



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 AM GMT

PDB ID : 2YQ5
Title : Crystal Structure of D-isomer specific 2-hydroxyacid dehydrogenase from *Lactobacillus delbrueckii* ssp. *bulgaricus*: NAD complexed form
Authors : Holton, S.J.; Anandhakrishnan, M.; Geerlof, A.; Wilmanns, M.
Deposited on : 2012-11-05
Resolution : 2.75 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 (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

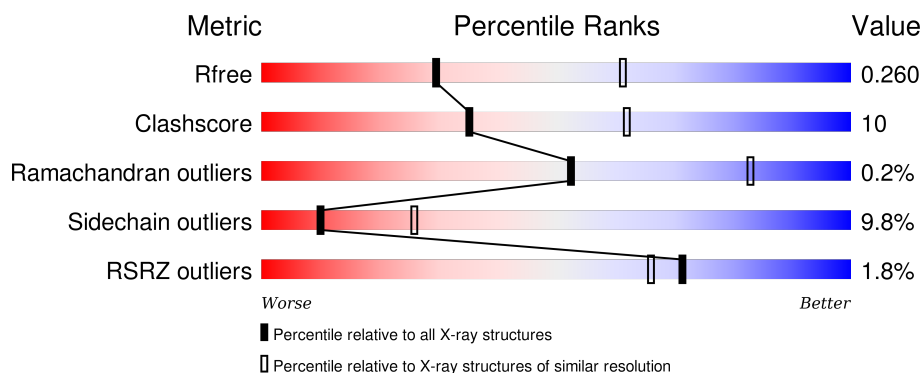
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	343	
1	B	343	
1	C	343	
1	D	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10369 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2545	1628	410	494	13			
1	B	328	Total	C	N	O	S	0	0	0
			2544	1626	410	495	13			
1	C	331	Total	C	N	O	S	0	0	0
			2573	1645	415	500	13			
1	D	321	Total	C	N	O	S	0	0	0
			2492	1593	399	487	13			

There are 40 discrepancies between the modelled and reference sequences:

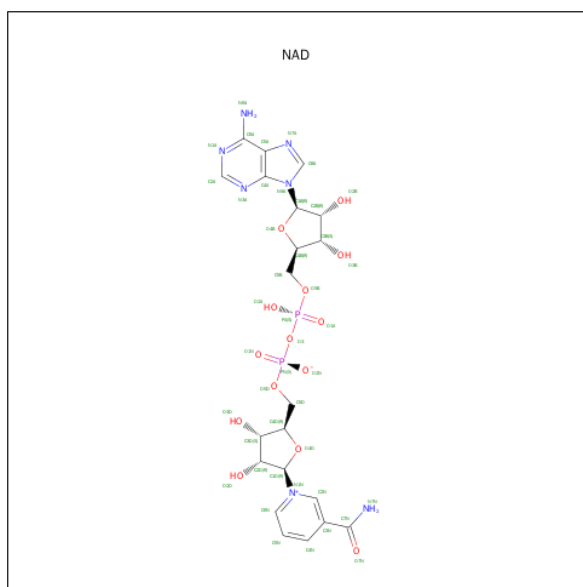
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
A	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
A	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
A	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
A	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
A	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
B	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
B	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
B	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
B	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
B	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
C	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
C	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
C	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
C	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
C	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	334	THR	-	EXPRESSION TAG	UNP Q1GAA2
D	335	ALA	-	EXPRESSION TAG	UNP Q1GAA2
D	336	SER	-	EXPRESSION TAG	UNP Q1GAA2
D	337	GLY	-	EXPRESSION TAG	UNP Q1GAA2
D	338	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	339	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	340	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	341	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	342	HIS	-	EXPRESSION TAG	UNP Q1GAA2
D	343	HIS	-	EXPRESSION TAG	UNP Q1GAA2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

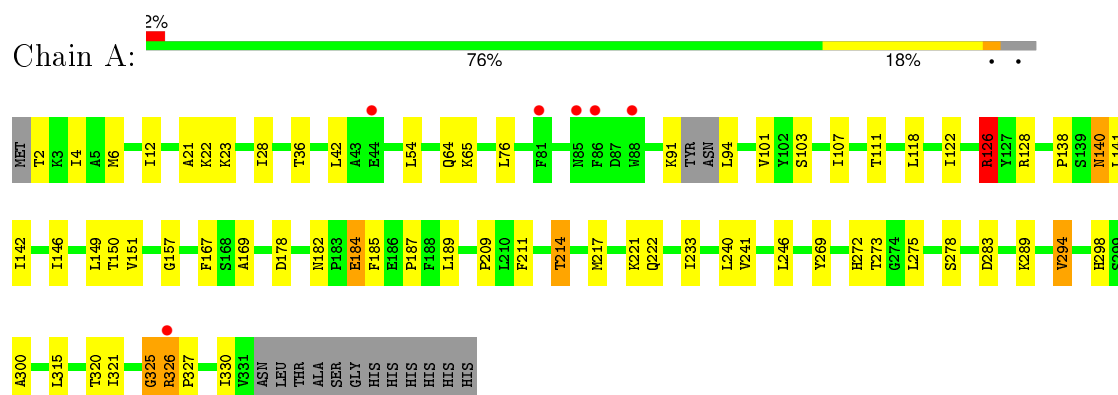
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	11	Total	O	0	0
			11	11		
3	C	9	Total	O	0	0
			9	9		
3	D	9	Total	O	0	0
			9	9		

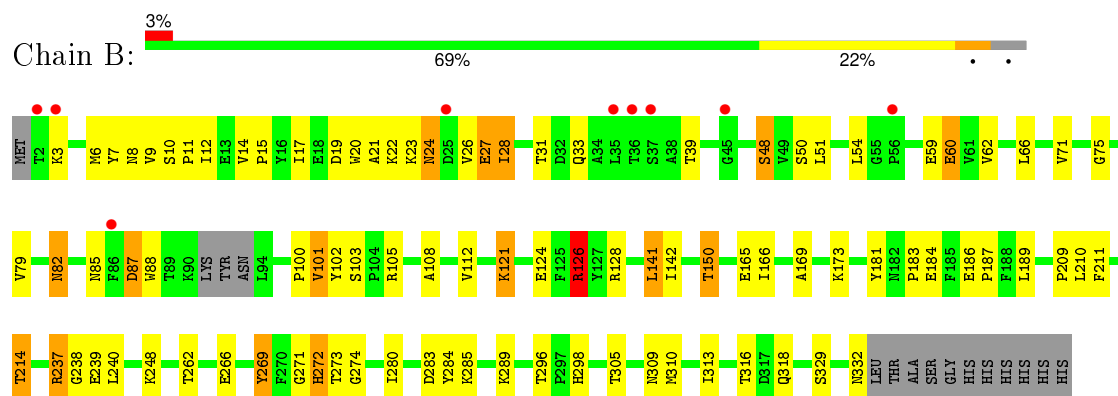
3 Residue-property plots [i](#)

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.

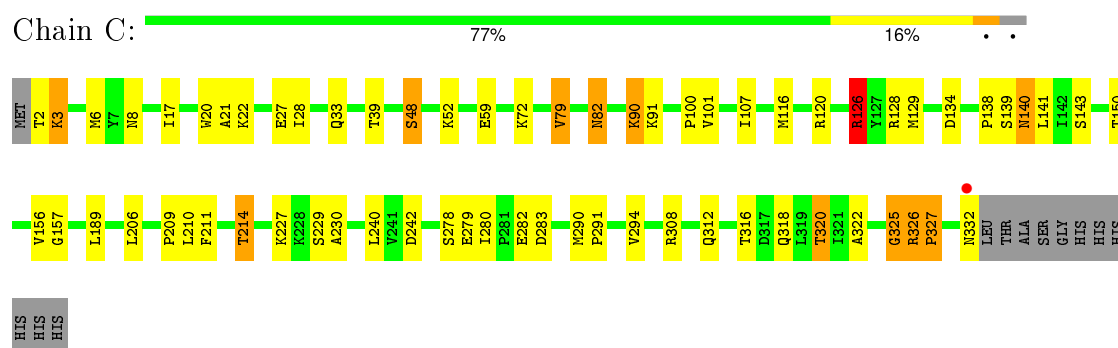
• Molecule 1: D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE



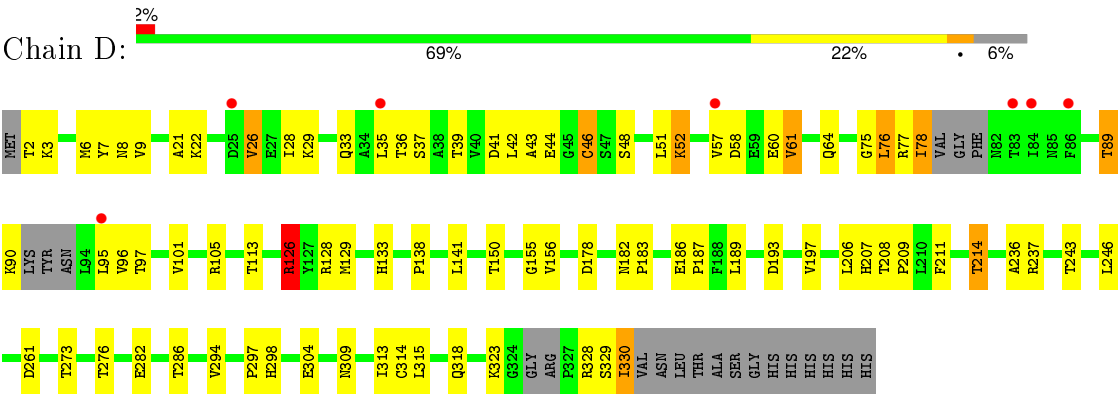
• Molecule 1: D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE



• Molecule 1: D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE



● Molecule 1: D-ISOMER SPECIFIC 2-HYDROXYACID DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.72Å 110.01Å 147.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.99 – 2.75 44.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.99-2.75) 99.1 (44.95-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.188 , 0.259 0.188 , 0.260	Depositor DCC
R_{free} test set	1955 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39677 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10369	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/2596	0.79	6/3528 (0.2%)
1	B	0.71	1/2595 (0.0%)	0.82	4/3528 (0.1%)
1	C	0.72	0/2626	0.86	5/3571 (0.1%)
1	D	0.63	0/2540	0.77	1/3450 (0.0%)
All	All	0.68	1/10357 (0.0%)	0.81	16/14077 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	GLU	CD-OE2	5.34	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	274	GLY	N-CA-C	-8.31	92.33	113.10
1	C	325	GLY	N-CA-C	7.50	131.85	113.10
1	B	273	THR	N-CA-C	-7.02	92.05	111.00
1	A	126	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	126	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	325	GLY	N-CA-C	5.95	127.97	113.10
1	C	126	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	326	ARG	C-N-CD	5.67	140.31	128.40
1	A	103	SER	C-N-CD	5.67	140.30	128.40
1	B	126	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	76	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	126	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	326	ARG	C-N-CD	5.38	139.70	128.40
1	C	327	PRO	CA-N-CD	-5.26	104.14	111.50
1	C	280	ILE	C-N-CD	5.21	139.34	128.40

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	2545	0	2543	42	0
1	B	2544	0	2536	64	0
1	C	2573	0	2565	50	0
1	D	2492	0	2483	52	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	A	10	0	0	0	0
3	B	11	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
All	All	10369	0	10231	201	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 10.

All (201) 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:B:6:MET:CE	1:B:28:ILE:HG21	1.74	1.16
1:D:126:ARG:HG2	1:D:126:ARG:HH11	1.05	1.10
1:B:6:MET:HE2	1:B:28:ILE:HG21	1.08	1.06
1:B:237:ARG:HH11	1:B:237:ARG:HG2	1.19	1.06
1:D:211:PHE:H	1:D:214:THR:HG22	1.22	1.05
1:B:126:ARG:HG2	1:B:126:ARG:HH11	1.21	1.03
1:B:6:MET:HE2	1:B:28:ILE:CG2	1.89	1.02
1:C:211:PHE:H	1:C:214:THR:HG22	1.27	0.98
1:A:126:ARG:HH11	1:A:126:ARG:HG2	1.27	0.97
1:C:20:TRP:HE1	1:C:316:THR:HG23	1.36	0.90
1:D:126:ARG:NH1	1:D:126:ARG:HG2	1.78	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:PHE:H	1:D:214:THR:CG2	1.85	0.90
1:C:79:VAL:HG13	1:C:100:PRO:HA	1.56	0.87
1:C:20:TRP:HE1	1:C:316:THR:CG2	1.87	0.86
1:D:95:LEU:HD23	1:D:330:ILE:HD12	1.57	0.85
1:C:140:ASN:HD22	1:C:140:ASN:H	1.24	0.84
1:D:2:THR:O	1:D:26:VAL:HG12	1.78	0.83
1:A:211:PHE:H	1:A:214:THR:HG22	1.45	0.81
1:B:211:PHE:H	1:B:214:THR:HG22	1.45	0.80
1:B:3:LYS:HD2	1:B:27:GLU:OE1	1.80	0.80
1:C:211:PHE:H	1:C:214:THR:CG2	1.96	0.78
1:A:209:PRO:O	1:A:214:THR:HG21	1.84	0.78
1:B:237:ARG:HG2	1:B:237:ARG:NH1	1.94	0.77
1:B:126:ARG:HG2	1:B:126:ARG:NH1	1.97	0.72
1:A:126:ARG:NH1	1:A:126:ARG:HG2	1.95	0.72
1:A:6:MET:HE1	1:A:315:LEU:HD11	1.73	0.71
1:A:178:ASP:OD1	2:A:0:NAD:O2B	2.09	0.70
1:C:211:PHE:N	1:C:214:THR:HG22	2.06	0.69
1:D:314:CYS:O	1:D:318:GLN:HG2	1.92	0.69
1:C:209:PRO:O	1:C:214:THR:HG21	1.94	0.68
1:C:90:LYS:HE3	1:C:90:LYS:HA	1.75	0.67
1:D:43:ALA:HA	1:D:46:CYS:SG	2.34	0.67
1:D:211:PHE:N	1:D:214:THR:HG22	2.04	0.67
1:C:21:ALA:HB2	1:C:28:ILE:HD12	1.76	0.67
1:D:52:LYS:O	1:D:52:LYS:HG3	1.95	0.67
1:B:237:ARG:HH11	1:B:237:ARG:CG	2.03	0.66
1:C:8:ASN:HD22	1:C:52:LYS:H	1.44	0.66
1:A:6:MET:HE3	1:A:28:ILE:HG21	1.78	0.65
1:A:320:THR:HG22	1:A:325:GLY:HA3	1.79	0.65
1:D:126:ARG:CG	1:D:126:ARG:HH11	1.95	0.64
1:A:91:LYS:O	1:A:94:LEU:N	2.30	0.64
1:D:89:THR:HG21	1:D:96:VAL:HG23	1.78	0.64
1:B:20:TRP:HE1	1:B:316:THR:CG2	2.10	0.63
1:D:41:ASP:O	1:D:44:GLU:HG3	1.99	0.63
1:C:48:SER:OG	1:C:318:GLN:NE2	2.28	0.63
1:D:2:THR:O	1:D:26:VAL:CG1	2.45	0.63
1:C:6:MET:HE1	1:C:17:ILE:HG23	1.81	0.63
1:B:66:LEU:HD22	1:B:71:VAL:HG21	1.82	0.62
1:D:33:GLN:HE21	1:D:39:THR:HG21	1.65	0.61
1:A:157:GLY:HA3	2:A:0:NAD:O5B	2.00	0.61
1:B:124:GLU:O	1:B:128:ARG:HG3	2.00	0.61
1:D:8:ASN:HD22	1:D:52:LYS:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:C	1:B:189:LEU:HD12	2.21	0.60
1:B:6:MET:HG2	1:B:50:SER:HB3	1.83	0.60
1:A:6:MET:CE	1:A:28:ILE:HG12	2.32	0.59
1:B:6:MET:HE1	1:B:17:ILE:HG23	1.82	0.59
1:D:33:GLN:HE21	1:D:39:THR:CG2	2.16	0.59
1:B:211:PHE:H	1:B:214:THR:CG2	2.15	0.59
1:B:150:THR:HB	1:B:173:LYS:HB3	1.85	0.58
1:B:82:ASN:ND2	1:B:82:ASN:H	2.02	0.58
1:C:140:ASN:N	1:C:140:ASN:HD22	1.99	0.57
1:B:66:LEU:HB3	1:B:71:VAL:HG22	1.86	0.57
1:D:211:PHE:O	1:D:214:THR:HG22	2.05	0.57
1:C:308:ARG:O	1:C:312:GLN:HG3	2.04	0.57
1:D:52:LYS:HB3	1:D:77:ARG:NH2	2.19	0.57
1:D:29:LYS:HB3	1:D:42:LEU:HD11	1.87	0.56
1:C:6:MET:CE	1:C:17:ILE:HG23	2.35	0.56
1:B:66:LEU:HB3	1:B:71:VAL:CG2	2.35	0.56
1:A:211:PHE:H	1:A:214:THR:CG2	2.18	0.55
1:D:261:ASP:O	1:D:298:HIS:HA	2.07	0.55
1:A:6:MET:HE3	1:A:28:ILE:CG2	2.37	0.55
1:B:21:ALA:O	1:B:24:ASN:O	2.24	0.55
1:B:20:TRP:HE1	1:B:316:THR:HG23	1.71	0.54
1:A:111:THR:HG23	1:A:233:ILE:HG21	1.89	0.54
1:C:90:LYS:HA	1:C:90:LYS:CE	2.37	0.54
1:B:280:ILE:O	1:B:285:LYS:HE3	2.08	0.54
1:D:8:ASN:ND2	1:D:52:LYS:H	2.05	0.54
1:D:52:LYS:O	1:D:52:LYS:CG	2.56	0.53
1:B:79:VAL:HG22	1:B:100:PRO:HA	1.89	0.53
1:C:6:MET:HE2	1:C:28:ILE:HG21	1.91	0.53
1:B:48:SER:OG	1:B:318:GLN:NE2	2.42	0.52
1:B:85:ASN:OD1	1:B:87:ASP:HB2	2.10	0.52
1:A:142:ILE:HD12	1:B:12:ILE:HG12	1.92	0.52
1:A:151:VAL:HG11	1:A:167:PHE:CD2	2.45	0.51
1:A:272:HIS:HB3	1:A:275:LEU:HD21	1.90	0.51
1:C:107:ILE:N	1:C:107:ILE:HD12	2.25	0.51
1:A:128:ARG:CZ	1:A:138:PRO:HG3	2.41	0.51
1:D:21:ALA:HB2	1:D:28:ILE:HD12	1.93	0.51
1:D:3:LYS:O	1:D:46:CYS:HA	2.11	0.51
1:D:3:LYS:O	1:D:46:CYS:HB3	2.11	0.51
1:A:21:ALA:HB2	1:A:28:ILE:HD13	1.93	0.50
1:A:327:PRO:O	1:A:330:ILE:HG12	2.11	0.50
1:A:6:MET:HE3	1:A:28:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:TYR:CZ	1:D:35:LEU:HD13	2.47	0.50
1:B:269:TYR:CD1	1:B:269:TYR:N	2.80	0.50
1:B:271:GLY:C	1:B:272:HIS:ND1	2.64	0.50
1:C:6:MET:CE	1:C:28:ILE:HG21	2.42	0.50
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.27	0.50
1:B:103:SER:HB2	1:B:305:THR:HG22	1.94	0.50
1:D:75:GLY:HA2	1:D:97:THR:OG1	2.12	0.50
1:D:6:MET:CE	1:D:315:LEU:HD21	2.42	0.49
1:B:101:VAL:O	1:B:101:VAL:HG22	2.12	0.49
1:B:3:LYS:HG3	1:B:27:GLU:HB3	1.94	0.49
1:A:300:ALA:HB3	2:A:0:NAD:N7N	2.27	0.49
1:B:14:VAL:HB	1:B:15:PRO:HD3	1.93	0.49
1:A:126:ARG:HH11	1:A:126:ARG:CG	2.11	0.49
1:B:209:PRO:O	1:B:214:THR:HG21	2.12	0.49
1:D:128:ARG:CZ	1:D:138:PRO:HG3	2.42	0.49
1:A:241:VAL:HG11	1:A:246:LEU:HD22	1.95	0.49
1:C:157:GLY:HA3	2:C:0:NAD:O5B	2.13	0.49
1:B:82:ASN:H	1:B:82:ASN:HD22	1.59	0.48
1:B:24:ASN:ND2	1:B:24:ASN:N	2.60	0.48
1:C:20:TRP:HE1	1:C:316:THR:HG22	1.70	0.48
1:B:6:MET:CE	1:B:28:ILE:CG2	2.66	0.48
1:C:6:MET:CE	1:C:17:ILE:CG2	2.92	0.48
1:A:140:ASN:H	1:A:140:ASN:HD22	1.61	0.48
1:C:140:ASN:H	1:C:140:ASN:ND2	2.04	0.47
1:C:82:ASN:HD22	1:C:82:ASN:H	1.60	0.47
1:D:57:VAL:O	1:D:57:VAL:HG12	2.14	0.47
1:B:309:ASN:HB3	1:B:313:ILE:HD12	1.97	0.47
1:C:128:ARG:NH1	1:C:138:PRO:HD3	2.29	0.47
1:A:107:ILE:HG12	2:A:0:NAD:C4N	2.43	0.47
1:A:214:THR:O	1:A:217:MET:HB2	2.13	0.47
1:D:3:LYS:O	1:D:46:CYS:CA	2.63	0.47
1:B:60:GLU:HB2	1:B:88:TRP:CE2	2.49	0.47
1:C:134:ASP:OD1	1:D:273:THR:HG22	2.15	0.47
1:C:320:THR:O	1:C:325:GLY:N	2.40	0.47
1:D:236:ALA:C	1:D:237:ARG:HG2	2.35	0.47
1:B:26:VAL:HG12	1:B:27:GLU:N	2.30	0.47
1:A:182:ASN:HB3	1:A:184:GLU:OE2	2.15	0.46
1:B:24:ASN:HD22	1:B:24:ASN:N	2.14	0.46
1:D:178:ASP:OD2	2:D:0:NAD:H1B	2.15	0.46
1:C:138:PRO:HG2	1:C:141:LEU:HB2	1.98	0.46
1:C:120:ARG:HD2	1:C:143:SER:OG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:MET:SD	1:D:297:PRO:HD3	2.56	0.45
1:B:266:GLU:HA	1:B:269:TYR:CE1	2.52	0.45
1:B:284:TYR:C	1:B:284:TYR:CD1	2.90	0.45
1:B:7:TYR:O	1:B:8:ASN:HB2	2.17	0.45
1:C:290:MET:HA	1:C:291:PRO:HD3	1.85	0.45
1:C:141:LEU:HA	1:C:141:LEU:HD12	1.73	0.45
1:D:243:THR:O	1:D:246:LEU:HB3	2.17	0.44
1:C:156:VAL:HG11	1:C:189:LEU:HD21	1.99	0.44
1:B:272:HIS:N	1:B:272:HIS:ND1	2.65	0.44
1:C:116:MET:HB3	1:D:113:THR:OG1	2.17	0.44
1:C:6:MET:HE2	1:C:28:ILE:HD13	1.99	0.44
1:A:140:ASN:N	1:A:140:ASN:HD22	2.14	0.44
2:C:0:NAD:H6N	2:C:0:NAD:H2D	1.74	0.44
1:D:209:PRO:O	1:D:214:THR:HG21	2.18	0.44
1:C:214:THR:HG23	1:C:240:LEU:CD2	2.48	0.44
1:C:72:LYS:HE2	1:C:322:ALA:HA	1.99	0.44
1:C:107:ILE:H	1:C:107:ILE:HD12	1.83	0.43
1:D:155:GLY:O	1:D:207:HIS:HB2	2.17	0.43
1:C:126:ARG:HH11	1:C:126:ARG:CG	2.31	0.43
1:A:118:LEU:HD21	1:A:294:VAL:HG12	2.00	0.43
1:B:283:ASP:OD1	1:B:284:TYR:N	2.51	0.43
1:A:321:ILE:HA	1:A:325:GLY:H	1.82	0.43
1:D:193:ASP:O	1:D:197:VAL:HG23	2.17	0.43
1:B:108:ALA:O	1:B:112:VAL:HG23	2.17	0.43
1:C:320:THR:OG1	1:C:327:PRO:HG3	2.18	0.43
1:D:309:ASN:O	1:D:313:ILE:HB	2.18	0.43
1:D:3:LYS:O	1:D:46:CYS:CB	2.67	0.43
1:D:89:THR:HG21	1:D:96:VAL:CG2	2.45	0.43
1:B:50:SER:HA	1:B:75:GLY:O	2.19	0.42
1:C:126:ARG:HG2	1:C:126:ARG:NH1	2.34	0.42
1:B:181:TYR:CE2	1:B:183:PRO:HD3	2.55	0.42
1:C:6:MET:HE3	1:C:17:ILE:HG21	2.01	0.42
1:A:182:ASN:HB2	1:A:185:PHE:CD2	2.55	0.42
1:B:121:LYS:HD2	1:B:141:LEU:HA	2.00	0.42
1:D:155:GLY:HA3	1:D:208:THR:HG22	2.02	0.42
1:C:227:LYS:HB2	1:C:230:ALA:HB2	2.02	0.42
1:C:3:LYS:HG3	1:C:27:GLU:HB3	2.01	0.42
1:D:189:LEU:C	1:D:189:LEU:HD12	2.40	0.42
1:C:20:TRP:NE1	1:C:316:THR:HG23	2.18	0.42
1:A:189:LEU:HD12	1:A:189:LEU:C	2.41	0.42
1:A:221:LYS:HB3	1:A:222:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HG12	1:B:296:THR:HG21	2.02	0.41
1:B:238:GLY:C	1:B:240:LEU:H	2.24	0.41
1:D:186:GLU:N	1:D:187:PRO:CD	2.83	0.41
1:A:4:ILE:O	1:A:28:ILE:HA	2.20	0.41
1:B:59:GLU:O	1:B:62:VAL:HG22	2.20	0.41
1:A:12:ILE:HG12	1:B:142:ILE:HD12	2.02	0.41
1:A:214:THR:HG23	1:A:240:LEU:CD2	2.50	0.41
1:B:210:LEU:HA	1:B:214:THR:HG21	2.02	0.41
1:A:169:ALA:HB1	1:B:169:ALA:HB1	2.03	0.41
1:A:91:LYS:HD3	1:A:91:LYS:HA	1.79	0.41
1:D:76:LEU:HD12	1:D:78:ILE:HD11	2.03	0.41
1:B:20:TRP:HE1	1:B:316:THR:HG22	1.84	0.41
1:B:102:TYR:CZ	1:B:310:MET:HE3	2.56	0.41
1:B:33:GLN:HG3	1:B:39:THR:HG21	2.02	0.41
1:A:146:ILE:HA	1:A:146:ILE:HD12	1.95	0.41
1:C:126:ARG:HH11	1:C:126:ARG:HG2	1.86	0.40
1:D:61:VAL:O	1:D:64:GLN:HB2	2.22	0.40
1:C:210:LEU:HA	1:C:214:THR:CG2	2.52	0.40
1:D:182:ASN:HA	1:D:183:PRO:HD3	1.85	0.40
1:A:187:PRO:HG3	1:D:105:ARG:HG3	2.03	0.40
1:B:186:GLU:N	1:B:187:PRO:CD	2.84	0.40
1:C:33:GLN:HE21	1:C:39:THR:HG21	1.87	0.40
1:C:242:ASP:OD1	1:C:242:ASP:C	2.60	0.40
1:D:129:MET:O	1:D:133:HIS:HA	2.21	0.40
1:B:105:ARG:NE	1:B:166:ILE:HD11	2.36	0.40
1:B:10:SER:O	1:B:11:PRO:C	2.60	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	324/343 (94%)	311 (96%)	13 (4%)	0	100	100
1	B	324/343 (94%)	313 (97%)	9 (3%)	2 (1%)	30	62
1	C	329/343 (96%)	322 (98%)	7 (2%)	0	100	100
1	D	313/343 (91%)	296 (95%)	17 (5%)	0	100	100
All	All	1290/1372 (94%)	1242 (96%)	46 (4%)	2 (0%)	52	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	GLU
1	B	239	GLU

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	281/294 (96%)	257 (92%)	24 (8%)	13	34
1	B	281/294 (96%)	252 (90%)	29 (10%)	9	23
1	C	284/294 (97%)	259 (91%)	25 (9%)	12	32
1	D	276/294 (94%)	244 (88%)	32 (12%)	7	18
All	All	1122/1176 (95%)	1012 (90%)	110 (10%)	10	26

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	22	LYS
1	A	23	LYS
1	A	36	THR
1	A	42	LEU
1	A	54	LEU
1	A	64	GLN
1	A	65	LYS
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	126	ARG
1	A	140	ASN
1	A	141	LEU
1	A	149	LEU
1	A	150	THR
1	A	184	GLU
1	A	214	THR
1	A	269	TYR
1	A	273	THR
1	A	278	SER
1	A	283	ASP
1	A	289	LYS
1	A	294	VAL
1	A	298	HIS
1	A	326	ARG
1	B	9	VAL
1	B	19	ASP
1	B	22	LYS
1	B	23	LYS
1	B	24	ASN
1	B	27	GLU
1	B	28	ILE
1	B	31	THR
1	B	48	SER
1	B	51	LEU
1	B	54	LEU
1	B	60	GLU
1	B	82	ASN
1	B	87	ASP
1	B	101	VAL
1	B	121	LYS
1	B	126	ARG
1	B	141	LEU
1	B	150	THR
1	B	214	THR
1	B	237	ARG
1	B	248	LYS
1	B	262	THR
1	B	269	TYR
1	B	272	HIS
1	B	289	LYS
1	B	298	HIS

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Mol	Chain	Res	Type
1	B	329	SER
1	B	332	ASN
1	C	2	THR
1	C	3	LYS
1	C	22	LYS
1	C	48	SER
1	C	59	GLU
1	C	79	VAL
1	C	82	ASN
1	C	90	LYS
1	C	91	LYS
1	C	101	VAL
1	C	126	ARG
1	C	139	SER
1	C	140	ASN
1	C	150	THR
1	C	206	LEU
1	C	214	THR
1	C	229	SER
1	C	278	SER
1	C	279	GLU
1	C	282	GLU
1	C	283	ASP
1	C	294	VAL
1	C	320	THR
1	C	326	ARG
1	C	332	ASN
1	D	9	VAL
1	D	22	LYS
1	D	26	VAL
1	D	36	THR
1	D	37	SER
1	D	46	CYS
1	D	48	SER
1	D	51	LEU
1	D	52	LYS
1	D	58	ASP
1	D	60	GLU
1	D	61	VAL
1	D	76	LEU
1	D	78	ILE
1	D	89	THR

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Mol	Chain	Res	Type
1	D	90	LYS
1	D	101	VAL
1	D	126	ARG
1	D	141	LEU
1	D	150	THR
1	D	156	VAL
1	D	206	LEU
1	D	214	THR
1	D	276	THR
1	D	282	GLU
1	D	286	THR
1	D	294	VAL
1	D	304	GLU
1	D	323	LYS
1	D	328	ARG
1	D	329	SER
1	D	330	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	64	GLN
1	A	82	ASN
1	A	140	ASN
1	B	8	ASN
1	B	24	ASN
1	B	82	ASN
1	B	318	GLN
1	C	8	ASN
1	C	33	GLN
1	C	82	ASN
1	C	140	ASN
1	C	318	GLN
1	D	8	ASN
1	D	33	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 ⓘ

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	0	-	38,48,48	2.05	9 (23%)	47,73,73	2.06	12 (25%)
2	NAD	B	0	-	38,48,48	2.17	16 (42%)	47,73,73	2.11	10 (21%)
2	NAD	C	0	-	38,48,48	1.56	4 (10%)	47,73,73	2.03	8 (17%)
2	NAD	D	0	-	38,48,48	1.54	4 (10%)	47,73,73	2.06	7 (14%)

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	0	-	-	0/22/62/62	0/5/5/5
2	NAD	B	0	-	-	0/22/62/62	0/5/5/5
2	NAD	C	0	-	-	0/22/62/62	0/5/5/5
2	NAD	D	0	-	-	0/22/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	0	NAD	O4B-C1B	-7.27	1.32	1.41
2	A	0	NAD	O4B-C4B	-4.80	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	NAD	PN-O2N	-3.96	1.38	1.54
2	B	0	NAD	PA-O1A	-3.56	1.38	1.51
2	B	0	NAD	C4A-N3A	-3.54	1.30	1.35
2	B	0	NAD	PN-O5D	-3.41	1.43	1.59
2	B	0	NAD	O4B-C4B	-3.37	1.37	1.45
2	B	0	NAD	O4B-C1B	-3.14	1.37	1.41
2	B	0	NAD	PA-O2A	-3.03	1.42	1.54
2	B	0	NAD	PA-O5B	-2.90	1.45	1.59
2	B	0	NAD	PN-O1N	-2.89	1.40	1.51
2	B	0	NAD	C5A-C4A	-2.85	1.34	1.40
2	B	0	NAD	C5A-N7A	-2.80	1.29	1.39
2	A	0	NAD	PN-O2N	-2.78	1.43	1.54
2	A	0	NAD	C4A-N3A	-2.58	1.31	1.35
2	A	0	NAD	C5A-N7A	-2.55	1.30	1.39
2	A	0	NAD	PA-O2A	-2.55	1.44	1.54
2	B	0	NAD	C2A-N1A	-2.52	1.29	1.33
2	B	0	NAD	C2D-C3D	-2.50	1.46	1.53
2	A	0	NAD	PA-O5B	-2.49	1.47	1.59
2	B	0	NAD	C8A-N7A	-2.37	1.30	1.34
2	B	0	NAD	C7N-N7N	-2.18	1.28	1.33
2	B	0	NAD	O2D-C2D	-2.14	1.37	1.43
2	A	0	NAD	O5B-C5B	-2.13	1.36	1.44
2	A	0	NAD	O4D-C1D	-2.08	1.38	1.41
2	D	0	NAD	C3N-C7N	2.31	1.54	1.50
2	C	0	NAD	C3N-C7N	2.45	1.54	1.50
2	C	0	NAD	C6N-N1N	2.49	1.42	1.35
2	D	0	NAD	PA-O1A	3.58	1.64	1.51
2	C	0	NAD	PA-O1A	3.64	1.64	1.51
2	D	0	NAD	O4B-C1B	4.36	1.46	1.41
2	D	0	NAD	O4D-C1D	5.47	1.48	1.41
2	C	0	NAD	O4D-C1D	7.38	1.50	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	NAD	N3A-C2A-N1A	-10.03	121.21	128.89
2	B	0	NAD	N3A-C2A-N1A	-9.10	121.92	128.89
2	C	0	NAD	N3A-C2A-N1A	-8.70	122.23	128.89
2	A	0	NAD	N3A-C2A-N1A	-7.35	123.27	128.89
2	D	0	NAD	C3N-C7N-N7N	-4.96	112.38	117.82
2	C	0	NAD	PN-O3-PA	-4.68	119.58	132.73
2	B	0	NAD	C3N-C7N-N7N	-4.52	112.87	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	0	NAD	O4D-C1D-N1N	-4.36	103.34	108.13
2	A	0	NAD	C4B-O4B-C1B	-3.88	105.46	109.72
2	C	0	NAD	C4D-O4D-C1D	-3.86	105.47	109.72
2	A	0	NAD	C3N-C7N-N7N	-3.82	113.63	117.82
2	A	0	NAD	C4D-O4D-C1D	-3.51	105.86	109.72
2	B	0	NAD	O2D-C2D-C3D	-3.32	101.02	111.83
2	C	0	NAD	C3N-C7N-N7N	-3.31	114.19	117.82
2	A	0	NAD	O4B-C1B-N9A	-3.23	101.33	108.10
2	D	0	NAD	C4D-O4D-C1D	-3.07	106.34	109.72
2	A	0	NAD	O4B-C4B-C5B	-3.06	98.39	109.32
2	A	0	NAD	C2B-C1B-N9A	-2.88	109.90	114.29
2	B	0	NAD	O3D-C3D-C2D	-2.84	102.58	111.83
2	D	0	NAD	C4A-C5A-N7A	-2.84	106.86	109.48
2	A	0	NAD	C4A-C5A-N7A	-2.67	107.03	109.48
2	D	0	NAD	PN-O3-PA	-2.38	126.04	132.73
2	B	0	NAD	C5D-C4D-C3D	-2.36	105.83	115.21
2	C	0	NAD	C4A-C5A-N7A	-2.21	107.45	109.48
2	B	0	NAD	O4D-C4D-C5D	2.00	116.49	109.32
2	A	0	NAD	O3-PA-O5B	2.18	108.71	102.94
2	C	0	NAD	O7N-C7N-C3N	2.18	121.97	119.59
2	C	0	NAD	O2A-PA-O3	2.24	115.27	105.09
2	B	0	NAD	O5D-C5D-C4D	2.31	117.63	109.12
2	A	0	NAD	C2N-C3N-C4N	2.35	120.90	118.29
2	A	0	NAD	O7N-C7N-C3N	2.70	122.53	119.59
2	D	0	NAD	O7N-C7N-C3N	2.77	122.61	119.59
2	B	0	NAD	O3-PA-O5B	2.79	110.33	102.94
2	B	0	NAD	O7N-C7N-C3N	3.31	123.20	119.59
2	B	0	NAD	O4D-C1D-N1N	3.56	112.04	108.13
2	D	0	NAD	O4D-C1D-N1N	3.72	112.22	108.13
2	C	0	NAD	O4D-C1D-N1N	5.18	113.83	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	0	NAD	4	0
2	C	0	NAD	2	0
2	D	0	NAD	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	328/343 (95%)	-0.13	6 (1%) 71 66	25, 45, 90, 116	0
1	B	328/343 (95%)	-0.08	9 (2%) 58 51	19, 38, 94, 109	0
1	C	331/343 (96%)	-0.39	1 (0%) 94 93	21, 35, 60, 77	0
1	D	321/343 (93%)	0.05	7 (2%) 65 59	23, 49, 93, 113	0
All	All	1308/1372 (95%)	-0.14	23 (1%) 71 66	19, 42, 89, 116	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	VAL	5.7
1	D	86	PHE	4.3
1	B	25	ASP	3.5
1	B	3	LYS	3.0
1	B	2	THR	3.0
1	B	56	PRO	2.8
1	D	84	ILE	2.8
1	A	86	PHE	2.8
1	B	35	LEU	2.7
1	B	86	PHE	2.7
1	A	88	TRP	2.6
1	D	35	LEU	2.6
1	A	326	ARG	2.5
1	C	332	ASN	2.4
1	D	25	ASP	2.4
1	B	37	SER	2.4
1	A	85	ASN	2.3
1	A	81	PHE	2.3
1	A	44	GLU	2.1
1	B	36	THR	2.1
1	B	45	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	95	LEU	2.0
1	D	83	THR	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(\AA^2)	Q<0.9
2	NAD	A	0	44/44	0.93	0.16	0.56	48,58,67,69	0
2	NAD	D	0	44/44	0.94	0.15	-0.21	47,59,65,67	0
2	NAD	C	0	44/44	0.97	0.12	-0.33	30,38,46,50	0
2	NAD	B	0	44/44	0.97	0.12	-1.10	31,38,41,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.