



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 AM GMT

PDB ID : 2OOR
Title : Structure of transhydrogenase (dI.NAD⁺)₂(dIII.H₂NADPH)₁ asymmetric complex
Authors : Bhakta, T.; Jackson J.B.
Deposited on : 2007-01-26
Resolution : 2.32 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

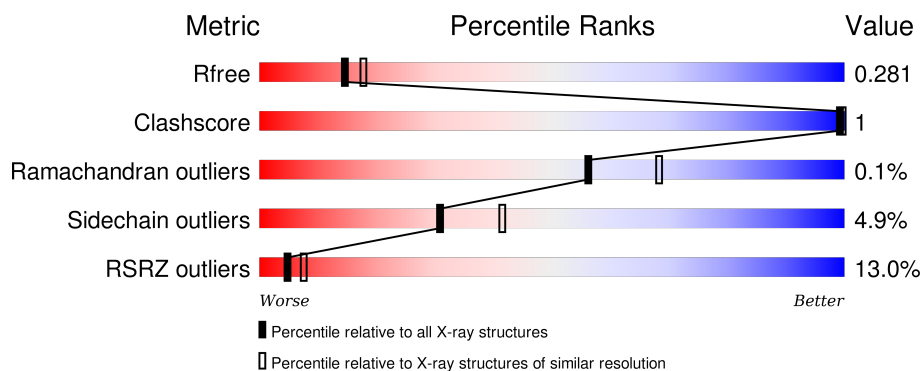
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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 $\leq 5\%$. 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	384	<div> <div>17%</div> <div>95%</div> <div>• •</div> </div>
1	B	384	<div> <div>6%</div> <div>89%</div> <div>5% • 5%</div> </div>
2	C	174	<div> <div>18%</div> <div>93%</div> <div>6% • •</div> </div>

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	TXP	C	400	X	-	-	-
5	GOL	B	700	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6981 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.

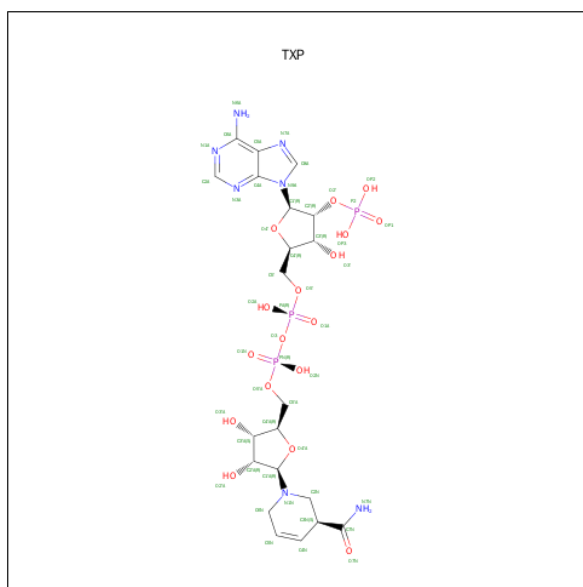
- Molecule 1 is a protein called NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2779	1753	479	529	18			
1	B	364	Total	C	N	O	S	0	0	0
			2675	1691	463	505	16			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

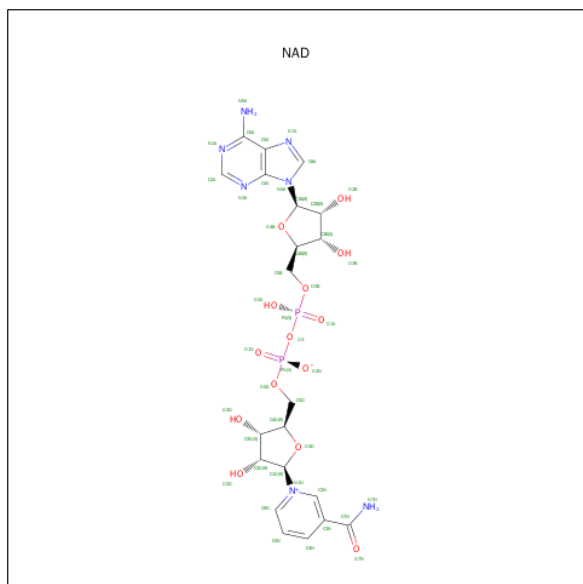
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	173	Total	C	N	O	S	0	0	0
			1302	826	215	250	11			

- Molecule 3 is 1,4,5,6-TETRAHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE PHOSPHATE (three-letter code: TXP) (formula: $C_{21}H_{32}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			36	15	6	13	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

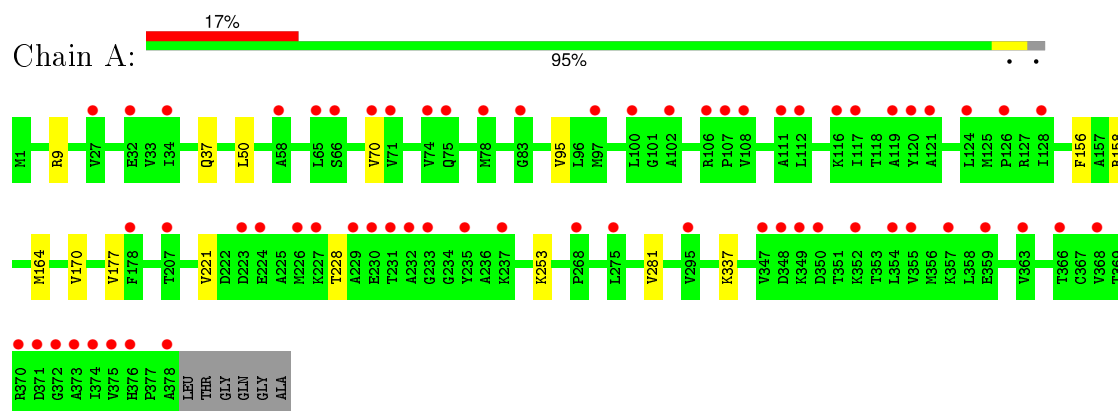
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	45	Total	O	0	0
			45	45		
6	C	11	Total	O	0	0
			11	11		

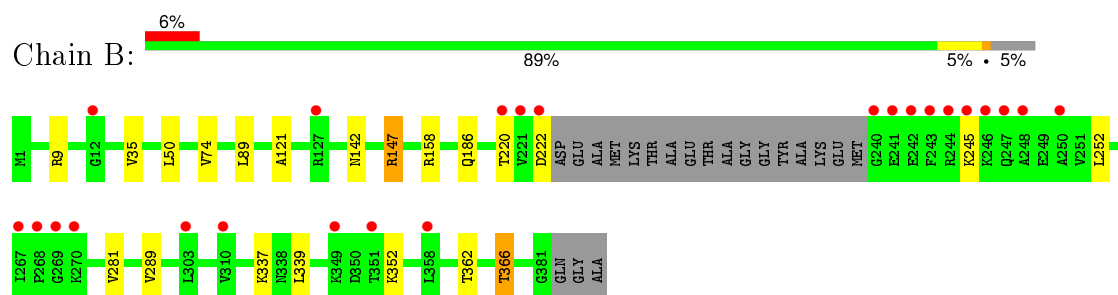
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

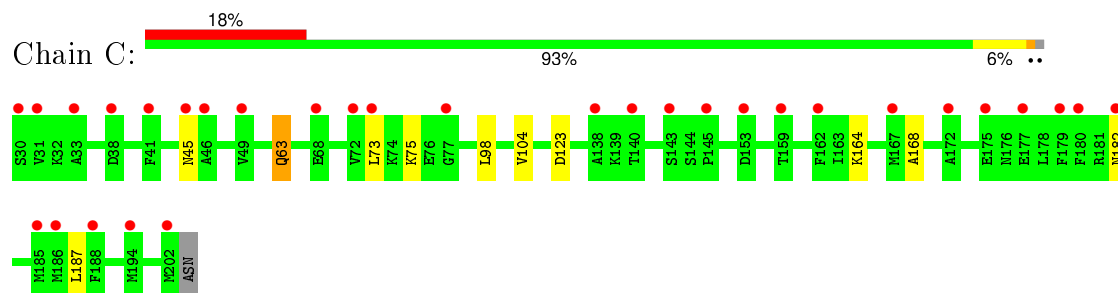
- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



- Molecule 2: NAD(P) transhydrogenase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.19Å 74.45Å 204.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.60 – 2.32 59.01 – 2.32	Depositor EDS
% Data completeness (in resolution range)	91.0 (102.60-2.32) 91.0 (59.01-2.32)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.247 , 0.275 0.253 , 0.281	Depositor DCC
R_{free} test set	2530 reflections (6.05%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
Estimated twinning fraction	0.017 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44315 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6981	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: GOL, NAD, TXP

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	0.42	0/2816	0.61	0/3816
1	B	0.42	0/2710	0.68	3/3674 (0.1%)
2	C	0.43	0/1325	0.64	0/1792
All	All	0.42	0/6851	0.64	3/9282 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	147	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	147	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2779	0	2904	2	0
1	B	2675	0	2809	4	0
2	C	1302	0	1297	2	0
3	C	48	0	27	0	0
4	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	36	0	20	0	0
5	B	6	0	8	0	0
6	A	35	0	0	0	0
6	B	45	0	0	0	0
6	C	11	0	0	0	0
All	All	6981	0	7091	8	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 (8) 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:142:ASN:HD21	1:B:186:GLN:HE21	1.19	0.89
1:A:70:VAL:HG23	1:A:95:VAL:HG23	1.87	0.57
1:B:142:ASN:ND2	1:B:186:GLN:HE21	1.98	0.56
1:B:121:ALA:O	1:B:366:THR:OG1	2.30	0.47
2:C:63:GLN:HG2	2:C:98:LEU:HB3	1.96	0.47
1:B:142:ASN:HD21	1:B:186:GLN:NE2	2.01	0.42
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.54	0.42
2:C:164:LYS:NZ	2:C:168:ALA:O	2.36	0.41

There are no symmetry-related clashes.

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	376/384 (98%)	355 (94%)	21 (6%)	0	100	100
1	B	360/384 (94%)	345 (96%)	15 (4%)	0	100	100
2	C	171/174 (98%)	163 (95%)	7 (4%)	1 (1%)	30	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	907/942 (96%)	863 (95%)	43 (5%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	182	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	293/296 (99%)	282 (96%)	11 (4%)	40 54
1	B	284/296 (96%)	267 (94%)	17 (6%)	24 31
2	C	137/138 (99%)	130 (95%)	7 (5%)	29 39
All	All	714/730 (98%)	679 (95%)	35 (5%)	31 41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	37	GLN
1	A	50	LEU
1	A	164	MET
1	A	170	VAL
1	A	177	VAL
1	A	221	VAL
1	A	228	THR
1	A	253	LYS
1	A	281	VAL
1	A	337	LYS
1	B	9	ARG
1	B	35	VAL
1	B	50	LEU
1	B	74	VAL

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Mol	Chain	Res	Type
1	B	89	LEU
1	B	147	ARG
1	B	220	THR
1	B	222	ASP
1	B	245	LYS
1	B	252	LEU
1	B	281	VAL
1	B	289	VAL
1	B	337	LYS
1	B	339	LEU
1	B	352	LYS
1	B	362	THR
1	B	366	THR
2	C	45	ASN
2	C	63	GLN
2	C	73	LEU
2	C	75	LYS
2	C	104	VAL
2	C	123	ASP
2	C	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	247	GLN
1	A	338	ASN
1	B	142	ASN
1	B	210	GLN
2	C	63	GLN
2	C	182	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

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	$\# Z > 2$
4	NAD	A	500	-	38,48,48	1.70	3 (7%)	47,73,73	2.05	5 (10%)
4	NAD	B	600	-	32,39,48	1.08	2 (6%)	37,60,73	2.22	6 (16%)
5	GOL	B	700	-	5,5,5	0.36	0	5,5,5	0.39	0
3	TXP	C	400	-	45,52,52	3.56	5 (11%)	54,80,80	2.10	11 (20%)

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
4	NAD	A	500	-	-	0/22/62/62	0/5/5/5
4	NAD	B	600	-	-	0/18/54/62	0/4/4/5
5	GOL	B	700	-	-	0/4/4/4	0/0/0/0
3	TXP	C	400	-	1/1/14/16	0/31/77/77	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	TXP	C2N-C3N	-17.69	1.35	1.52
3	C	400	TXP	C2N-N1N	-11.51	1.27	1.47
3	C	400	TXP	C3N-C7N	-4.73	1.47	1.53
4	B	600	NAD	C2A-N1A	2.60	1.38	1.33
4	A	500	NAD	C2A-N1A	2.62	1.38	1.33
4	B	600	NAD	C2A-N3A	3.71	1.38	1.32
4	A	500	NAD	C2A-N3A	3.74	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	TXP	O7N-C7N	4.88	1.32	1.23
3	C	400	TXP	C4N-C5N	7.31	1.52	1.32
4	A	500	NAD	O7N-C7N	8.29	1.41	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	NAD	N3A-C2A-N1A	-11.80	119.86	128.89
4	A	500	NAD	N3A-C2A-N1A	-11.76	119.89	128.89
3	C	400	TXP	N3A-C2A-N1A	-10.05	121.20	128.89
3	C	400	TXP	C6N-C5N-C4N	-6.68	111.20	123.08
3	C	400	TXP	C3N-C4N-C5N	-3.64	109.42	121.88
4	B	600	NAD	PN-O3-PA	-2.76	124.97	132.73
3	C	400	TXP	C1'-N9A-C4A	-2.67	122.92	126.94
3	C	400	TXP	PA-O3-PN	-2.61	125.40	132.73
4	A	500	NAD	PN-O3-PA	-2.60	125.44	132.73
3	C	400	TXP	C4A-C5A-N7A	-2.40	107.27	109.48
3	C	400	TXP	O7N-C7N-N7N	-2.33	119.62	123.08
4	B	600	NAD	C1B-N9A-C4A	-2.22	123.59	126.94
3	C	400	TXP	C4'-O4'-C1'	-2.12	107.39	109.72
4	B	600	NAD	O3-PA-O5B	2.16	108.67	102.94
4	B	600	NAD	O4B-C1B-N9A	2.16	112.62	108.10
4	B	600	NAD	C1D-C2D-C3D	2.21	105.84	101.40
4	A	500	NAD	O4B-C1B-N9A	2.22	112.74	108.10
3	C	400	TXP	OP3-P2-OP2	2.34	116.28	107.38
4	A	500	NAD	C3N-C7N-N7N	2.68	120.75	117.82
3	C	400	TXP	C2N-N1N-C1'A	2.94	122.32	115.34
3	C	400	TXP	C3N-C7N-N7N	3.45	120.62	117.06
4	A	500	NAD	O4D-C1D-N1N	3.79	112.30	108.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	400	TXP	C3N

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	378/384 (98%)	1.14	64 (16%) 2 4	29, 63, 96, 108	0
1	B	364/384 (94%)	0.54	24 (6%) 22 29	26, 45, 74, 121	0
2	C	173/174 (99%)	1.22	31 (17%) 2 3	35, 66, 91, 99	0
All	All	915/942 (97%)	0.92	119 (13%) 5 7	26, 54, 93, 121	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	GLU	8.2
1	A	112	LEU	7.8
1	B	243	PHE	7.8
1	B	242	GLU	7.4
1	A	350	ASP	7.0
1	A	349	LYS	6.7
2	C	33	ALA	6.4
1	A	232	ALA	6.4
1	B	245	LYS	6.1
1	A	102	ALA	6.1
2	C	41	PHE	6.0
1	B	248	ALA	5.7
1	A	371	ASP	5.7
1	A	233	GLY	5.6
1	B	240	GLY	5.5
1	B	244	ARG	5.4
1	A	368	VAL	5.3
1	A	227	LYS	5.2
2	C	172	ALA	5.2
1	A	111	ALA	5.2
1	B	247	GLN	5.0
1	A	375	VAL	5.0
1	A	376	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	235	TYR	4.9
1	B	351	THR	4.7
1	A	124	LEU	4.6
2	C	31	VAL	4.5
2	C	159	THR	4.4
1	B	221	VAL	4.4
1	A	223	ASP	4.3
1	A	126	PRO	4.3
2	C	162	PHE	4.2
1	A	108	VAL	4.1
1	A	363	VAL	4.1
2	C	49	VAL	4.1
1	A	128	ILE	4.0
1	A	229	ALA	4.0
2	C	143	SER	4.0
1	A	120	TYR	3.9
1	A	100	LEU	3.7
1	A	347	VAL	3.7
2	C	202	MET	3.7
2	C	188	PHE	3.6
1	A	378	ALA	3.5
2	C	179	PHE	3.4
1	B	246	LYS	3.4
2	C	180	PHE	3.4
1	A	370	ARG	3.4
1	A	226	MET	3.4
2	C	167	MET	3.3
1	A	224	GLU	3.3
1	A	119	ALA	3.3
1	A	374	ILE	3.2
1	A	359	GLU	3.2
1	A	117	ILE	3.2
2	C	145	PRO	3.2
1	A	107	PRO	3.1
1	A	354	LEU	3.1
1	A	207	THR	3.1
1	A	348	ASP	3.1
1	B	220	THR	3.0
2	C	140	THR	3.0
2	C	185	MET	3.0
1	B	222	ASP	2.9
1	B	303	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	175	GLU	2.9
2	C	177	GLU	2.8
1	A	75	GLN	2.8
1	A	231	THR	2.8
1	A	355	VAL	2.8
2	C	45	ASN	2.8
2	C	46	ALA	2.8
1	A	352	LYS	2.7
1	A	178	PHE	2.7
1	A	65	LEU	2.7
1	B	268	PRO	2.7
1	A	373	ALA	2.7
1	A	78	MET	2.7
1	A	275	LEU	2.7
1	A	357	LYS	2.7
1	A	58	ALA	2.7
1	A	34	ILE	2.6
1	B	270	LYS	2.6
1	B	349	LYS	2.6
2	C	68	GLU	2.5
1	B	267	ILE	2.5
2	C	30	SER	2.5
1	A	121	ALA	2.5
1	A	83	GLY	2.5
2	C	182	ASN	2.5
2	C	138	ALA	2.5
1	A	70	VAL	2.4
1	A	366	THR	2.4
1	A	106	ARG	2.4
1	A	116	LYS	2.4
2	C	153	ASP	2.4
2	C	186	MET	2.3
1	A	27	VAL	2.2
1	A	71	VAL	2.2
1	A	230	GLU	2.2
1	A	268	PRO	2.2
1	A	237	LYS	2.2
1	B	358	LEU	2.2
2	C	194	MET	2.2
2	C	77	GLY	2.2
1	A	97	MET	2.2
1	B	127	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	74	VAL	2.2
1	B	12	GLY	2.2
2	C	38	ASP	2.2
1	A	32	GLU	2.1
2	C	72	VAL	2.1
2	C	73	LEU	2.1
1	A	66	SER	2.1
1	B	269	GLY	2.1
1	A	295	VAL	2.1
1	A	372	GLY	2.1
1	B	310	VAL	2.1
1	B	250	ALA	2.1

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
5	GOL	B	700	6/6	0.82	0.24	6.23	48,49,49,50	0
4	NAD	B	600	36/44	0.86	0.21	0.16	76,78,81,81	0
3	TXP	C	400	48/48	0.93	0.17	-0.15	42,48,51,53	0
4	NAD	A	500	44/44	0.91	0.16	-0.47	48,53,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.