



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:22 AM GMT

PDB ID : 1LI4
Title : Human S-adenosylhomocysteinehydrolase complexed with neplanocin
Authors : Yang, X.; Hu, Y.; Yin, D.H.; Turner, M.A.; Wang, M.; Borchardt, R.T.;
Howell, P.L.; Kuczera, K.; Schowen, R.L.
Deposited on : 2002-04-17
Resolution : 2.01 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

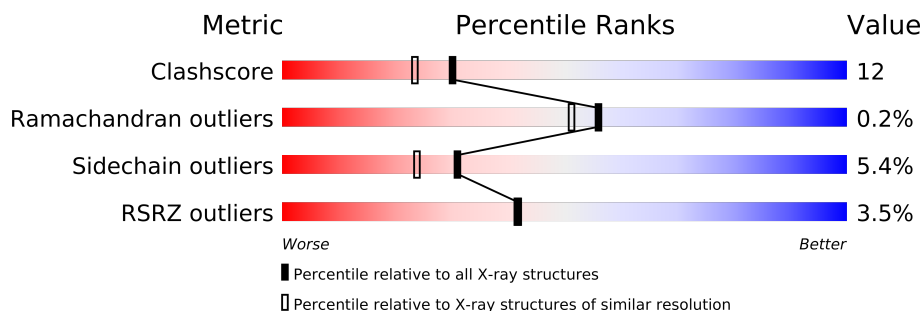
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	432	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	IPA	A	900	-	X

2 Entry composition i

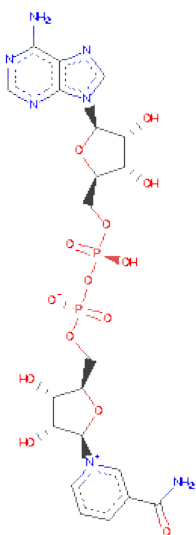
There are 5 unique types of molecules in this entry. The entry contains 3606 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-adenosylhomocysteinehydrolase.

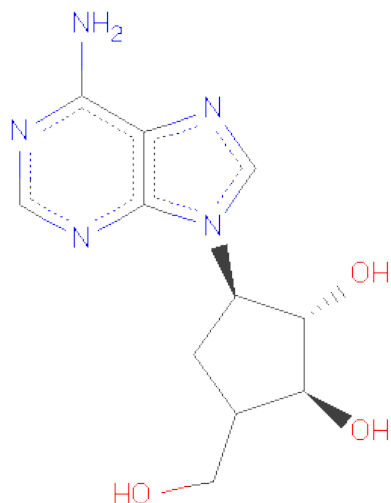
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	3322	2106	569	622	25	0	0	0

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



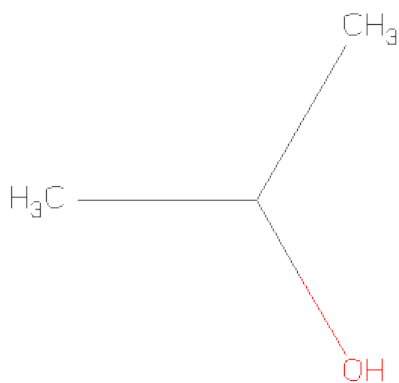
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0

- Molecule 3 is 3-(6-AMINO-PURIN-9-YL)-5-HYDROXYMETHYL-CYCLOPENTANE-1,2-DIOL (three-letter code: NOC) (formula: $C_{11}H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	19	11	5	3	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	3	1	0	0
4	A	1	4	3	1	0	0

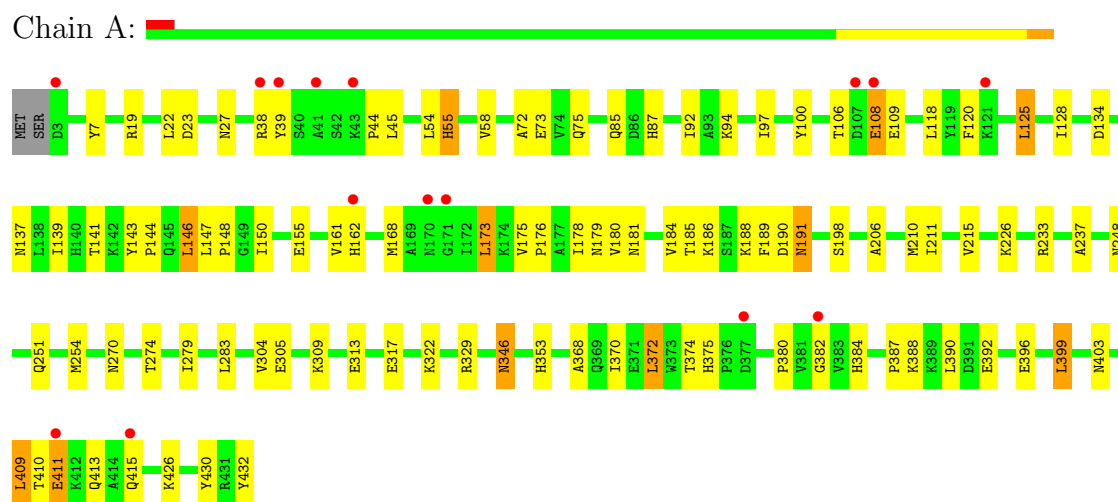
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total 213	O 213	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: S-adenosylhomocysteinehydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 135.67Å 171.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.01 29.71 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.71-2.01) 95.1 (29.71-2.01)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.236 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34435 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3606	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, NAD, NOC

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	0.78	0/3386	0.85	1/4585 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	409	LEU	CA-CB-CG	5.75	128.53	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3321	81	0
2	A	44	0	24	1	0
3	A	19	0	12	1	0
4	A	8	0	16	0	0
5	A	213	0	0	9	0
All	All	3606	0	3373	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:TYR:HB3	1:A:146:LEU:HD13	1.51	0.92
1:A:128:ILE:HD11	1:A:139:ILE:HD12	1.54	0.86
1:A:215:VAL:H	1:A:270:ASN:HD22	1.21	0.85
1:A:188:LYS:HE2	5:A:1100:HOH:O	1.77	0.85
1:A:410:THR:H	1:A:413:GLN:HE21	1.28	0.81
1:A:426:LYS:HG2	1:A:430:TYR:CD2	2.17	0.80
1:A:143:TYR:O	1:A:146:LEU:HD13	1.84	0.77
1:A:146:LEU:N	1:A:146:LEU:HD12	2.02	0.73
1:A:191:ASN:HD22	1:A:191:ASN:H	1.36	0.72
1:A:125:LEU:HD13	1:A:125:LEU:H	1.55	0.72
1:A:191:ASN:HD22	1:A:191:ASN:N	1.89	0.71
1:A:23:ASP:HB3	5:A:1111:HOH:O	1.90	0.70
1:A:125:LEU:HD22	1:A:125:LEU:O	1.91	0.70
1:A:143:TYR:HB3	1:A:146:LEU:CD1	2.20	0.70
1:A:188:LYS:CE	5:A:1100:HOH:O	2.35	0.69
1:A:106:THR:OG1	1:A:109:GLU:HG3	1.93	0.68
1:A:374:THR:HG22	1:A:375:HIS:CE1	2.30	0.66
1:A:118:LEU:HA	1:A:125:LEU:HD12	1.78	0.65
1:A:184:VAL:HG21	1:A:432:TYR:CE1	2.37	0.60
1:A:370:ILE:O	1:A:374:THR:HB	2.03	0.59
1:A:346:ASN:HD22	1:A:346:ASN:H	1.51	0.58
1:A:75:GLN:HG3	1:A:120:PHE:CE2	2.39	0.57
1:A:411:GLU:O	1:A:415:GLN:HG3	2.05	0.57
1:A:186:LYS:HZ2	1:A:191:ASN:HD21	1.51	0.57
1:A:346:ASN:HD21	2:A:433:NAD:H72N	1.51	0.57
1:A:346:ASN:HD22	1:A:346:ASN:N	2.03	0.56
1:A:39:TYR:CD2	1:A:44:PRO:HG3	2.41	0.56
1:A:146:LEU:N	1:A:146:LEU:CD1	2.69	0.55
1:A:426:LYS:HG2	1:A:430:TYR:CG	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:380:PRO:O	1:A:384:HIS:HE1	1.90	0.53
1:A:387:PRO:HD2	1:A:390:LEU:HD12	1.90	0.52
1:A:73:GLU:HG3	5:A:1061:HOH:O	2.10	0.52
1:A:19:ARG:NH1	1:A:22:LEU:HD12	2.24	0.51
1:A:396:GLU:HA	1:A:399:LEU:HD22	1.93	0.51
1:A:108:GLU:CD	1:A:108:GLU:H	2.11	0.51
1:A:143:TYR:CB	1:A:146:LEU:HD13	2.33	0.50
1:A:161:VAL:HG21	1:A:179:ASN:OD1	2.12	0.50
1:A:125:LEU:HD23	1:A:150:ILE:HG12	1.94	0.49
1:A:125:LEU:HD21	1:A:150:ILE:HD11	1.93	0.49
1:A:181:ASN:HA	1:A:186:LYS:HD2	1.93	0.49
1:A:178:ILE:HD12	1:A:372:LEU:HD22	1.94	0.48
1:A:175:VAL:HG13	1:A:176:PRO:HD2	1.95	0.48
1:A:168:MET:SD	1:A:382:GLY:HA2	2.53	0.48
1:A:415:GLN:NE2	5:A:1112:HOH:O	2.46	0.48
1:A:274:THR:HB	1:A:305:GLU:OE1	2.13	0.48
1:A:410:THR:H	1:A:413:GLN:NE2	2.03	0.48
1:A:191:ASN:ND2	1:A:191:ASN:N	2.60	0.47
1:A:108:GLU:N	1:A:108:GLU:CD	2.68	0.47
1:A:309:LYS:O	1:A:313:GLU:HG3	2.14	0.47
1:A:317:GLU:HB2	1:A:329:ARG:HB3	1.96	0.46
1:A:388:LYS:O	1:A:392:GLU:HG3	2.16	0.46
1:A:125:LEU:CD1	1:A:125:LEU:H	2.26	0.46
1:A:54:LEU:O	1:A:55:HIS:C	2.53	0.46
1:A:206:ALA:O	1:A:322:LYS:HE3	2.15	0.46
1:A:233:ARG:HG3	5:A:1048:HOH:O	2.14	0.46
1:A:58:VAL:H	1:A:85:GLN:NE2	2.14	0.46
1:A:368:ALA:O	1:A:372:LEU:HD22	2.16	0.46
1:A:380:PRO:O	1:A:384:HIS:CE1	2.69	0.45
1:A:137:ASN:O	1:A:141:THR:HG23	2.16	0.45
1:A:155:GLU:O	1:A:180:VAL:HB	2.16	0.45
1:A:92:ILE:HG23	1:A:97:ILE:HB	1.99	0.45
1:A:374:THR:CG2	1:A:375:HIS:CE1	3.00	0.44
1:A:55:HIS:CD2	3:A:434:NOC:H5'2	2.53	0.44
1:A:186:LYS:NZ	1:A:191:ASN:HD21	2.15	0.44
1:A:248:ASN:HA	1:A:251:GLN:HE21	1.82	0.44
1:A:191:ASN:ND2	1:A:191:ASN:H	2.11	0.43
1:A:226:LYS:NZ	1:A:251:GLN:HE22	2.16	0.43
1:A:134:ASP:HB2	5:A:1018:HOH:O	2.18	0.43
1:A:45:LEU:HB3	1:A:72:ALA:HB2	2.00	0.43
1:A:198:SER:OG	1:A:353:HIS:HD2	2.01	0.43
1:A:173:LEU:HD22	1:A:175:VAL:H	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:HIS:CE1	5:A:998:HOH:O	2.72	0.42
1:A:188:LYS:HD3	5:A:1100:HOH:O	2.20	0.42
1:A:106:THR:HG1	1:A:109:GLU:HG3	1.85	0.42
1:A:248:ASN:H	1:A:248:ASN:HD22	1.68	0.42
1:A:279:ILE:HG22	1:A:304:VAL:HB	2.02	0.41
1:A:143:TYR:N	1:A:144:PRO:CD	2.82	0.41
1:A:185:THR:HA	1:A:189:PHE:CD1	2.56	0.41
1:A:211:ILE:HG22	1:A:237:ALA:HB2	2.04	0.40
1:A:147:LEU:HB2	1:A:148:PRO:HD3	2.04	0.40
1:A:7:TYR:C	1:A:7:TYR:CD1	2.94	0.40

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	428/432 (99%)	414 (97%)	13 (3%)	1 (0%)	56 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	HIS

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	352/356 (99%)	333 (95%)	19 (5%)	31 24

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	38	ARG
1	A	87	HIS
1	A	94	LYS
1	A	108	GLU
1	A	125	LEU
1	A	146	LEU
1	A	173	LEU
1	A	190	ASP
1	A	191	ASN
1	A	210	MET
1	A	254	MET
1	A	283	LEU
1	A	346	ASN
1	A	372	LEU
1	A	399	LEU
1	A	403	ASN
1	A	409	LEU
1	A	411	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	85	GLN
1	A	162	HIS
1	A	181	ASN
1	A	191	ASN
1	A	248	ASN
1	A	251	GLN
1	A	270	ASN
1	A	346	ASN
1	A	353	HIS
1	A	365	GLN
1	A	384	HIS
1	A	413	GLN
1	A	415	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	433	-	48,48,48	5.20	29 (60%)	73,73,73	3.19	36 (49%)
3	NOC	A	434	-	21,21,21	3.00	8 (38%)	31,31,31	2.51	8 (25%)
4	IPA	A	900	-	3,3,3	0.95	0	3,3,3	0.51	0
4	IPA	A	901	-	3,3,3	0.84	0	3,3,3	0.32	0

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	433	-	-	0/30/62/62	0/3/5/5
3	NOC	A	434	-	1/1/4/4	0/5/22/22	0/1/3/3
4	IPA	A	900	-	-	0/0/0/0	0/0/0/0
4	IPA	A	901	-	-	0/0/0/0	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	433	NAD	C8A-N9A	14.40	1.58	1.36
2	A	433	NAD	C4N-C3N	13.73	1.63	1.39
2	A	433	NAD	C2B-C1B	-10.31	1.38	1.53
2	A	433	NAD	C4A-N9A	-10.04	1.23	1.37
2	A	433	NAD	PN-O5D	-9.22	1.30	1.60
3	A	434	NOC	O3'-C3'	-8.98	1.21	1.43
2	A	433	NAD	C2N-N1N	7.82	1.45	1.35
2	A	433	NAD	O4B-C4B	-7.53	1.27	1.45
2	A	433	NAD	PA-O3	7.25	1.73	1.59
2	A	433	NAD	C2A-N1A	7.20	1.48	1.33
2	A	433	NAD	O4D-C1D	6.23	1.50	1.41
3	A	434	NOC	C5'-C4'	-5.81	1.38	1.53
2	A	433	NAD	O5B-C5B	-5.76	1.20	1.44
2	A	433	NAD	C5A-C4A	5.75	1.53	1.40
2	A	433	NAD	O4B-C1B	5.48	1.49	1.41
2	A	433	NAD	C3B-C4B	-4.76	1.39	1.53
2	A	433	NAD	O3B-C3B	4.62	1.54	1.43
2	A	433	NAD	C2N-C3N	4.60	1.45	1.38
2	A	433	NAD	C6N-C5N	4.48	1.49	1.38
3	A	434	NOC	C6'-C4'	-4.37	1.42	1.52
2	A	433	NAD	C6N-N1N	4.29	1.47	1.35
2	A	433	NAD	C3D-C4D	4.22	1.64	1.53
2	A	433	NAD	C3N-C7N	4.12	1.57	1.50
3	A	434	NOC	C2'-C1'	4.04	1.58	1.53
2	A	433	NAD	O4D-C4D	3.59	1.53	1.45
2	A	433	NAD	PN-O2N	3.23	1.56	1.48
2	A	433	NAD	C6A-N1A	3.22	1.51	1.37
2	A	433	NAD	C1B-N9A	-3.17	1.38	1.48
2	A	433	NAD	O2B-C2B	-3.13	1.35	1.43
2	A	433	NAD	C5A-N7A	-3.00	1.29	1.40
2	A	433	NAD	PA-O2A	-2.88	1.42	1.55
3	A	434	NOC	C8-N7	-2.74	1.29	1.34
3	A	434	NOC	C4-N9	-2.34	1.34	1.37
3	A	434	NOC	C4-N3	2.23	1.39	1.35
3	A	434	NOC	C8-N9	2.17	1.39	1.36
2	A	433	NAD	C5B-C4B	-2.14	1.44	1.51
2	A	433	NAD	C6A-N6A	-2.11	1.28	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	433	NAD	O7N-C7N-C3N	-9.34	109.05	119.58
2	A	433	NAD	N3A-C2A-N1A	-8.19	121.86	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	433	NAD	C6N-N1N-C2N	7.58	130.60	122.04
2	A	433	NAD	PA-O5B-C5B	6.47	168.59	122.03
3	A	434	NOC	O3'-C3'-C4'	6.47	128.77	112.70
3	A	434	NOC	C5'-C4'-C6'	5.93	123.69	113.90
2	A	433	NAD	O5B-C5B-C4B	5.92	130.67	108.94
2	A	433	NAD	C3N-C2N-N1N	-5.90	110.42	120.36
2	A	433	NAD	C4A-C5A-N7A	5.57	114.29	109.52
3	A	434	NOC	C6'-C4'-C3'	5.27	124.02	113.89
2	A	433	NAD	C2N-C3N-C4N	5.25	124.26	118.31
2	A	433	NAD	C2D-C1D-N1N	5.15	122.57	113.86
2	A	433	NAD	O5D-C5D-C4D	4.73	126.29	108.94
2	A	433	NAD	C3N-C7N-N7N	4.59	122.99	117.77
3	A	434	NOC	C2'-C1'-N9	4.55	121.27	112.93
2	A	433	NAD	PN-O3-PA	-4.32	114.38	132.95
2	A	433	NAD	C4B-O4B-C1B	-4.30	105.08	109.75
2	A	433	NAD	C2N-C3N-C7N	-4.26	106.66	119.35
3	A	434	NOC	C5'-C4'-C3'	4.06	112.04	102.24
2	A	433	NAD	C2B-C3B-C4B	3.82	110.27	102.65
2	A	433	NAD	O4D-C1D-N1N	-3.79	104.08	107.95
2	A	433	NAD	O2A-PA-O5B	3.75	127.44	108.51
2	A	433	NAD	PN-O5D-C5D	3.58	132.61	120.24
2	A	433	NAD	O2N-PN-O3	3.51	118.26	108.79
2	A	433	NAD	O4D-C1D-C2D	-3.43	101.52	106.77
2	A	433	NAD	C5N-C4N-C3N	-3.42	115.89	120.32
2	A	433	NAD	O7N-C7N-N7N	3.35	127.43	122.59
3	A	434	NOC	O3'-C3'-C2'	3.08	121.84	111.83
3	A	434	NOC	C5'-C1'-C2'	-3.07	99.97	104.17
2	A	433	NAD	C2N-N1N-C1D	-2.99	111.93	119.33
2	A	433	NAD	C5N-C6N-N1N	-2.97	115.43	120.43
2	A	433	NAD	C5A-C6A-N6A	2.96	127.41	120.72
2	A	433	NAD	C3D-C2D-C1D	2.88	105.42	100.91
2	A	433	NAD	O2A-PA-O3	2.82	118.50	105.14
2	A	433	NAD	C4N-C3N-C7N	2.82	128.59	121.10
2	A	433	NAD	N3A-C4A-N9A	2.78	130.45	125.43
2	A	433	NAD	O5B-PA-O1A	-2.67	98.92	109.37
2	A	433	NAD	O2B-C2B-C1B	2.67	119.30	111.23
2	A	433	NAD	C2A-N3A-C4A	2.36	120.74	114.01
3	A	434	NOC	C5'-C1'-N9	2.30	117.13	113.51
2	A	433	NAD	C1B-N9A-C4A	2.20	130.43	126.64
2	A	433	NAD	C8A-N9A-C4A	-2.13	105.27	106.90
2	A	433	NAD	C5D-C4D-C3D	-2.09	106.85	115.21
2	A	433	NAD	C3B-C2B-C1B	-2.05	97.70	100.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	434	NOC	C4'

There are no torsion outliers.

There are no ring outliers.

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	430/432 (99%)	0.19	15 (3%) 42 41	14, 27, 44, 51	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	TYR	4.4
1	A	41	ALA	4.1
1	A	377	ASP	4.0
1	A	121	LYS	3.8
1	A	3	ASP	3.8
1	A	171	GLY	3.6
1	A	415	GLN	2.8
1	A	162	HIS	2.8
1	A	411	GLU	2.8
1	A	108	GLU	2.7
1	A	38	ARG	2.7
1	A	382	GLY	2.4
1	A	170	ASN	2.2
1	A	43	LYS	2.2
1	A	107	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	IPA	A	900	4/4	0.24	4.88	27,27,28,28	0
4	IPA	A	901	4/4	0.16	1.27	33,34,34,34	0
3	NOC	A	434	19/19	0.14	0.18	18,19,19,19	0
2	NAD	A	433	44/44	0.11	-0.29	16,19,20,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.