



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:01 PM GMT

PDB ID : 1D4F
Title : CRYSTAL STRUCTURE OF RECOMBINANT RAT-LIVER D244E MUTANT S-ADENOSYLHOMOCYSTEINEHYDROLASE
Authors : Komoto, J.; Huang, Y.; Takusagawa, F.; Gomi, T.; Ogawa, H.; Takata, Y.; Fujioka, M.
Deposited on : 2000-06-22
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

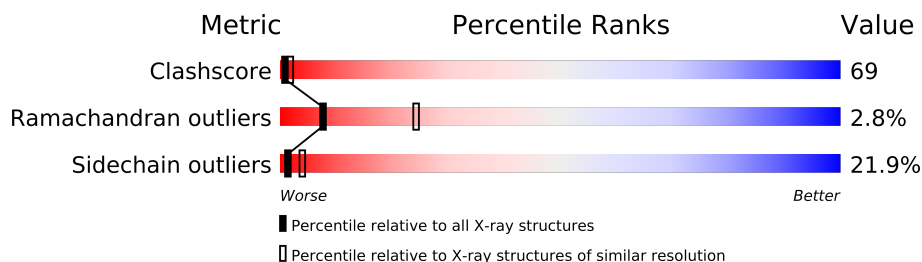
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.80 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	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14005 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
1	A	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			

There are 4 discrepancies between the modelled and reference sequences:

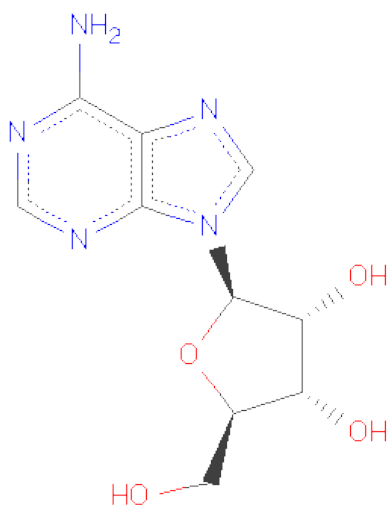
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	ENGINEERED	UNP P10760
B	244	GLU	ASP	ENGINEERED	UNP P10760
C	244	GLU	ASP	ENGINEERED	UNP P10760
D	244	GLU	ASP	ENGINEERED	UNP P10760

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	118	Total	O	0	0
			118	118		
4	C	120	Total	O	0	0
			120	120		
4	D	98	Total	O	0	0
			98	98		

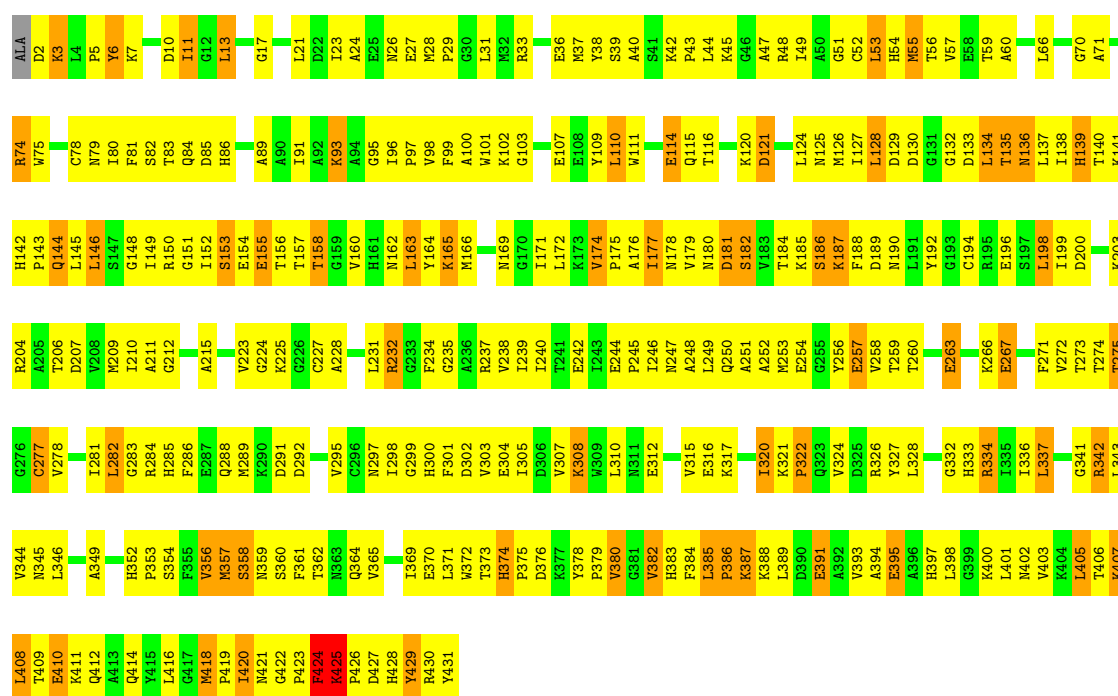
3 Residue-property plots

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.

Note EDS was not executed.

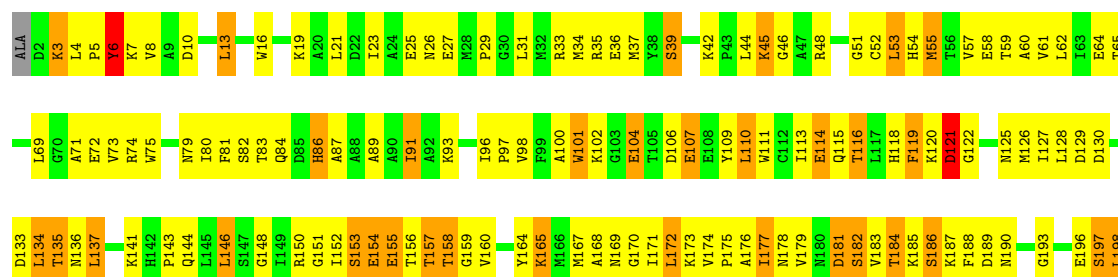
• Molecule 1: S-ADENOSYLHOMOCYSTEINEHYDROLASE

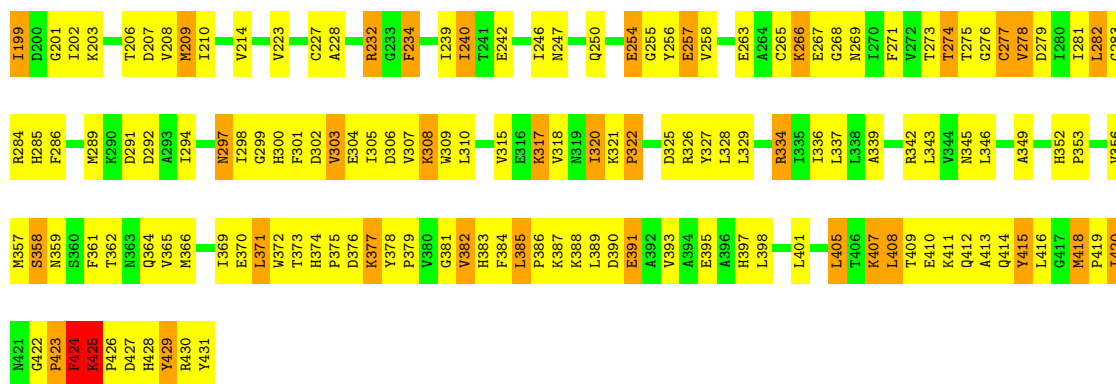
Chain A:



• Molecule 1: S-ADENOSYLHOMOCYSTEINEHYDROLASE

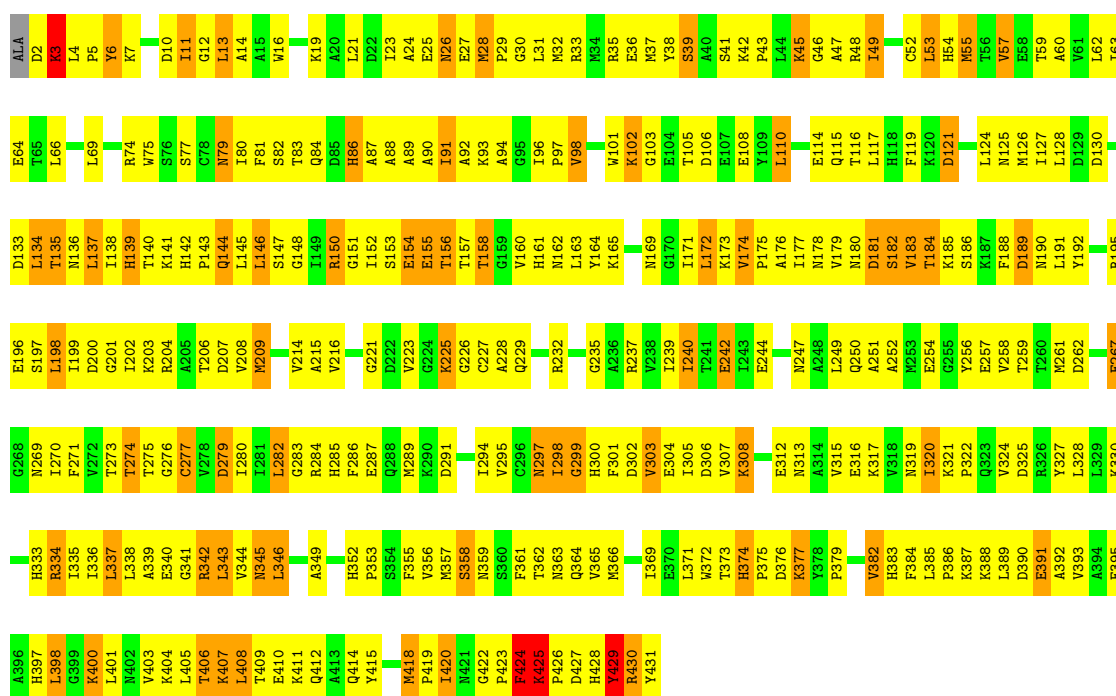
Chain B:





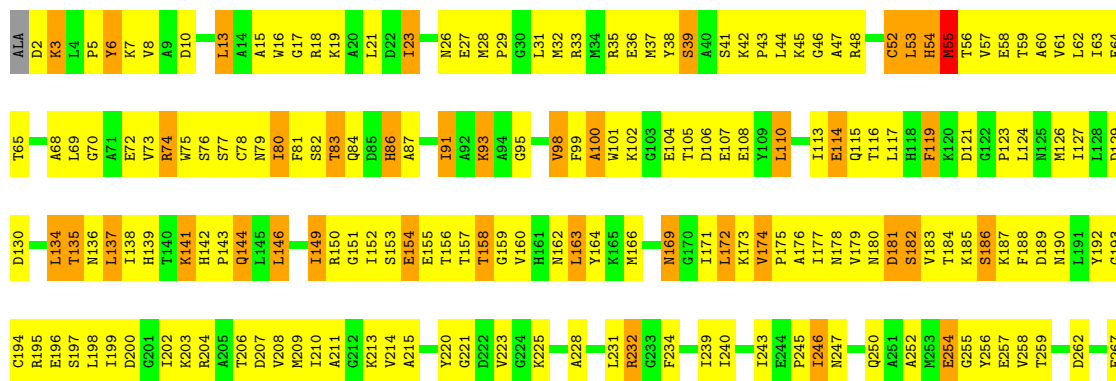
• Molecule 1: S-ADENOSYLHOMOCYSTEINEHYDROLASE

Chain C:



• Molecule 1: S-ADENOSYLHOMOCYSTEINEHYDROLASE

Chain D:



A339	A268
E340	N269
G341	
T273	T273
R342	T274
T409	T275
E410	T276
K411	C277
Q412	C277
A413	D277
Q414	D279
Y415	D279
Y416	H352
G417	P353
M418	
P419	V356
N421	M357
G422	S358
P423	
F424	F361
K425	T362
P426	N363
D427	Q364
H428	V365
Y429	M366
R430	
Y431	I369
	E370
	L371
	W372
	T373
	H374
	P375
	D376
	K377
	Y378
	P379
	V380
	G381
	V382
	H383
	F384
	L385
	P386
	K387
	K388
	L389
	D390
	E391
	A392
	V393
	A394
	E395
	A396
	H397
	L398
	L401
	M402
	V403
	K404
	L405
	K317
	V318
	N319
	T320
	K321
	P322
	Q323
	V324
	V325
	R326
	Y327
	L328
	N331
	R334
	I335
	I336
	L337
	L338

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 223.00Å 91.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (8.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.197 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14005	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

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

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	0.31	0/3385	0.59	0/4580
1	B	0.31	0/3385	0.59	0/4580
1	C	0.32	0/3385	0.59	0/4580
1	D	0.32	0/3385	0.58	0/4580
All	All	0.32	0/13540	0.59	0/18320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3343	465	0
1	B	3320	0	3343	480	0
1	C	3320	0	3343	497	0
1	D	3320	0	3343	513	0
2	A	44	0	26	22	0
2	B	44	0	26	16	0
2	C	44	0	26	7	0
2	D	44	0	26	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	19	0	13	3	0
3	B	19	0	13	2	0
3	C	19	0	13	1	0
3	D	19	0	13	1	0
4	A	137	0	0	3	0
4	B	118	0	0	8	0
4	C	120	0	0	7	0
4	D	98	0	0	3	0
All	All	14005	0	13528	1856	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 69.

The worst 5 of 1856 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:419:PRO:CG	1:A:422:GLY:HA3	1.36	1.53
1:A:419:PRO:HG2	1:A:422:GLY:C	1.23	1.52
1:A:419:PRO:HG2	1:A:422:GLY:CA	1.40	1.51
1:D:419:PRO:HG2	1:D:422:GLY:C	1.31	1.45
1:A:419:PRO:CG	1:A:422:GLY:CA	1.91	1.40

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	428/431 (99%)	367 (86%)	50 (12%)	11 (3%)	8	26
1	B	428/431 (99%)	373 (87%)	43 (10%)	12 (3%)	8	24
1	C	428/431 (99%)	374 (87%)	42 (10%)	12 (3%)	8	24
1	D	428/431 (99%)	358 (84%)	57 (13%)	13 (3%)	7	22
All	All	1712/1724 (99%)	1472 (86%)	192 (11%)	48 (3%)	8	24

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	425	LYS
1	B	425	LYS
1	C	184	THR
1	D	415	TYR

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	353/353 (100%)	282 (80%)	71 (20%)	2	5
1	B	353/353 (100%)	271 (77%)	82 (23%)	1	3
1	C	353/353 (100%)	269 (76%)	84 (24%)	1	3
1	D	353/353 (100%)	281 (80%)	72 (20%)	2	5
All	All	1412/1412 (100%)	1103 (78%)	309 (22%)	1	4

5 of 309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	ASP
1	C	110	LEU
1	D	321	LYS
1	B	407	LYS
1	C	26	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	HIS
1	C	269	ASN
1	D	374	HIS
1	C	26	ASN
1	C	178	ASN

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 ⓘ

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	501	-	48,48,48	1.54	6 (12%)	73,73,73	2.90	21 (28%)
3	ADN	A	601	-	21,21,21	1.06	2 (9%)	31,31,31	2.40	9 (29%)
2	NAD	B	502	-	48,48,48	1.44	6 (12%)	73,73,73	2.57	17 (23%)
3	ADN	B	602	-	21,21,21	1.07	2 (9%)	31,31,31	2.48	10 (32%)
2	NAD	C	503	-	48,48,48	1.30	5 (10%)	73,73,73	2.21	14 (19%)
3	ADN	C	603	-	21,21,21	1.03	2 (9%)	31,31,31	2.64	12 (38%)
2	NAD	D	504	-	48,48,48	1.28	4 (8%)	73,73,73	2.11	17 (23%)
3	ADN	D	604	-	21,21,21	1.05	2 (9%)	31,31,31	2.64	10 (32%)

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	-	-	0/30/62/62	0/3/5/5
3	ADN	A	601	-	-	0/6/22/22	0/1/3/3
2	NAD	B	502	-	-	0/30/62/62	0/3/5/5
3	ADN	B	602	-	-	0/6/22/22	0/1/3/3
2	NAD	C	503	-	-	0/30/62/62	0/3/5/5
3	ADN	C	603	-	-	0/6/22/22	0/1/3/3
2	NAD	D	504	-	-	0/30/62/62	0/3/5/5
3	ADN	D	604	-	-	0/6/22/22	0/1/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2N-N1N	5.84	1.42	1.35
2	D	504	NAD	C2N-N1N	5.59	1.42	1.35
2	C	503	NAD	C2N-N1N	5.34	1.42	1.35
2	A	501	NAD	O4B-C1B	5.29	1.49	1.41
2	B	502	NAD	C2N-N1N	5.22	1.42	1.35

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	O4B-C1B-N9A	13.30	120.81	108.44
2	B	502	NAD	O4B-C1B-N9A	12.45	120.02	108.44
2	A	501	NAD	C4D-O4D-C1D	10.06	120.67	109.75
2	B	502	NAD	O4D-C1D-N1N	8.66	116.81	107.95
2	C	503	NAD	O4B-C1B-N9A	7.20	115.14	108.44

There are no chirality outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.