



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:21 pm GMT

PDB ID : 1T2F
Title : Human B lactate dehydrogenase complexed with NAD⁺ and 4-hydroxy-1,2,5-oxadiazole-3-carboxylic acid
Authors : Cameron, A.; Read, J.; Tranter, R.; Winter, V.J.; Sessions, R.B.; Brady, R.L.; Vivas, L.; Easton, A.; Kendrick, H.; Croft, S.L.; Barros, D.; Lavandera, J.L.; Martin, J.J.; Risco, F.; Garcia-Ochoa, S.; Gamo, F.J.; Sanz, L.; Leon, L.; Ruiz, J.R.; Gabarro, R.; Mallo, A.; De Las Heras, F.G.
Deposited on : 2004-04-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

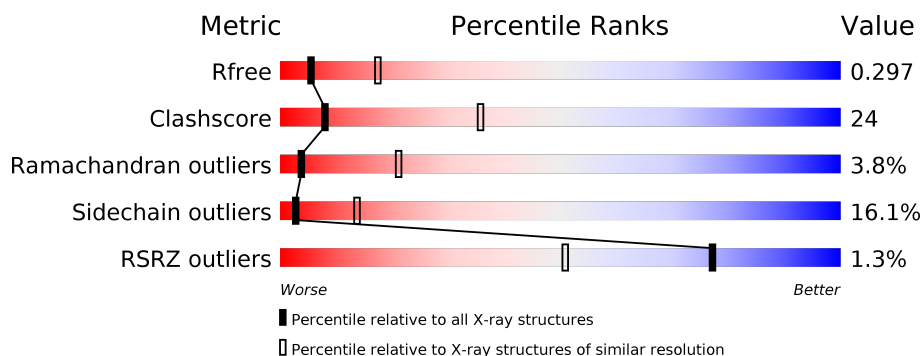
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	333	<div> <div>2%</div> <div>53%</div> <div>34%</div> <div>11%</div> <div>.</div> </div>
1	B	333	<div> <div>%</div> <div>45%</div> <div>45%</div> <div>8%</div> <div>.</div> </div>
1	C	333	<div> <div>%</div> <div>56%</div> <div>32%</div> <div>10%</div> <div>.</div> </div>
1	D	333	<div> <div>%</div> <div>50%</div> <div>38%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10665 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.

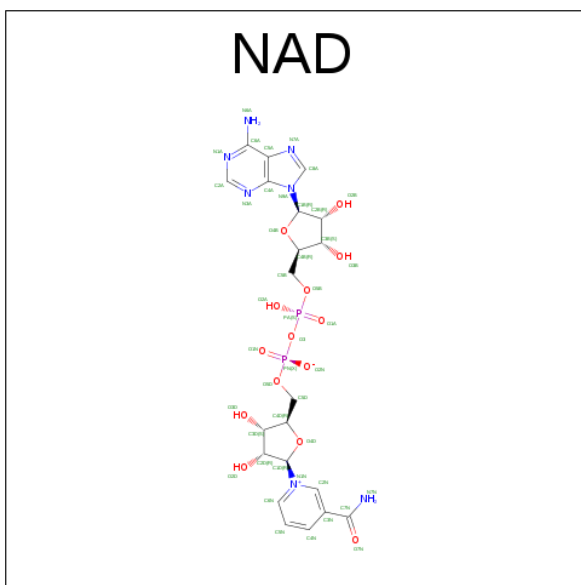
- Molecule 1 is a protein called L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	51	0	0
			2555	1627	430	484	14			
1	B	332	Total	C	N	O	S	71	0	0
			2555	1627	430	484	14			
1	C	332	Total	C	N	O	S	65	0	0
			2555	1627	430	484	14			
1	D	332	Total	C	N	O	S	78	0	0
			2555	1627	430	484	14			

There are 4 discrepancies between the modelled and reference sequences:

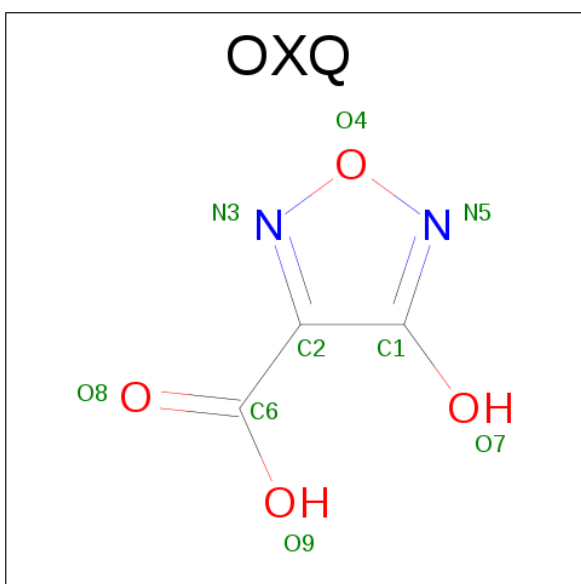
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	PHE	ASP	ENGINEERED	UNP P07195
B	332	PHE	ASP	ENGINEERED	UNP P07195
C	332	PHE	ASP	ENGINEERED	UNP P07195
D	332	PHE	ASP	ENGINEERED	UNP P07195

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



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

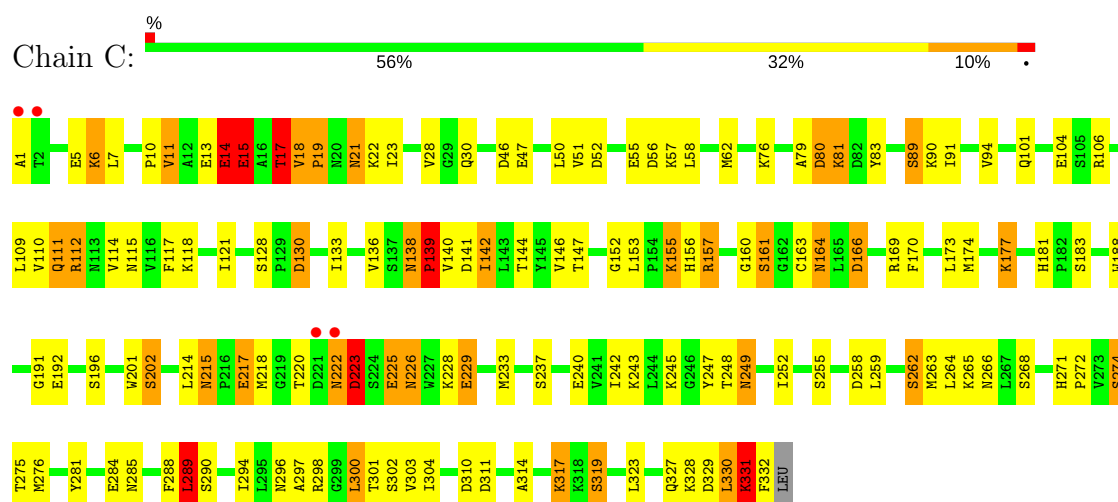
- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLIC ACID (three-letter code: OXQ) (formula: $C_3H_2N_2O_4$).



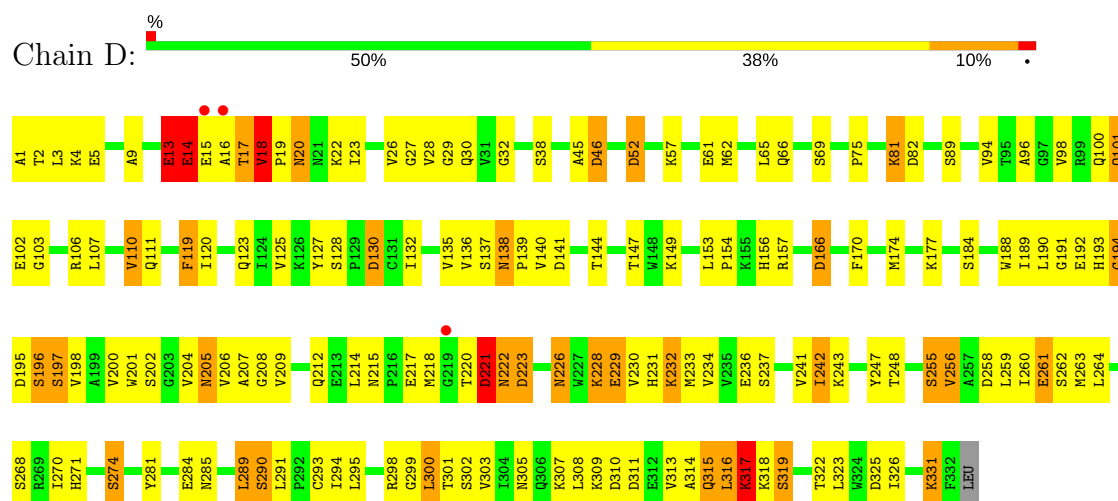
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 3 2 4	0	0
3	B	1	Total C N O 9 3 2 4	0	0
3	C	1	Total C N O 9 3 2 4	0	0
3	D	1	Total C N O 9 3 2 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	76	Total O 76 76	0	0
4	C	48	Total O 48 48	0	0
4	D	43	Total O 43 43	0	0



• Molecule 1: L-lactate dehydrogenase B chain



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	137.40Å 160.44Å 59.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 28.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.88-3.00) 90.3 (28.90-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.321 0.201 , 0.297	Depositor DCC
R_{free} test set	1238 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10665	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 46.79 % 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 1.0889e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXQ, 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	1.26	8/2597 (0.3%)	1.28	18/3520 (0.5%)
1	B	1.19	6/2597 (0.2%)	1.19	24/3520 (0.7%)
1	C	1.24	8/2597 (0.3%)	1.28	29/3520 (0.8%)
1	D	1.49	13/2597 (0.5%)	1.52	36/3520 (1.0%)
All	All	1.30	35/10388 (0.3%)	1.32	107/14080 (0.8%)

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	1	2
1	B	1	3
1	C	2	2
1	D	4	0
All	All	8	7

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	GLU	CA-CB	-33.15	0.81	1.53
1	D	119	PHE	CB-CG	29.10	2.00	1.51
1	A	222	ASN	CA-CB	27.49	2.24	1.53
1	D	318	LYS	CA-CB	-27.04	0.94	1.53
1	D	217	GLU	CB-CG	-26.53	1.01	1.52

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	27.37	173.62	113.40
1	D	318	LYS	CA-CB-CG	27.25	173.35	113.40
1	D	119	PHE	CB-CG-CD2	20.86	135.40	120.80
1	A	221	ASP	N-CA-CB	20.71	147.88	110.60
1	D	331	LYS	N-CA-CB	20.29	147.12	110.60

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	221	ASP	CA
1	B	222	ASN	CA
1	C	6	LYS	CA
1	C	284	GLU	CA
1	D	221	ASP	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	15	GLU	Peptide
1	B	1	ALA	Peptide
1	B	139	PRO	Peptide
1	B	222	ASN	Peptide

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	2555	0	2627	126	4
1	B	2555	0	2627	149	4
1	C	2555	0	2627	113	3
1	D	2555	0	2627	109	3
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	4	0
3	A	9	0	0	1	0
3	B	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	0	3	0
3	D	9	0	0	2	0
4	A	66	0	0	17	0
4	B	76	0	0	34	0
4	C	48	0	0	27	0
4	D	43	0	0	13	0
All	All	10665	0	10612	485	7

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 24.

The worst 5 of 485 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:C:294:ILE:HB	4:C:452:HOH:O	1.29	1.24
1:B:324:TRP:HB3	4:B:456:HOH:O	1.38	1.23
1:C:152:GLY:HA3	4:C:454:HOH:O	1.42	1.18
1:C:302:SER:HB2	4:C:452:HOH:O	1.49	1.12
1:A:229:GLU:HG3	4:A:456:HOH:O	1.48	1.10

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:CA	1:B:14:GLU:OE2[1_554]	1.19	1.01
1:C:14:GLU:OE1	1:D:149:LYS:NZ[1_554]	1.69	0.51
1:A:148:TRP:O	1:B:14:GLU:OE1[1_554]	1.75	0.45
1:A:149:LYS:C	1:B:14:GLU:OE2[1_554]	1.78	0.42
1:C:14:GLU:OE2	1:D:149:LYS:NZ[1_554]	1.82	0.38

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/333 (99%)	272 (82%)	45 (14%)	13 (4%)	3	20
1	B	330/333 (99%)	264 (80%)	51 (16%)	15 (4%)	3	17
1	C	330/333 (99%)	275 (83%)	45 (14%)	10 (3%)	5	27
1	D	330/333 (99%)	269 (82%)	49 (15%)	12 (4%)	4	22
All	All	1320/1332 (99%)	1080 (82%)	190 (14%)	50 (4%)	4	21

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	221	ASP
1	A	222	ASN
1	A	224	SER
1	A	226	ASN

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	288/289 (100%)	236 (82%)	52 (18%)	2	10
1	B	288/289 (100%)	248 (86%)	40 (14%)	4	18
1	C	288/289 (100%)	241 (84%)	47 (16%)	3	13
1	D	288/289 (100%)	241 (84%)	47 (16%)	3	13
All	All	1152/1156 (100%)	966 (84%)	186 (16%)	3	14

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	LEU
1	C	81	LYS
1	D	261	GLU
1	B	310	ASP
1	C	11	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	315	GLN
1	C	181	HIS
1	D	266	ASN
1	C	21	ASN
1	C	108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

8 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	401	-	41,48,48	1.90	5 (12%)	43,73,73	1.83	5 (11%)
3	OXQ	A	402	-	2,9,9	1.03	0	0,12,12	0.00	-
2	NAD	B	403	-	41,48,48	1.94	5 (12%)	43,73,73	2.73	8 (18%)
3	OXQ	B	404	-	2,9,9	1.01	0	0,12,12	0.00	-
2	NAD	C	405	-	41,48,48	1.74	6 (14%)	43,73,73	2.31	9 (20%)
3	OXQ	C	406	-	2,9,9	1.02	0	0,12,12	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	407	-	41,48,48	2.02	4 (9%)	43,73,73	1.72	6 (13%)
3	OXQ	D	408	-	2,9,9	0.89	0	0,12,12	0.00	-

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	401	-	-	0/22/62/62	0/5/5/5
3	OXQ	A	402	-	-	0/0/4/4	0/0/1/1
2	NAD	B	403	-	-	0/22/62/62	0/5/5/5
3	OXQ	B	404	-	-	0/0/4/4	0/0/1/1
2	NAD	C	405	-	-	0/22/62/62	0/5/5/5
3	OXQ	C	406	-	-	0/0/4/4	0/0/1/1
2	NAD	D	407	-	-	0/22/62/62	0/5/5/5
3	OXQ	D	408	-	-	0/0/4/4	0/0/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	405	NAD	C2D-C1D	-2.99	1.48	1.53
2	A	401	NAD	C2D-C1D	-2.67	1.49	1.53
2	C	405	NAD	O4B-C1B	-2.53	1.37	1.41
2	A	401	NAD	O4D-C4D	-2.29	1.39	1.45
2	C	405	NAD	O3D-C3D	-2.09	1.38	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	NAD	N3A-C2A-N1A	-14.07	116.60	128.86
2	C	405	NAD	N3A-C2A-N1A	-8.76	121.23	128.86
2	A	401	NAD	N3A-C2A-N1A	-8.22	121.70	128.86
2	D	407	NAD	N3A-C2A-N1A	-7.40	122.42	128.86
2	C	405	NAD	C1B-N9A-C4A	-5.86	116.51	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	1	0
3	A	402	OXQ	1	0
2	B	403	NAD	4	0
3	B	404	OXQ	1	0
2	C	405	NAD	4	0
3	C	406	OXQ	3	0
2	D	407	NAD	4	0
3	D	408	OXQ	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	332/333 (99%)	-0.39	6 (1%)	69 40	37, 50, 82, 93	11 (3%)
1	B	332/333 (99%)	-0.10	4 (1%)	79 53	38, 61, 85, 90	15 (4%)
1	C	332/333 (99%)	-0.29	4 (1%)	79 53	37, 54, 84, 92	14 (4%)
1	D	332/333 (99%)	-0.32	3 (0%)	84 61	37, 53, 85, 93	18 (5%)
All	All	1328/1332 (99%)	-0.28	17 (1%)	77 51	37, 54, 84, 93	58 (4%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	ASN	6.1
1	D	15	GLU	4.5
1	C	221	ASP	3.7
1	A	221	ASP	3.3
1	D	219	GLY	3.2

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
3	OXQ	A	402	9/9	0.94	0.20	0.90	63,64,65,65	0
2	NAD	C	405	44/44	0.93	0.18	-0.01	33,43,52,57	0
2	NAD	B	403	44/44	0.90	0.21	-0.09	46,61,84,87	0
2	NAD	A	401	44/44	0.94	0.16	-0.29	29,40,50,51	0
2	NAD	D	407	44/44	0.93	0.16	-0.30	33,42,47,49	0
3	OXQ	B	404	9/9	0.92	0.19	-0.35	53,56,60,62	0
3	OXQ	C	406	9/9	0.94	0.16	-0.44	56,58,59,59	0
3	OXQ	D	408	9/9	0.97	0.17	-0.88	63,65,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.