Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:18 PM GMT

PDB ID	:	1EZ4
Title	:	CRYSTAL STRUCTURE OF NON-ALLOSTERIC L-LACTATE DEHYDROGENASE FROM LACTOBACILLUS PENTOSUS AT 2.3 ANGSTROM RESOLUTION
Authors	:	Uchikoba, H.; Fushinobu, S.; Wakagi, T.; Konno, M.; Taguchi, H.; Matsuzawa, H.
Deposited on	:	2000-05-10
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

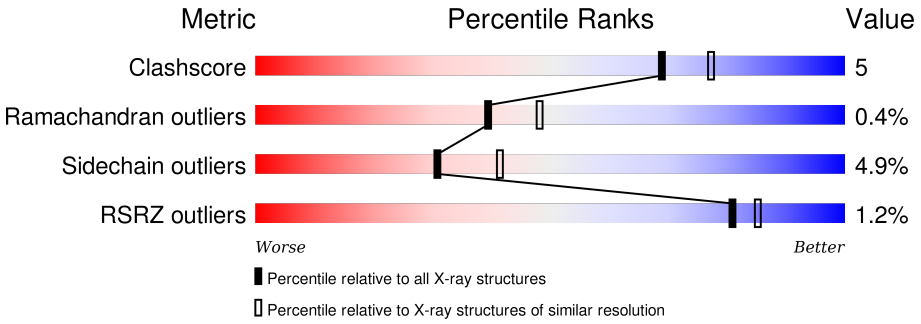
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	318	2% 83% 10%
1	B	318	85% 11%
1	C	318	2% 81% 12%
1	D	318	% 84% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	1353	-	-	-	X
2	NAD	C	1354	-	-	-	X
2	NAD	D	1355	-	-	-	X

2 Entry composition

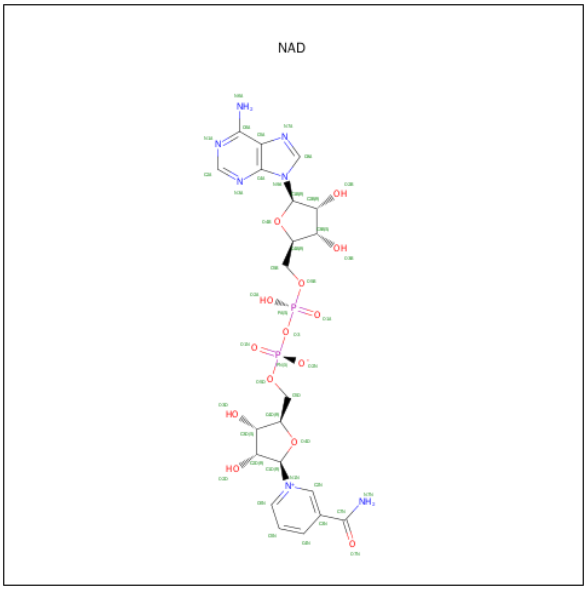
There are 3 unique types of molecules in this entry. The entry contains 10353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2304	1455	384	458	7			
1	B	318	Total	C	N	O	S	0	0	0
			2392	1508	401	476	7			
1	C	307	Total	C	N	O	S	0	0	0
			2304	1455	384	458	7			
1	D	318	Total	C	N	O	S	0	0	0
			2392	1508	401	476	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is water.

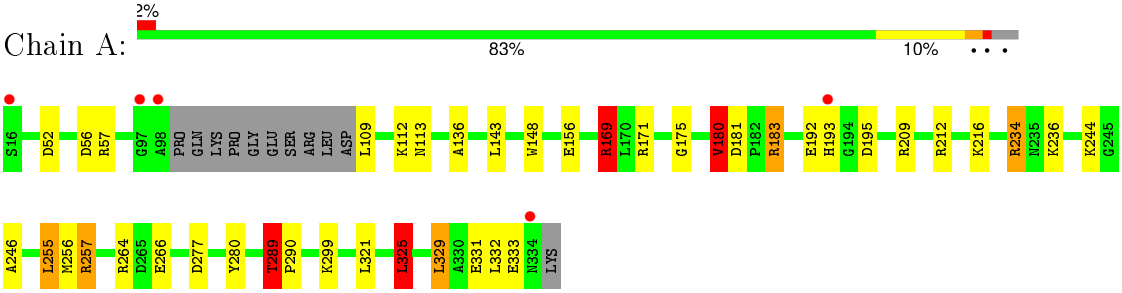
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total	O	0	0
			184	184		
3	B	219	Total	O	0	0
			219	219		
3	C	189	Total	O	0	0
			189	189		
3	D	193	Total	O	0	0
			193	193		

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 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.

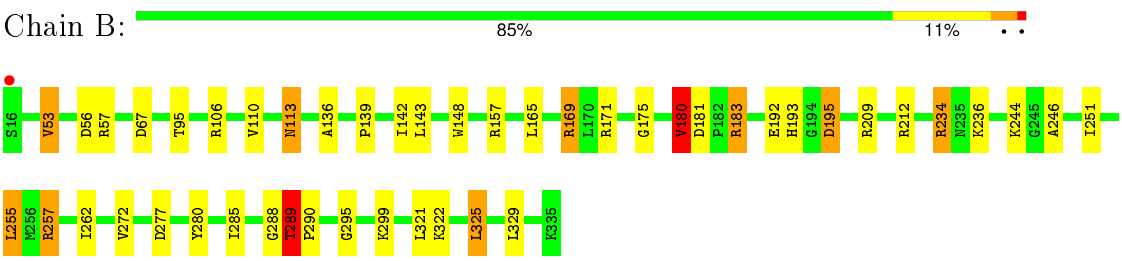
- Molecule 1: LACTATE DEHYDROGENASE

Chain A:



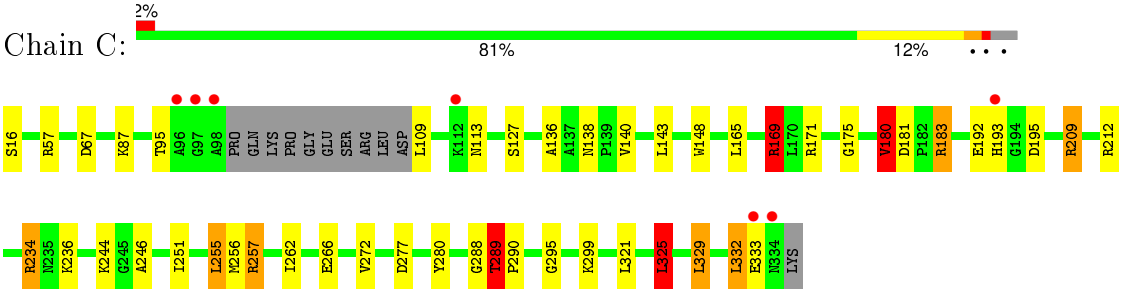
- Molecule 1: LACTATE DEHYDROGENASE

Chain B:



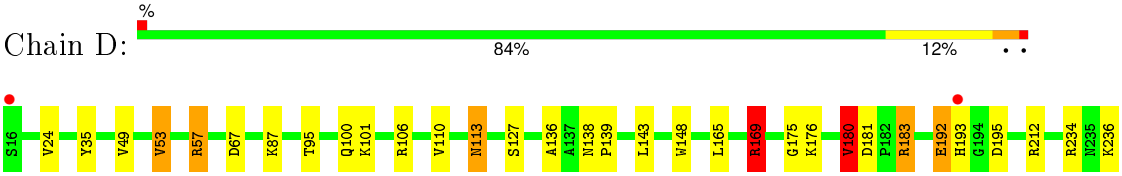
- Molecule 1: LACTATE DEHYDROGENASE

Chain C:



- Molecule 1: LACTATE DEHYDROGENASE

Chain D:




K244
G245
A246
I251
L255
M256
R257
I262
L263
R264
D277
Y280
T289
P290
G295
T320
L321
K322
L325
L329
L332
K335

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.35Å 145.54Å 111.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.30 76.28 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (80.00-2.30) 99.0 (76.28-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.241 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.0	EDS
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 123624 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10353	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.79	0/2337	1.53	26/3162 (0.8%)
1	B	0.82	0/2428	1.54	25/3284 (0.8%)
1	C	0.79	0/2337	1.55	21/3162 (0.7%)
1	D	0.80	0/2428	1.48	21/3284 (0.6%)
All	All	0.80	0/9530	1.53	93/12892 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	3
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	ARG	NE-CZ-NH2	19.51	130.06	120.30
1	B	169	ARG	NE-CZ-NH2	18.60	129.60	120.30
1	B	257	ARG	NE-CZ-NH1	-17.50	111.55	120.30
1	C	257	ARG	NE-CZ-NH1	-16.72	111.94	120.30
1	D	257	ARG	NE-CZ-NH1	-16.27	112.16	120.30
1	C	169	ARG	NE-CZ-NH2	16.13	128.37	120.30
1	A	183	ARG	NE-CZ-NH2	15.82	128.21	120.30
1	A	257	ARG	NE-CZ-NH1	-15.81	112.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	ARG	NE-CZ-NH1	-15.43	112.58	120.30
1	A	257	ARG	NE-CZ-NH2	14.72	127.66	120.30
1	D	169	ARG	NE-CZ-NH2	13.46	127.03	120.30
1	B	57	ARG	NE-CZ-NH2	12.63	126.62	120.30
1	B	257	ARG	NE-CZ-NH2	12.57	126.59	120.30
1	A	169	ARG	NE-CZ-NH2	12.35	126.48	120.30
1	C	257	ARG	NE-CZ-NH2	11.73	126.16	120.30
1	B	57	ARG	NE-CZ-NH1	-10.91	114.84	120.30
1	A	212	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	C	183	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	D	183	ARG	NE-CZ-NH2	10.83	125.71	120.30
1	D	169	ARG	NE-CZ-NH1	-10.66	114.97	120.30
1	B	183	ARG	NE-CZ-NH2	10.30	125.45	120.30
1	D	257	ARG	NE-CZ-NH2	10.25	125.42	120.30
1	C	171	ARG	NE-CZ-NH2	10.20	125.40	120.30
1	D	212	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	C	169	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	D	183	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	A	171	ARG	NE-CZ-NH2	8.34	124.47	120.30
1	C	212	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	A	180	VAL	CB-CA-C	-8.20	95.81	111.40
1	D	148	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	B	171	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	169	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	C	332	LEU	CA-CB-CG	7.68	132.97	115.30
1	C	180	VAL	CB-CA-C	-7.64	96.88	111.40
1	B	180	VAL	CB-CA-C	-7.52	97.11	111.40
1	C	148	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	C	148	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	C	57	ARG	CB-CG-CD	-7.30	92.62	111.60
1	D	180	VAL	CB-CA-C	-7.18	97.76	111.40
1	C	256	MET	CG-SD-CE	7.08	111.54	100.20
1	D	148	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	A	148	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	B	212	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	D	332	LEU	CA-CB-CG	6.78	130.90	115.30
1	B	148	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	B	148	TRP	CD1-CG-CD2	6.60	111.58	106.30
1	A	148	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	B	53	VAL	N-CA-CB	-6.55	97.10	111.50
1	B	53	VAL	CG1-CB-CG2	6.40	121.14	110.90
1	A	209	ARG	NE-CZ-NH1	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	209	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	A	234	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	B	57	ARG	CG-CD-NE	-6.15	98.89	111.80
1	A	183	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	57	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	A	52	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	183	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	A	212	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	C	209	ARG	CG-CD-NE	-5.89	99.44	111.80
1	B	289	THR	CB-CA-C	-5.87	95.75	111.60
1	C	325	LEU	CA-CB-CG	5.80	128.64	115.30
1	D	257	ARG	CG-CD-NE	-5.77	99.68	111.80
1	A	209	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	D	53	VAL	N-CA-CB	-5.75	98.85	111.50
1	A	256	MET	CG-SD-CE	5.70	109.32	100.20
1	C	289	THR	CB-CA-C	-5.69	96.23	111.60
1	A	57	ARG	CB-CG-CD	-5.67	96.87	111.60
1	D	113	ASN	OD1-CG-ND2	-5.57	109.09	121.90
1	D	289	THR	CB-CA-C	-5.56	96.58	111.60
1	B	192	GLU	CA-C-N	-5.44	105.24	117.20
1	A	192	GLU	CA-C-N	-5.43	105.25	117.20
1	A	289	THR	CB-CA-C	-5.43	96.95	111.60
1	A	257	ARG	CG-CD-NE	-5.39	100.49	111.80
1	C	192	GLU	CA-C-N	-5.36	105.42	117.20
1	B	157	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	264	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	264	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	57	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	C	234	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	257	ARG	CG-CD-NE	-5.28	100.72	111.80
1	D	192	GLU	CA-C-N	-5.22	105.71	117.20
1	B	234	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	325	LEU	CA-CB-CG	5.14	127.11	115.30
1	D	321	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	180	VAL	CG1-CB-CG2	5.13	119.12	110.90
1	D	53	VAL	CB-CA-C	5.11	121.11	111.40
1	A	209	ARG	CG-CD-NE	-5.10	101.08	111.80
1	B	257	ARG	CG-CD-NE	-5.10	101.09	111.80
1	D	322	LYS	CB-CG-CD	-5.09	98.36	111.60
1	B	53	VAL	CA-CB-CG2	-5.09	103.27	110.90
1	B	209	ARG	CG-CD-NE	-5.09	101.12	111.80
1	B	113	ASN	OD1-CG-ND2	-5.06	110.25	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	ARG	Sidechain
1	B	257	ARG	Sidechain
1	B	289	THR	Peptide
1	C	209	ARG	Sidechain
1	C	257	ARG	Sidechain
1	C	289	THR	Peptide
1	D	289	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2304	0	2309	19	0
1	B	2392	0	2400	21	0
1	C	2304	0	2309	24	0
1	D	2392	0	2400	25	0
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0
2	D	44	0	26	2	0
3	A	184	0	0	1	0
3	B	219	0	0	2	0
3	C	189	0	0	2	0
3	D	193	0	0	0	0
All	All	10353	0	9522	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (88) 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:A:169:ARG:HD2	1:A:236:LYS:HD3	1.62	0.81
1:C:169:ARG:HD2	1:C:236:LYS:HD3	1.63	0.79
1:D:169:ARG:HD2	1:D:236:LYS:HD3	1.68	0.73
1:C:136:ALA:O	2:C:1354:NAD:H2N	1.91	0.70
1:B:169:ARG:HD2	1:B:236:LYS:HD3	1.75	0.67
1:C:95:THR:O	2:C:1354:NAD:H4D	1.97	0.64
1:A:325:LEU:HD22	1:A:329:LEU:HD22	1.81	0.61
1:B:136:ALA:O	2:B:1353:NAD:H2N	2.01	0.59
1:C:325:LEU:HD22	1:C:329:LEU:HD22	1.82	0.59
1:A:136:ALA:HB2	1:A:255:LEU:HD11	1.85	0.59
1:D:95:THR:O	2:D:1355:NAD:H4D	2.03	0.59
1:B:169:ARG:CD	1:B:236:LYS:HD3	2.34	0.57
1:B:95:THR:O	2:B:1353:NAD:H4D	2.05	0.57
1:D:244:LYS:HE3	1:D:246:ALA:O	2.04	0.57
1:D:136:ALA:HB2	1:D:255:LEU:HD11	1.85	0.57
1:A:109:LEU:HA	1:A:112:LYS:HG2	1.89	0.55
1:C:169:ARG:CD	1:C:236:LYS:HD3	2.35	0.55
1:D:192:GLU:HG3	1:D:321:LEU:HD22	1.89	0.55
1:B:244:LYS:HE3	1:B:246:ALA:O	2.07	0.54
1:C:67:ASP:OD2	1:D:169:ARG:HD3	2.08	0.54
1:D:110:VAL:HG22	1:D:139:PRO:HG3	1.90	0.54
1:D:325:LEU:HD22	1:D:329:LEU:HD22	1.89	0.53
1:B:136:ALA:HB2	1:B:255:LEU:HD11	1.90	0.53
2:C:1354:NAD:H52A	2:C:1354:NAD:H52N	1.92	0.52
1:A:169:ARG:HD3	1:B:67:ASP:OD2	2.10	0.52
3:C:1498:HOH:O	1:D:176:LYS:HE2	2.10	0.51
1:A:136:ALA:O	2:A:1352:NAD:H2N	2.11	0.51
1:B:142:ILE:HG23	1:B:325:LEU:HD23	1.93	0.51
1:D:138:ASN:HB2	2:D:1355:NAD:O2D	2.11	0.50
1:A:289:THR:HG22	1:A:290:PRO:HD2	1.94	0.49
1:C:280:TYR:CE2	1:C:289:THR:HG23	2.48	0.49
1:B:195:ASP:HA	1:B:234:ARG:HD2	1.93	0.49
1:D:169:ARG:CD	1:D:236:LYS:HD3	2.40	0.49
1:C:136:ALA:HB2	1:C:255:LEU:HD11	1.93	0.49
1:C:169:ARG:HD3	1:D:67:ASP:OD2	2.12	0.49
1:C:175:GLY:HA2	1:C:180:VAL:HG23	1.96	0.48
1:A:175:GLY:HA2	1:A:180:VAL:HG23	1.96	0.48
1:A:280:TYR:CE2	1:A:289:THR:HG23	2.48	0.48
1:D:280:TYR:CE2	1:D:289:THR:HG23	2.49	0.47
1:C:280:TYR:HE2	1:C:289:THR:HG23	1.80	0.47
1:B:165:LEU:HD22	1:B:251:ILE:HB	1.96	0.47
1:C:244:LYS:HE3	1:C:246:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:HD22	1:C:140:VAL:H	1.63	0.47
1:C:165:LEU:HD22	1:C:251:ILE:HB	1.96	0.47
1:B:285:ILE:HG21	1:B:322:LYS:HG2	1.97	0.46
1:A:195:ASP:HA	1:A:234:ARG:HD2	1.98	0.46
1:A:244:LYS:HE3	1:A:246:ALA:O	2.15	0.45
1:D:35:TYR:CD1	1:D:255:LEU:HB3	2.51	0.45
1:A:181:ASP:HB2	1:C:266:GLU:O	2.16	0.45
1:A:113:ASN:HB3	1:A:143:LEU:HD11	1.97	0.45
1:D:280:TYR:HE2	1:D:289:THR:HG23	1.82	0.45
1:B:110:VAL:HG22	1:B:139:PRO:HG3	1.99	0.45
1:D:113:ASN:HB3	1:D:143:LEU:HD11	1.99	0.44
2:C:1354:NAD:H5N	3:C:1528:HOH:O	2.18	0.44
1:B:289:THR:HG22	1:B:290:PRO:HD2	1.99	0.44
1:B:113:ASN:HB3	1:B:143:LEU:HD11	2.00	0.44
1:B:280:TYR:CE2	1:B:289:THR:HG23	2.52	0.44
1:D:175:GLY:HA2	1:D:180:VAL:HG23	2.00	0.43
1:D:289:THR:HG22	1:D:290:PRO:HD2	2.00	0.43
1:C:262:ILE:O	1:C:295:GLY:HA2	2.18	0.43
1:A:280:TYR:HE2	1:A:289:THR:HG23	1.83	0.43
1:A:181:ASP:OD1	1:A:183:ARG:HD3	2.19	0.43
1:B:285:ILE:CG2	1:B:322:LYS:HG2	2.48	0.43
1:D:181:ASP:OD1	1:D:183:ARG:HD3	2.19	0.43
1:C:181:ASP:OD1	1:C:183:ARG:HD3	2.18	0.43
1:D:262:ILE:O	1:D:295:GLY:HA2	2.19	0.42
1:B:181:ASP:OD1	1:B:183:ARG:HD3	2.19	0.42
1:B:272:VAL:O	1:B:288:GLY:HA2	2.20	0.42
2:B:1353:NAD:H2A	3:B:1457:HOH:O	2.20	0.42
1:C:272:VAL:O	1:C:288:GLY:HA2	2.19	0.42
1:A:299:LYS:HA	1:A:299:LYS:HD2	1.96	0.42
1:C:289:THR:HG22	1:C:290:PRO:HD2	2.01	0.42
1:A:266:GLU:O	1:C:181:ASP:HB2	2.20	0.42
1:C:195:ASP:HA	1:C:234:ARG:HD2	2.02	0.42
1:B:262:ILE:O	1:B:295:GLY:HA2	2.20	0.41
1:C:113:ASN:HB3	1:C:143:LEU:HD11	2.00	0.41
2:B:1353:NAD:H5N	3:B:1544:HOH:O	2.20	0.41
1:B:175:GLY:HA2	1:B:180:VAL:HG23	2.01	0.41
1:A:156:GLU:HB3	3:A:1438:HOH:O	2.20	0.41
1:C:87:LYS:HG3	1:C:127:SER:O	2.21	0.41
1:C:299:LYS:HD2	1:C:299:LYS:HA	1.92	0.41
1:B:299:LYS:HD2	1:B:299:LYS:HA	1.86	0.41
1:D:165:LEU:HD22	1:D:251:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:VAL:HG22	1:D:49:VAL:HB	2.02	0.40
1:D:234:ARG:HH21	1:D:234:ARG:HD3	1.77	0.40
1:A:109:LEU:HA	1:A:112:LYS:HE2	2.02	0.40
1:D:195:ASP:HA	1:D:234:ARG:HD2	2.03	0.40
1:D:87:LYS:HG3	1:D:127:SER:O	2.21	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	303/318 (95%)	288 (95%)	14 (5%)	1 (0%)	46	57
1	B	316/318 (99%)	300 (95%)	14 (4%)	2 (1%)	30	36
1	C	303/318 (95%)	291 (96%)	11 (4%)	1 (0%)	46	57
1	D	316/318 (99%)	299 (95%)	16 (5%)	1 (0%)	46	57
All	All	1238/1272 (97%)	1178 (95%)	55 (4%)	5 (0%)	39	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	HIS
1	B	193	HIS
1	C	193	HIS
1	D	193	HIS
1	B	195	ASP

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/255 (96%)	232 (95%)	13 (5%)	28	37
1	B	255/255 (100%)	246 (96%)	9 (4%)	43	58
1	C	245/255 (96%)	233 (95%)	12 (5%)	31	41
1	D	255/255 (100%)	240 (94%)	15 (6%)	24	32
All	All	1000/1020 (98%)	951 (95%)	49 (5%)	31	41

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	169	ARG
1	A	180	VAL
1	A	216	LYS
1	A	255	LEU
1	A	277	ASP
1	A	289	THR
1	A	321	LEU
1	A	325	LEU
1	A	329	LEU
1	A	331	GLU
1	A	332	LEU
1	A	333	GLU
1	B	53	VAL
1	B	106	ARG
1	B	180	VAL
1	B	255	LEU
1	B	277	ASP
1	B	289	THR
1	B	321	LEU
1	B	325	LEU
1	B	329	LEU
1	C	16	SER
1	C	109	LEU
1	C	169	ARG
1	C	180	VAL
1	C	255	LEU
1	C	277	ASP

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Mol	Chain	Res	Type
1	C	289	THR
1	C	321	LEU
1	C	325	LEU
1	C	329	LEU
1	C	332	LEU
1	C	333	GLU
1	D	53	VAL
1	D	57	ARG
1	D	100	GLN
1	D	101	LYS
1	D	106	ARG
1	D	169	ARG
1	D	180	VAL
1	D	255	LEU
1	D	277	ASP
1	D	289	THR
1	D	320	THR
1	D	321	LEU
1	D	325	LEU
1	D	329	LEU
1	D	332	LEU

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	138	ASN
1	A	193	HIS
1	B	334	ASN
1	C	138	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	NAD	A	1352	-	38,48,48	1.13	4 (10%)	47,73,73	2.34	11 (23%)
2	NAD	B	1353	-	38,48,48	1.11	3 (7%)	47,73,73	2.34	13 (27%)
2	NAD	C	1354	-	38,48,48	1.21	4 (10%)	47,73,73	2.42	12 (25%)
2	NAD	D	1355	-	38,48,48	1.21	4 (10%)	47,73,73	2.29	13 (27%)

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	1352	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1353	-	-	0/22/62/62	0/5/5/5
2	NAD	C	1354	-	-	0/22/62/62	0/5/5/5
2	NAD	D	1355	-	-	0/22/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1354	NAD	C6N-N1N	2.39	1.41	1.35
2	B	1353	NAD	C6N-N1N	2.46	1.42	1.35
2	A	1352	NAD	C6N-N1N	2.49	1.42	1.35
2	D	1355	NAD	O4B-C1B	2.50	1.44	1.41
2	A	1352	NAD	O4B-C1B	2.57	1.44	1.41
2	C	1354	NAD	O4B-C1B	2.65	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1355	NAD	C6N-N1N	2.81	1.43	1.35
2	A	1352	NAD	C3N-C7N	2.89	1.55	1.50
2	B	1353	NAD	C3N-C7N	2.89	1.55	1.50
2	A	1352	NAD	O4D-C1D	3.00	1.45	1.41
2	D	1355	NAD	C3N-C7N	3.01	1.55	1.50
2	B	1353	NAD	O4D-C1D	3.15	1.45	1.41
2	C	1354	NAD	O4D-C1D	3.22	1.45	1.41
2	C	1354	NAD	C3N-C7N	3.55	1.56	1.50
2	D	1355	NAD	O4D-C1D	3.60	1.45	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1354	NAD	N3A-C2A-N1A	-10.91	120.54	128.89
2	B	1353	NAD	N3A-C2A-N1A	-9.70	121.47	128.89
2	A	1352	NAD	N3A-C2A-N1A	-9.66	121.50	128.89
2	D	1355	NAD	N3A-C2A-N1A	-8.51	122.38	128.89
2	B	1353	NAD	C4B-O4B-C1B	-5.89	103.25	109.72
2	A	1352	NAD	C4B-O4B-C1B	-5.73	103.42	109.72
2	A	1352	NAD	C4D-O4D-C1D	-5.49	103.68	109.72
2	D	1355	NAD	C4B-O4B-C1B	-4.75	104.50	109.72
2	C	1354	NAD	C4B-O4B-C1B	-3.70	105.65	109.72
2	C	1354	NAD	C4D-O4D-C1D	-3.65	105.70	109.72
2	B	1353	NAD	C4D-O4D-C1D	-3.08	106.33	109.72
2	B	1353	NAD	C1B-N9A-C4A	-2.72	122.84	126.94
2	D	1355	NAD	C4D-O4D-C1D	-2.64	106.81	109.72
2	B	1353	NAD	O3-PN-O5D	-2.62	95.99	102.94
2	D	1355	NAD	C1B-N9A-C4A	-2.34	123.41	126.94
2	A	1352	NAD	C1B-N9A-C4A	-2.33	123.42	126.94
2	C	1354	NAD	C1B-N9A-C4A	-2.13	123.73	126.94
2	D	1355	NAD	O7N-C7N-N7N	-2.11	119.63	122.59
2	B	1353	NAD	C2B-C1B-N9A	-2.10	111.08	114.29
2	C	1354	NAD	O3D-C3D-C4D	2.04	117.17	111.05
2	D	1355	NAD	O3B-C3B-C2B	2.04	118.46	111.83
2	D	1355	NAD	C3N-C2N-N1N	2.05	122.72	120.36
2	A	1352	NAD	O3B-C3B-C2B	2.07	118.55	111.83
2	B	1353	NAD	C2A-N1A-C6A	2.08	122.48	118.77
2	B	1353	NAD	O2B-C2B-C3B	2.12	118.72	111.83
2	A	1352	NAD	O7N-C7N-C3N	2.12	121.90	119.59
2	B	1353	NAD	O4D-C4D-C3D	2.24	109.66	105.15
2	C	1354	NAD	C2B-C1B-N9A	2.32	117.83	114.29
2	D	1355	NAD	O4D-C4D-C3D	2.34	109.85	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1352	NAD	O2B-C2B-C3B	2.38	119.57	111.83
2	D	1355	NAD	C4A-C5A-N7A	2.38	111.67	109.48
2	C	1354	NAD	C3N-C2N-N1N	2.42	123.15	120.36
2	A	1352	NAD	O4B-C1B-N9A	2.44	113.20	108.10
2	D	1355	NAD	O2B-C2B-C3B	2.48	119.89	111.83
2	C	1354	NAD	O4D-C4D-C3D	2.52	110.22	105.15
2	D	1355	NAD	O7N-C7N-C3N	2.67	122.50	119.59
2	B	1353	NAD	O3D-C3D-C2D	2.74	120.75	111.83
2	C	1354	NAD	O4B-C1B-N9A	2.79	113.94	108.10
2	C	1354	NAD	C4A-C5A-N7A	2.95	112.19	109.48
2	B	1353	NAD	C4A-C5A-N7A	2.99	112.23	109.48
2	A	1352	NAD	O4D-C4D-C3D	3.02	111.23	105.15
2	B	1353	NAD	O4B-C1B-N9A	3.16	114.71	108.10
2	D	1355	NAD	O4B-C1B-N9A	3.24	114.87	108.10
2	A	1352	NAD	C4A-C5A-N7A	3.47	112.67	109.48
2	C	1354	NAD	O7N-C7N-C3N	3.54	123.45	119.59
2	A	1352	NAD	O4D-C1D-N1N	3.68	112.18	108.13
2	B	1353	NAD	O4D-C1D-N1N	5.15	113.78	108.13
2	C	1354	NAD	O4D-C1D-N1N	6.12	114.85	108.13
2	D	1355	NAD	O4D-C1D-N1N	7.88	116.79	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1352	NAD	1	0
2	B	1353	NAD	4	0
2	C	1354	NAD	4	0
2	D	1355	NAD	2	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, 95^{th} 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	307/318 (96%)	-0.49	5 (1%) 74 80	8, 18, 40, 78	0
1	B	318/318 (100%)	-0.51	1 (0%) 94 96	9, 19, 44, 68	0
1	C	307/318 (96%)	-0.50	7 (2%) 64 72	8, 18, 43, 87	0
1	D	318/318 (100%)	-0.49	2 (0%) 90 93	8, 20, 42, 66	0
All	All	1250/1272 (98%)	-0.50	15 (1%) 81 85	8, 19, 43, 87	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	HIS	7.2
1	C	334	ASN	5.4
1	A	334	ASN	5.0
1	C	193	HIS	4.6
1	A	98	ALA	4.1
1	C	98	ALA	3.8
1	C	333	GLU	3.3
1	A	97	GLY	3.3
1	B	16	SER	2.9
1	C	97	GLY	2.8
1	D	193	HIS	2.6
1	C	96	ALA	2.6
1	D	16	SER	2.4
1	C	112	LYS	2.1
1	A	16	SER	2.1

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 (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, 95^{th} 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
2	NAD	B	1353	44/44	0.72	0.29	5.86	51,69,79,83	0
2	NAD	D	1355	44/44	0.70	0.29	4.64	53,74,85,86	0
2	NAD	C	1354	44/44	0.62	0.40	3.20	66,77,86,89	0
2	NAD	A	1352	44/44	0.73	0.31	1.73	62,70,82,84	0

6.5 Other polymers (i)

There are no such residues in this entry.