
1	G	292	ALA	2.7
1	F	298	GLU	2.7
1	G	311	ASN	2.7
1	D	206	PRO	2.7
1	F	176	PRO	2.7
1	H	313	VAL	2.7
1	D	229	PHE	2.7
1	H	302	ARG	2.7
1	B	70	LEU	2.7
1	F	175	THR	2.7
1	F	133	TRP	2.7
1	H	269	SER	2.7
1	H	144	ILE	2.7
1	E	306	GLY	2.6
1	H	86	ARG	2.6
1	E	297	VAL	2.6
1	G	192	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	183	SER	2.6
1	D	67	PHE	2.6
1	D	52	ARG	2.6
1	C	100	PRO	2.5
1	F	229	PHE	2.5
1	C	99	ASP	2.5
1	D	32	LEU	2.5
1	F	304	GLU	2.5
1	G	99	ASP	2.5
1	B	5	ALA	2.5
1	D	28	ALA	2.5
1	G	304	GLU	2.5
1	D	216	ASN	2.5
1	D	294	PRO	2.5
1	D	315	PRO	2.5
1	G	84	VAL	2.4
1	F	208	THR	2.4
1	D	132	ARG	2.4
1	D	311	ASN	2.4
1	E	288	ILE	2.4
1	J	5	ALA	2.4
1	B	313	VAL	2.4
1	F	217	ALA	2.4
1	G	82	ALA	2.4
1	B	87	ASP	2.4
1	B	308	PRO	2.4
1	F	71	LYS	2.4
1	F	9	LEU	2.4
1	F	174	ARG	2.4
1	H	271	LEU	2.4
1	F	248	ARG	2.3
1	G	306	GLY	2.3
1	G	319	TYR	2.3
1	D	272	TRP	2.3
1	F	89	LEU	2.3
1	F	245	ALA	2.3
1	D	26	GLN	2.3
1	D	9	LEU	2.3
1	D	191	LEU	2.3
1	E	64	PHE	2.3
1	F	147	GLY	2.3
1	F	29	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	30	PRO	2.3
1	F	100	PRO	2.3
1	D	271	LEU	2.3
1	G	178	ALA	2.3
1	G	316	ARG	2.3
1	F	73	VAL	2.3
1	H	314	ASP	2.3
1	D	80	VAL	2.3
1	D	168	ASP	2.3
1	F	213	GLY	2.3
1	F	185	PHE	2.3
1	B	300	ILE	2.3
1	F	207	LEU	2.2
1	D	98	SER	2.2
1	B	138	PRO	2.2
1	B	297	VAL	2.2
1	D	215	MET	2.2
1	B	94	VAL	2.2
1	D	22	LYS	2.2
1	H	85	ALA	2.2
1	D	25	LEU	2.2
1	F	30	PRO	2.2
1	B	98	SER	2.2
1	D	73	VAL	2.2
1	D	63	PHE	2.2
1	F	48	PRO	2.2
1	H	91	ASP	2.2
1	G	299	ASN	2.2
1	E	93	PRO	2.2
1	F	198	SER	2.1
1	H	294	PRO	2.1
1	B	299	ASN	2.1
1	F	319	TYR	2.1
1	G	153	ASP	2.1
1	G	314	ASP	2.1
1	F	156	ALA	2.1
1	F	293	ALA	2.1
1	F	98	SER	2.1
1	I	315	PRO	2.1
1	H	179	LEU	2.1
1	G	290	ARG	2.1
1	E	83	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	51	VAL	2.1
1	F	318	GLY	2.1
1	E	53	TYR	2.1
1	E	304	GLU	2.0
1	E	100	PRO	2.0
1	G	312	GLN	2.0
1	H	137	HIS	2.0
1	G	79	GLY	2.0
1	B	301	ARG	2.0
1	G	144	ILE	2.0
1	H	153	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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 [i](#)

There are no such residues in this entry.