Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:32 PM GMT

PDB ID	:	4P63
Title	:	CRYSTAL STRUCTURE OF DEOXYHYPUSINE SYNTHASE FROM PYROCOCCUS HORIKOSHII
Authors	:	Gai, Z.Q.; Okada, C.; Yu, J.; Wakabayashi, H.; Tanaka, I.; Yao, M.
Deposited on	:	2014-03-21
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

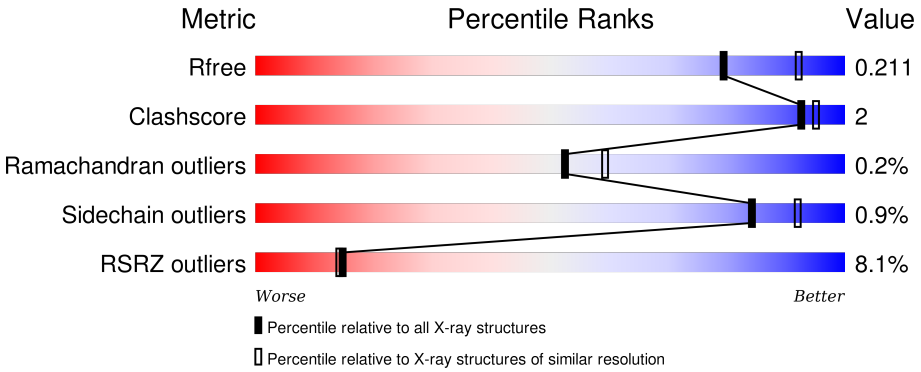
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	342	10%, 87%, 5%, 8%
1	B	342	3%, 85%, 12%
1	C	342	4%, 84%, 13%
1	D	342	12%, 85%, 5%, 9%

2 Entry composition

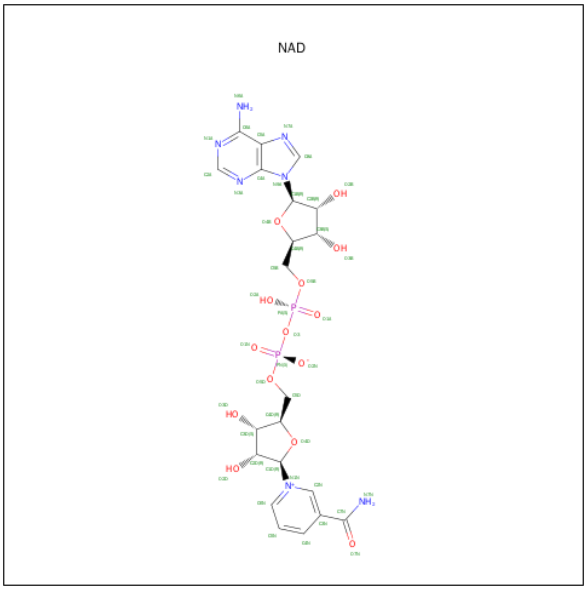
There are 3 unique types of molecules in this entry. The entry contains 20893 atoms, of which 10244 are hydrogens and 0 are deuteriums.

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 Probable deoxyhypusine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	12	0
			5280	1712	2641	435	485	7			
1	B	302	Total	C	H	N	O	S	0	0	0
			4931	1597	2473	404	450	7			
1	C	299	Total	C	H	N	O	S	0	0	0
			4886	1578	2459	401	441	7			
1	D	312	Total	C	H	N	O	S	0	13	0
			5232	1694	2619	431	481	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	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

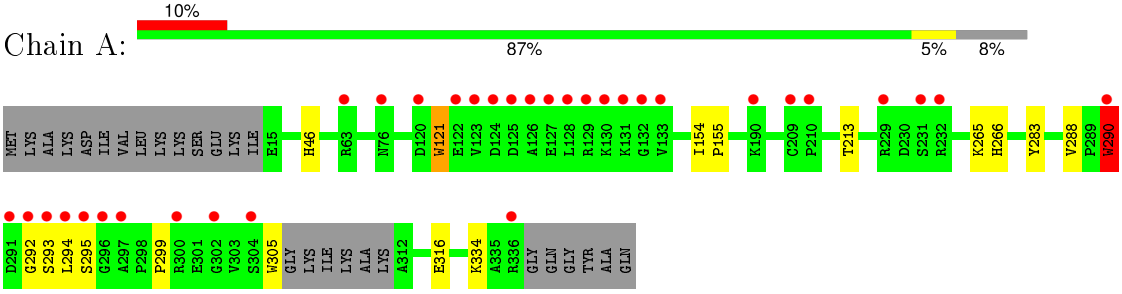
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	132	Total O 132 132	0	0
3	C	123	Total O 123 123	0	0
3	D	63	Total O 63 63	0	0

3 Residue-property plots

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.

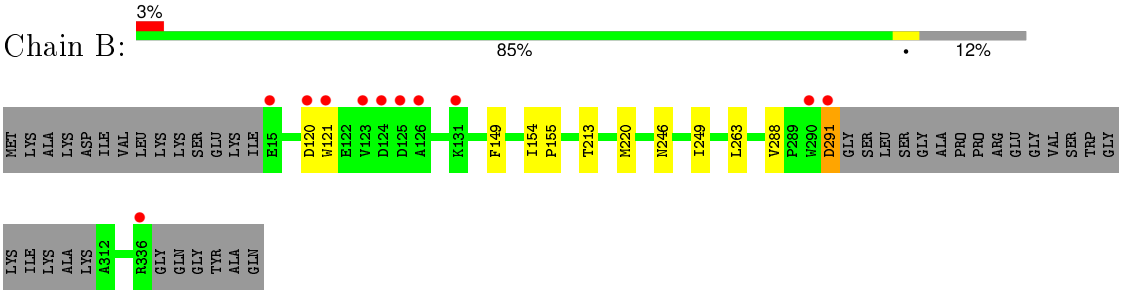
- Molecule 1: Probable deoxyhypusine synthase

Chain A:



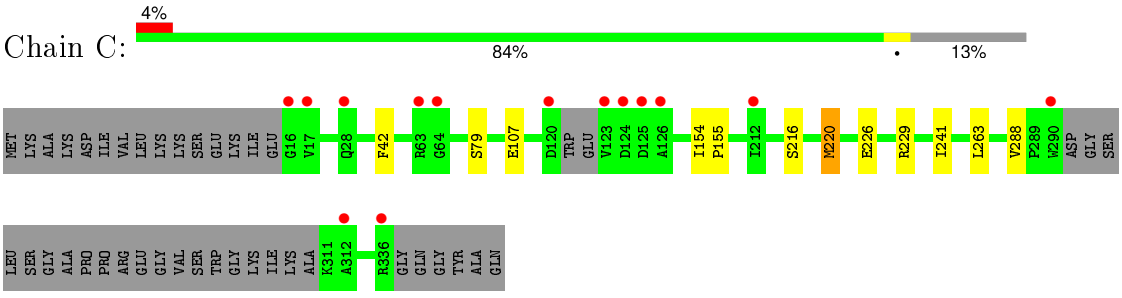
- Molecule 1: Probable deoxyhypusine synthase

Chain B:



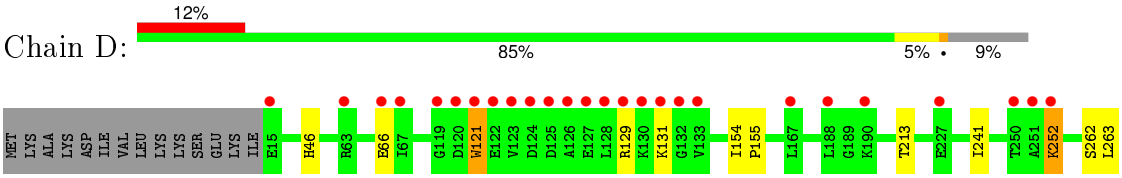
- Molecule 1: Probable deoxyhypusine synthase

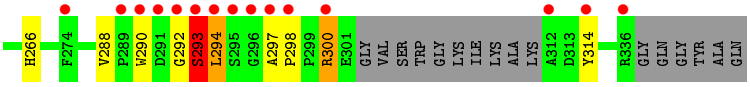
Chain C:



- Molecule 1: Probable deoxyhypusine synthase

Chain D:




H266
F274
V288
P289
W290
D291
G292
S293
L294
S295
G296
A297
P298
P299
R300
E301
GLY
VAL
SER
TRP
GLY
LYS
ILE
LYS
ALA
LYS
A312
D313
Y314
R336
GLY
GLN
GLY
TYR
ALA
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.28Å 89.91Å 164.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.44 – 2.20 35.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.44-2.20) 100.0 (35.44-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.20 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.166 , 0.203 0.175 , 0.211	Depositor DCC
R_{free} test set	3322 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 60.8	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 66523 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20893	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.24	0/2702	0.46	0/3658
1	B	0.23	0/2512	0.44	0/3394
1	C	0.23	0/2478	0.45	0/3344
1	D	0.23	0/2674	0.42	0/3619
All	All	0.23	0/10366	0.44	0/14015

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	293[B]	SER	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	2639	2641	2642	18	0
1	B	2458	2473	2475	8	0
1	C	2427	2459	2461	8	0
1	D	2613	2619	2620	14	0
2	A	44	26	25	0	0
2	D	44	26	26	0	0
3	A	106	0	0	2	0
3	B	132	0	0	0	0
3	C	123	0	0	0	0
3	D	63	0	0	1	0
All	All	10649	10244	10249	40	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 2.

All (40) 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:263:LEU:HD11	1:C:263:LEU:HD11	1.79	0.65
1:B:246:ASN:HA	1:B:249:ILE:HG22	1.86	0.56
1:C:226:GLU:O	1:C:229:ARG:NH1	2.38	0.55
1:A:288[A]:VAL:HG11	1:C:288:VAL:HG11	1.88	0.55
1:A:292[B]:GLY:HA3	1:C:42:PHE:CE1	2.41	0.55
1:D:213:THR:OG1	3:D:543:HOH:O	2.19	0.53
1:D:66:GLU:HB3	1:D:252:LYS:HE3	1.93	0.51
1:B:213:THR:HB	1:C:241:ILE:HG21	1.94	0.50
1:B:120:ASP:OD1	1:B:121:TRP:N	2.46	0.48
1:C:154:ILE:HB	1:C:155:PRO:HD3	1.95	0.48
1:A:154:ILE:HB	1:A:155:PRO:HD3	1.96	0.48
1:C:216:SER:O	1:C:220:MET:HG2	2.13	0.48
1:A:121:TRP:CE2	1:D:290[B]:TRP:HB3	2.48	0.48
1:D:292[B]:GLY:C	1:D:294[B]:LEU:N	2.66	0.48
1:A:266:HIS:HB2	1:A:294[B]:LEU:CD2	2.44	0.47
1:D:266:HIS:HB2	1:D:294[A]:LEU:CD2	2.45	0.47
1:B:154:ILE:HB	1:B:155:PRO:HD3	1.96	0.47
1:D:154:ILE:HB	1:D:155:PRO:HD3	1.96	0.46
1:A:266:HIS:HB2	1:A:294[B]:LEU:HD22	1.98	0.46
1:B:149:PHE:CE2	1:B:220:MET:HE1	2.50	0.46
1:A:290[A]:TRP:HB3	1:D:121:TRP:CE2	2.51	0.45
1:D:297[B]:ALA:N	1:D:298[B]:PRO:HD2	2.31	0.45
1:D:293[B]:SER:O	1:D:294[B]:LEU:HG	2.17	0.45
1:A:265:LYS:NZ	1:A:295[B]:SER:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASP:OD1	1:B:291:ASP:N	2.50	0.45
1:A:316:GLU:OE2	3:A:568:HOH:O	2.21	0.45
1:A:334:LYS:NZ	3:A:557:HOH:O	2.48	0.45
1:A:213:THR:HB	1:D:241:ILE:HG21	1.99	0.45
1:A:294[A]:LEU:HD13	1:A:316:GLU:O	2.17	0.44
1:D:46:HIS:HD2	1:D:294[B]:LEU:HD12	1.83	0.44
1:A:292[A]:GLY:O	1:A:294[A]:LEU:HA	2.18	0.44
1:B:288:VAL:HG11	1:D:288[B]:VAL:HG11	1.99	0.44
1:A:290[A]:TRP:C	1:A:292[A]:GLY:N	2.72	0.43
1:A:46:HIS:CE1	1:A:294[A]:LEU:HB2	2.54	0.43
1:A:283:TYR:CE2	1:A:299[B]:PRO:HA	2.55	0.42
1:A:46:HIS:HE1	1:A:294[A]:LEU:HB2	1.84	0.42
1:A:293[A]:SER:HA	1:A:294[A]:LEU:HG	2.02	0.41
1:D:262:SER:OG	1:D:263:LEU:N	2.49	0.40
1:C:79:SER:OG	1:C:107:GLU:OE1	2.26	0.40
1:D:300:ARG:NH1	1:D:314:TYR:HB2	2.36	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	324/342 (95%)	314 (97%)	8 (2%)	2 (1%)	30 29
1	B	298/342 (87%)	294 (99%)	4 (1%)	0	100 100
1	C	293/342 (86%)	290 (99%)	3 (1%)	0	100 100
1	D	321/342 (94%)	310 (97%)	7 (2%)	4 (1%)	16 12
All	All	1236/1368 (90%)	1208 (98%)	22 (2%)	6 (0%)	52 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294[A]	LEU
1	D	294[B]	LEU
1	D	293[A]	SER
1	D	293[B]	SER
1	A	290[A]	TRP
1	A	290[B]	TRP

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	280/291 (96%)	276 (99%)	4 (1%)	74 85
1	B	261/291 (90%)	260 (100%)	1 (0%)	93 97
1	C	258/291 (89%)	257 (100%)	1 (0%)	93 97
1	D	277/291 (95%)	272 (98%)	5 (2%)	66 79
All	All	1076/1164 (92%)	1065 (99%)	11 (1%)	84 91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	TRP
1	A	290[A]	TRP
1	A	290[B]	TRP
1	A	305	TRP
1	B	291	ASP
1	C	220	MET
1	D	121	TRP
1	D	129	ARG
1	D	131	LYS
1	D	252	LYS
1	D	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	46	HIS

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)

2 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	-	38,48,48	0.88	2 (5%)	47,73,73	1.99	8 (17%)
2	NAD	D	401	-	38,48,48	0.82	1 (2%)	47,73,73	2.13	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	401	-	-	0/22/62/62	0/5/5/5
2	NAD	D	401	-	-	0/22/62/62	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	O4B-C1B	2.27	1.44	1.41
2	D	401	NAD	C5A-C4A	2.96	1.47	1.40
2	A	401	NAD	C5A-C4A	3.06	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAD	N3A-C2A-N1A	-7.94	122.81	128.89
2	A	401	NAD	N3A-C2A-N1A	-7.44	123.20	128.89
2	D	401	NAD	PN-O3-PA	-5.14	118.30	132.73
2	D	401	NAD	C4D-O4D-C1D	-4.49	104.78	109.72
2	D	401	NAD	C2B-C1B-N9A	-3.70	108.63	114.29
2	A	401	NAD	PN-O3-PA	-3.67	122.42	132.73
2	A	401	NAD	C2B-C1B-N9A	-3.31	109.23	114.29
2	D	401	NAD	C4A-C5A-N7A	-3.02	106.70	109.48
2	A	401	NAD	C4A-C5A-N7A	-2.97	106.75	109.48
2	A	401	NAD	C4D-O4D-C1D	-2.52	106.94	109.72
2	D	401	NAD	O4B-C1B-N9A	2.03	112.35	108.10
2	A	401	NAD	C3N-C7N-N7N	3.32	121.45	117.82
2	A	401	NAD	O2B-C2B-C3B	3.51	123.23	111.83
2	A	401	NAD	O4D-C1D-N1N	6.17	114.91	108.13
2	D	401	NAD	O4D-C1D-N1N	7.35	116.21	108.13

There are no chirality outliers.

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, 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	316/342 (92%)	0.38	33 (10%) 8 8	17, 32, 72, 114	0
1	B	302/342 (88%)	-0.29	11 (3%) 46 45	16, 27, 54, 114	0
1	C	299/342 (87%)	-0.05	14 (4%) 35 34	18, 30, 67, 110	0
1	D	312/342 (91%)	0.61	41 (13%) 5 4	21, 43, 83, 125	0
All	All	1229/1368 (89%)	0.17	99 (8%) 15 14	16, 33, 73, 125	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	11.6
1	A	294[A]	LEU	9.4
1	A	293[A]	SER	9.1
1	D	126	ALA	8.5
1	D	294[A]	LEU	8.5
1	D	123	VAL	8.3
1	D	293[A]	SER	7.8
1	A	292[A]	GLY	7.3
1	A	126	ALA	7.1
1	A	295[A]	SER	6.8
1	D	290[A]	TRP	6.8
1	D	122	GLU	6.8
1	A	291[A]	ASP	6.8
1	A	297[A]	ALA	6.3
1	A	304	SER	6.3
1	D	336	ARG	6.2
1	D	295[A]	SER	6.2
1	D	292[A]	GLY	6.1
1	D	124	ASP	6.0
1	C	123	VAL	6.0
1	D	300	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	291	ASP	5.8
1	A	122	GLU	5.8
1	A	290[A]	TRP	5.6
1	B	121	TRP	5.6
1	D	296[A]	GLY	5.5
1	B	15	GLU	5.5
1	D	128	LEU	5.5
1	D	132	GLY	5.5
1	D	119	GLY	5.4
1	D	129	ARG	5.3
1	A	130	LYS	5.3
1	A	129	ARG	5.2
1	D	130	LYS	5.2
1	D	312	ALA	5.2
1	C	126	ALA	5.2
1	A	296[A]	GLY	5.0
1	A	125	ASP	5.0
1	D	120	ASP	5.0
1	A	127	GLU	5.0
1	A	124	ASP	4.9
1	D	131	LYS	4.8
1	D	297[A]	ALA	4.6
1	A	128	LEU	4.2
1	D	291[A]	ASP	4.0
1	B	124	ASP	3.9
1	B	290	TRP	3.9
1	A	63	ARG	3.9
1	A	120	ASP	3.8
1	C	290	TRP	3.8
1	C	63	ARG	3.8
1	C	336	ARG	3.8
1	B	120	ASP	3.7
1	C	124	ASP	3.7
1	D	15	GLU	3.6
1	B	336	ARG	3.6
1	D	298[A]	PRO	3.5
1	B	126	ALA	3.5
1	B	123	VAL	3.4
1	A	210	PRO	3.3
1	C	125	ASP	3.2
1	A	131	LYS	3.2
1	D	314	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	252	LYS	3.1
1	A	133	VAL	3.0
1	D	125	ASP	3.0
1	D	190	LYS	3.0
1	D	127	GLU	3.0
1	A	190	LYS	2.9
1	D	63	ARG	2.9
1	A	336	ARG	2.9
1	C	212	ILE	2.8
1	A	300	ARG	2.7
1	C	120	ASP	2.7
1	D	251	ALA	2.6
1	A	302	GLY	2.6
1	B	125	ASP	2.6
1	D	133	VAL	2.6
1	A	231	SER	2.5
1	D	167	LEU	2.5
1	D	289[A]	PRO	2.5
1	D	66	GLU	2.5
1	D	250	THR	2.5
1	D	188	LEU	2.5
1	D	121	TRP	2.4
1	C	17	VAL	2.4
1	A	232	ARG	2.3
1	A	209	CYS	2.3
1	A	76	ASN	2.3
1	D	274	PHE	2.3
1	A	132	GLY	2.2
1	C	16	GLY	2.2
1	D	67	ILE	2.2
1	A	229	ARG	2.2
1	C	28	GLN	2.2
1	C	64	GLY	2.1
1	B	131	LYS	2.1
1	D	227	GLU	2.1
1	C	312	ALA	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, 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	D	401	44/44	0.69	0.33	0.78	48,104,147,156	0
2	NAD	A	401	44/44	0.81	0.27	0.47	42,90,113,116	0

6.5 Other polymers (i)

There are no such residues in this entry.