Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:37 PM GMT

PDB ID	:	4PGF
Title	:	The structure of mono-acetylated SAHH
Authors	:	Kavran, J.M.; Wang, Y.; Cole, P.A.; Leahy, D.J.
Deposited on	:	2014-05-01
Resolution	:	2.59 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 (i) symbol.

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

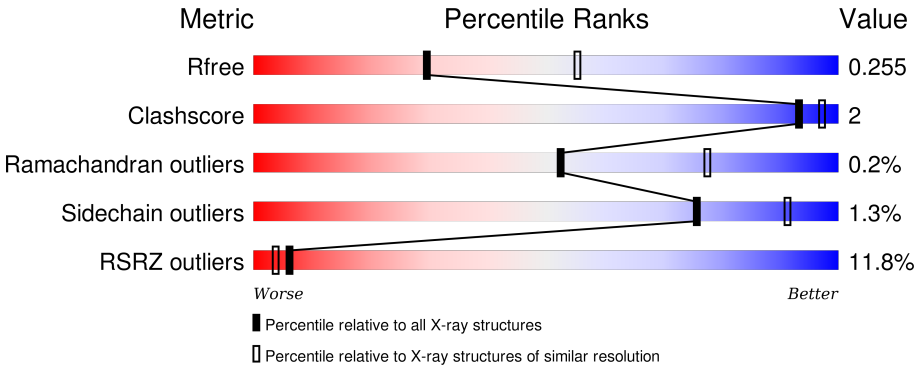
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	432	5% 95% 5%
1	B	432	19% 92% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13514 atoms, of which 6715 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.

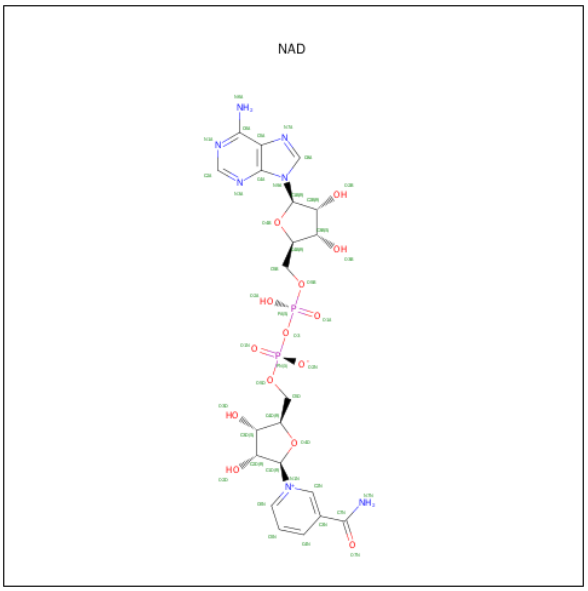
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	H	N	O	S	0	1	0
			6671	2116	3335	572	622	26			
1	B	428	Total	C	H	N	O	S	0	0	0
			6615	2102	3302	569	616	26			

There are 4 discrepancies between the modelled and reference sequences:

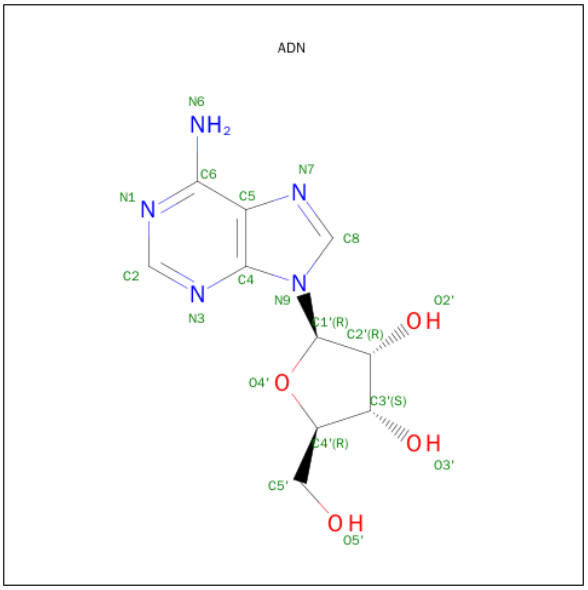
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ASN	ASP	variant	UNP P23526
A	396	CYS	GLU	engineered mutation	UNP P23526
B	86	ASN	ASP	variant	UNP P23526
B	396	CYS	GLU	engineered mutation	UNP P23526

- 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	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			32	10	13	5	4		
3	B	1	Total	C	H	N	O	0	0
			32	10	13	5	4		

- Molecule 4 is water.

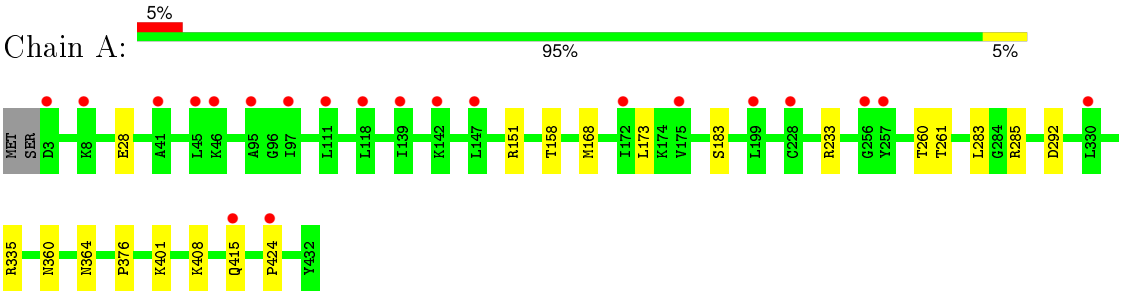
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	11	Total	O	0	0
			11	11		

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 (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.

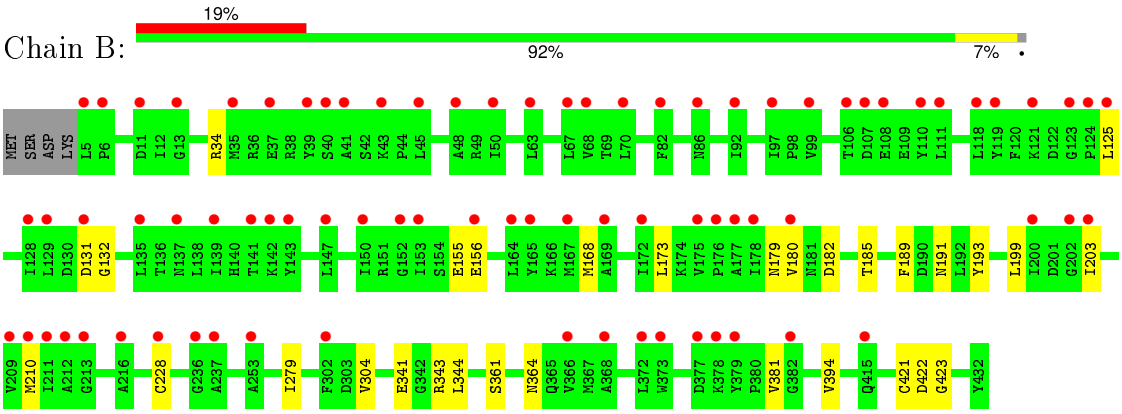
- Molecule 1: Adenosylhomocysteinase

Chain A:



- Molecule 1: Adenosylhomocysteinase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	97.60Å 102.74Å 175.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 2.59 44.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.00-2.59) 99.7 (44.00-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.248 0.213 , 0.255	Depositor DCC
R_{free} test set	1377 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 38.7	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 27636 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13514	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: ADN, NAD, ALY

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	0.30	0/3390	0.46	0/4587
1	B	0.28	0/3364	0.45	1/4553 (0.0%)
All	All	0.29	0/6754	0.46	1/9140 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	422	ASP	C-N-CA	8.94	141.07	122.30

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	3336	3335	3350	9	0
1	B	3313	3302	3327	17	0
2	A	44	26	26	0	0
2	B	44	26	26	0	0
3	A	19	13	13	0	0
3	B	19	13	13	0	0
4	A	13	0	0	1	0
4	B	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6799	6715	6755	26	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 (26) 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:132:GLY:N	1:B:155:GLU:OE2	2.29	0.57
1:A:292:ASP:OD2	1:A:335:ARG:NH2	2.41	0.53
1:B:131:ASP:HA	1:B:155:GLU:OE2	2.11	0.50
1:B:168:MET:HE1	1:B:381:VAL:HG12	1.95	0.49
1:B:179:ASN:ND2	1:B:182:ASP:OD2	2.46	0.49
1:A:283:LEU:HD12	1:A:285:ARG:NH1	2.29	0.48
1:A:168:MET:HE2	1:A:173:LEU:HB3	1.96	0.46
1:B:180:VAL:HG13	1:B:364:ASN:HB3	1.96	0.46
1:A:151:ARG:HD3	1:A:376:PRO:HG3	1.98	0.45
1:B:168:MET:HE3	1:B:173:LEU:HD23	1.98	0.45
1:B:279:ILE:HG22	1:B:304:VAL:HB	1.99	0.45
1:A:260:THR:OG1	1:A:261:THR:N	2.48	0.44
1:B:185:THR:HG21	1:B:394:VAL:HG11	2.00	0.43
1:A:28:GLU:OE2	1:A:401:LYS:HE2	2.18	0.43
1:B:131:ASP:HB3	1:B:156:GLU:HB3	2.00	0.43
1:B:156:GLU:OE2	1:B:361:SER:HB3	2.19	0.43
1:A:360:ASN:O	1:A:364:ASN:ND2	2.49	0.43
1:B:199:LEU:HD22	1:B:228:CYS:SG	2.60	0.42
1:A:408:ALY:HE3	1:A:408:ALY:HH31	1.86	0.42
1:B:341:GLU:HB2	1:B:343:ARG:NH1	2.34	0.42
1:A:415:GLN:NE2	4:A:612:HOH:O	2.44	0.41
1:B:199:LEU:HD11	1:B:203:ILE:HD11	2.02	0.41
1:B:185:THR:HG21	1:B:394:VAL:CG1	2.50	0.41
1:B:131:ASP:CB	1:B:156:GLU:HB3	2.51	0.41
1:B:168:MET:HE2	1:B:173:LEU:HB3	2.02	0.40
1:B:189:PHE:HA	1:B:193:TYR:CD2	2.57	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	428/432 (99%)	405 (95%)	22 (5%)	1 (0%)	52 77
1	B	425/432 (98%)	402 (95%)	22 (5%)	1 (0%)	52 77
All	All	853/864 (99%)	807 (95%)	44 (5%)	2 (0%)	52 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	PRO
1	B	423	GLY

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	354/355 (100%)	351 (99%)	3 (1%)	86 95
1	B	351/355 (99%)	345 (98%)	6 (2%)	68 88
All	All	705/710 (99%)	696 (99%)	9 (1%)	76 91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	THR
1	A	183	SER
1	A	233	ARG
1	B	34	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	LEU
1	B	191	ASN
1	B	210	MET
1	B	344	LEU
1	B	421	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	ALY	A	408	1	10,11,12	0.90	1 (10%)	10,12,14	1.44	2 (20%)
1	ALY	B	408	1	10,11,12	1.02	1 (10%)	10,12,14	1.62	3 (30%)

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
1	ALY	A	408	1	-	2/8/10/12	0/0/0/0
1	ALY	B	408	1	-	2/8/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	ALY	CH-NZ	2.13	1.39	1.33
1	B	408	ALY	CH-NZ	2.47	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	ALY	CB-CA-N	2.20	116.78	110.52
1	B	408	ALY	CH3-CH-NZ	2.43	119.88	116.19
1	B	408	ALY	CB-CA-N	2.63	118.00	110.52
1	A	408	ALY	CE-NZ-CH	3.06	127.36	122.36
1	B	408	ALY	CE-NZ-CH	3.09	127.41	122.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	408	ALY	CH3-CH-NZ-CE
1	B	408	ALY	CH3-CH-NZ-CE
1	B	408	ALY	OH-CH-NZ-CE
1	A	408	ALY	OH-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	408	ALY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	501	-	38,48,48	1.47	4 (10%)	47,73,73	1.85	10 (21%)
3	ADN	A	502	-	16,21,21	0.81	1 (6%)	16,31,31	1.09	2 (12%)
2	NAD	B	501	-	38,48,48	1.43	4 (10%)	47,73,73	1.92	10 (21%)
3	ADN	B	502	-	16,21,21	0.80	0	16,31,31	1.01	2 (12%)

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	501	-	-	0/22/62/62	0/5/5/5
3	ADN	A	502	-	-	0/2/22/22	0/3/3/3
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	ADN	B	502	-	-	0/2/22/22	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O2D-C2D	-2.19	1.37	1.43
3	A	502	ADN	C2-N3	2.02	1.35	1.32
2	A	501	NAD	C2A-N1A	2.05	1.37	1.33
2	B	501	NAD	C7N-N7N	2.44	1.37	1.33
2	A	501	NAD	C7N-N7N	2.51	1.38	1.33
2	A	501	NAD	PA-O5B	3.59	1.75	1.59
2	B	501	NAD	PA-O5B	3.69	1.75	1.59
2	A	501	NAD	PN-O5D	4.26	1.78	1.59
2	B	501	NAD	PN-O5D	4.61	1.80	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	PN-O3-PA	-6.79	113.67	132.73
2	A	501	NAD	PN-O3-PA	-5.88	116.22	132.73
2	B	501	NAD	C4B-O4B-C1B	-4.59	104.67	109.72
2	A	501	NAD	O4D-C1D-N1N	-3.89	103.86	108.13
2	A	501	NAD	C4B-O4B-C1B	-3.84	105.50	109.72
2	B	501	NAD	C1B-N9A-C4A	-3.22	122.09	126.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAD	C1B-N9A-C4A	-3.06	122.32	126.94
2	B	501	NAD	O5D-PN-O1N	-2.66	99.28	109.62
2	B	501	NAD	C5B-C4B-C3B	-2.66	104.66	115.21
2	A	501	NAD	O2N-PN-O5D	-2.52	95.74	108.46
2	A	501	NAD	O5D-PN-O1N	-2.51	99.87	109.62
2	A	501	NAD	C5B-C4B-C3B	-2.47	105.39	115.21
2	B	501	NAD	O2N-PN-O5D	-2.26	97.08	108.46
3	A	502	ADN	C1'-N9-C4	-2.24	123.57	126.94
2	B	501	NAD	O4D-C1D-N1N	-2.16	105.76	108.13
3	B	502	ADN	C1'-N9-C4	-2.11	123.75	126.94
3	A	502	ADN	C4'-O4'-C1'	-2.01	107.51	109.72
3	B	502	ADN	C4-C5-N7	2.11	111.42	109.48
2	B	501	NAD	O2A-PA-O3	2.60	116.88	105.09
2	A	501	NAD	O2A-PA-O3	2.81	117.83	105.09
2	A	501	NAD	O2N-PN-O1N	2.94	128.46	112.53
2	B	501	NAD	O2N-PN-O1N	3.08	129.23	112.53
2	A	501	NAD	O2A-PA-O1A	3.18	129.78	112.53
2	B	501	NAD	O2A-PA-O1A	3.23	130.02	112.53

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	429/432 (99%)	0.51	21 (4%) 33 26	44, 58, 72, 106	0
1	B	427/432 (98%)	1.09	80 (18%) 2 1	44, 72, 103, 226	0
All	All	856/864 (99%)	0.80	101 (11%) 6 4	44, 61, 100, 226	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	7.1
1	B	111	LEU	6.6
1	B	378	LYS	6.2
1	B	175	VAL	5.8
1	B	118	LEU	5.4
1	B	379	TYR	5.3
1	B	124	PRO	5.1
1	B	150	ILE	4.9
1	B	86	ASN	4.7
1	B	152	GLY	4.6
1	B	372	LEU	4.4
1	B	39	TYR	4.3
1	B	129	LEU	4.2
1	B	177	ALA	4.1
1	B	97	ILE	3.9
1	B	143	TYR	3.8
1	B	92	ILE	3.7
1	B	377	ASP	3.7
1	B	121	LYS	3.7
1	B	373	TRP	3.7
1	B	123	GLY	3.6
1	B	107	ASP	3.5
1	B	45	LEU	3.4
1	A	172	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	99	VAL	3.3
1	B	141	THR	3.3
1	B	135	LEU	3.3
1	B	82	PHE	3.3
1	B	165	TYR	3.2
1	A	45	LEU	3.2
1	B	67	LEU	3.2
1	B	40	SER	3.1
1	B	366	VAL	3.0
1	B	125	LEU	3.0
1	B	164	LEU	2.9
1	B	108	GLU	2.9
1	B	382	GLY	2.9
1	B	237	ALA	2.9
1	B	119	TYR	2.9
1	B	37	GLU	2.9
1	B	203	ILE	2.9
1	B	415	GLN	2.8
1	B	6	PRO	2.8
1	B	110	TYR	2.8
1	B	302	PHE	2.8
1	B	131	ASP	2.8
1	B	142	LYS	2.8
1	B	236	GLY	2.8
1	B	106	THR	2.7
1	B	137	ASN	2.7
1	B	11	ASP	2.7
1	B	35	MET	2.7
1	B	212	ALA	2.7
1	B	70	LEU	2.6
1	B	180	VAL	2.6
1	B	68	VAL	2.6
1	B	128	ILE	2.6
1	B	48	ALA	2.5
1	A	3	ASP	2.5
1	B	176	PRO	2.5
1	A	142	LYS	2.5
1	B	63	LEU	2.5
1	B	147	LEU	2.5
1	B	156	GLU	2.4
1	B	202	GLY	2.4
1	B	216	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	CYS	2.4
1	B	172	ILE	2.4
1	B	169	ALA	2.4
1	A	147	LEU	2.4
1	B	5	LEU	2.4
1	B	43	LYS	2.3
1	A	424	PRO	2.3
1	A	111	LEU	2.3
1	A	330	LEU	2.3
1	A	175	VAL	2.3
1	B	200	ILE	2.3
1	A	97	ILE	2.2
1	B	211	ILE	2.2
1	A	41	ALA	2.2
1	B	41	ALA	2.2
1	B	253	ALA	2.2
1	B	139	ILE	2.2
1	B	167	MET	2.2
1	A	257	TYR	2.2
1	A	415	GLN	2.2
1	A	139	ILE	2.2
1	A	46	LYS	2.2
1	B	228	CYS	2.1
1	A	118	LEU	2.1
1	B	210	MET	2.1
1	A	256	GLY	2.1
1	B	213	GLY	2.1
1	A	8	LYS	2.1
1	A	95	ALA	2.1
1	B	368	ALA	2.1
1	B	13	GLY	2.0
1	B	178	ILE	2.0
1	A	199	LEU	2.0
1	B	209	VAL	2.0
1	B	50	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	ALY	B	408	12/13	0.88	0.32	-	55,68,79,79	0
1	ALY	A	408	12/13	0.88	0.23	-	53,73,88,89	0

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
3	ADN	B	502	19/19	0.92	0.23	0.61	71,78,94,96	0
3	ADN	A	502	19/19	0.92	0.20	0.40	56,60,72,73	0
2	NAD	B	501	44/44	0.95	0.17	-0.41	53,66,82,87	0
2	NAD	A	501	44/44	0.97	0.16	-0.54	47,56,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.