wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 08:33 AM EDT

PDB ID	:	1A7A
Title	:	STRUCTURE OF HUMAN PLACENTAL S-ADENOSYLHOMOCYSTEINE HYDROLASE: DETERMINATION OF A 30 SELENIUM ATOM SUBSTRUCTURE FROM DATA AT A SINGLE WAVELENGTH
Authors	:	Turner, M.A.; Yuan, C.-S.; Borchardt, R.T.; Hershfield, M.S.; Smith, G.D.; Howell, P.L.
Deposited on	:	1998-03-10
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

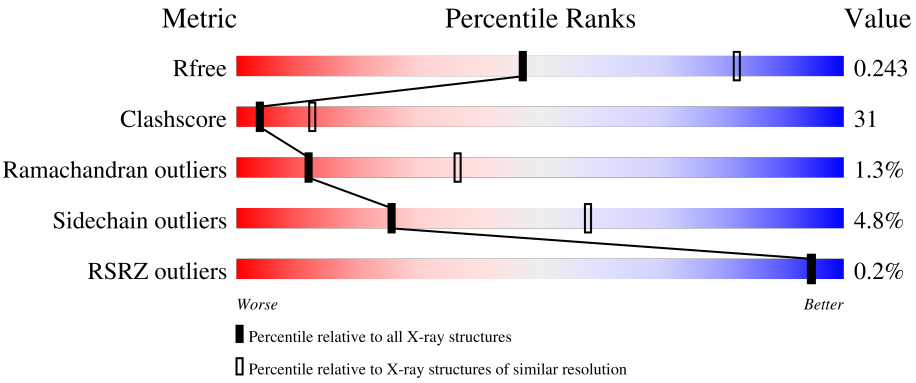
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	53% 43% .
1	B	432	52% 43% .

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	ADC	B	436	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6834 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 S-ADENOSYLHOMOCYSTEINE HYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	Se	0	0	0
			3336	2115	573	623	10	15			
1	B	430	Total	C	N	O	S	Se	0	0	0
			3330	2112	572	621	10	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	engineered mutation	UNP P23526
A	33	MSE	MET	engineered mutation	UNP P23526
A	35	MSE	MET	engineered mutation	UNP P23526
A	56	MSE	MET	engineered mutation	UNP P23526
A	127	MSE	MET	engineered mutation	UNP P23526
A	167	MSE	MET	engineered mutation	UNP P23526
A	168	MSE	MET	engineered mutation	UNP P23526
A	210	MSE	MET	engineered mutation	UNP P23526
A	254	MSE	MET	engineered mutation	UNP P23526
A	262	MSE	MET	engineered mutation	UNP P23526
A	290	MSE	MET	engineered mutation	UNP P23526
A	351	MSE	MET	engineered mutation	UNP P23526
A	358	MSE	MET	engineered mutation	UNP P23526
A	367	MSE	MET	engineered mutation	UNP P23526
A	419	MSE	MET	engineered mutation	UNP P23526
B	29	MSE	MET	engineered mutation	UNP P23526
B	33	MSE	MET	engineered mutation	UNP P23526
B	35	MSE	MET	engineered mutation	UNP P23526
B	56	MSE	MET	engineered mutation	UNP P23526
B	127	MSE	MET	engineered mutation	UNP P23526
B	167	MSE	MET	engineered mutation	UNP P23526
B	168	MSE	MET	engineered mutation	UNP P23526
B	210	MSE	MET	engineered mutation	UNP P23526
B	254	MSE	MET	engineered mutation	UNP P23526
B	262	MSE	MET	engineered mutation	UNP P23526

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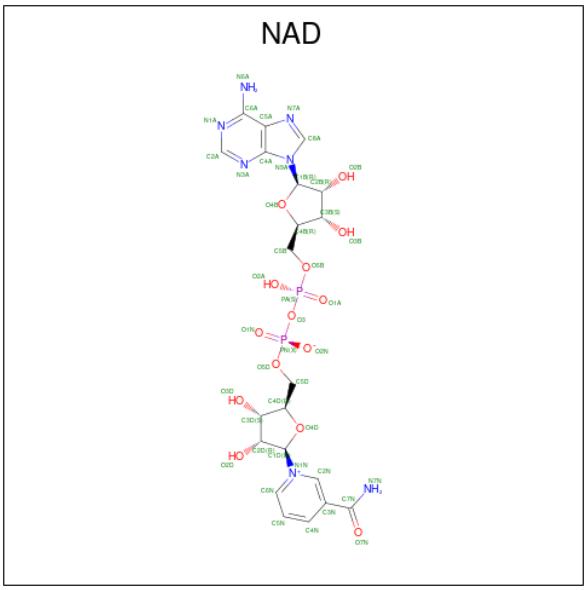
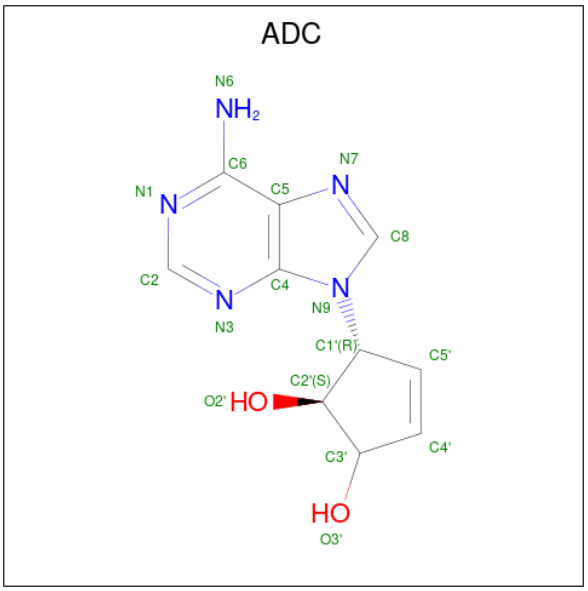
Chain	Residue	Modelled	Actual	Comment	Reference
B	290	MSE	MET	engineered mutation	UNP P23526
B	351	MSE	MET	engineered mutation	UNP P23526
B	358	MSE	MET	engineered mutation	UNP P23526
B	367	MSE	MET	engineered mutation	UNP P23526
B	419	MSE	MET	engineered mutation	UNP P23526

- 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	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		

- Molecule 3 is (1'R,2'S)-9-(2-HYDROXY-3'-KETO-CYCLOPENTEN-1-YL)ADENINE (three-letter code: ADC) (formula: $C_{10}H_{11}N_5O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 10 5 2	0	0
3	B	1	Total C N O 17 10 5 2	0	0

- Molecule 4 is water.

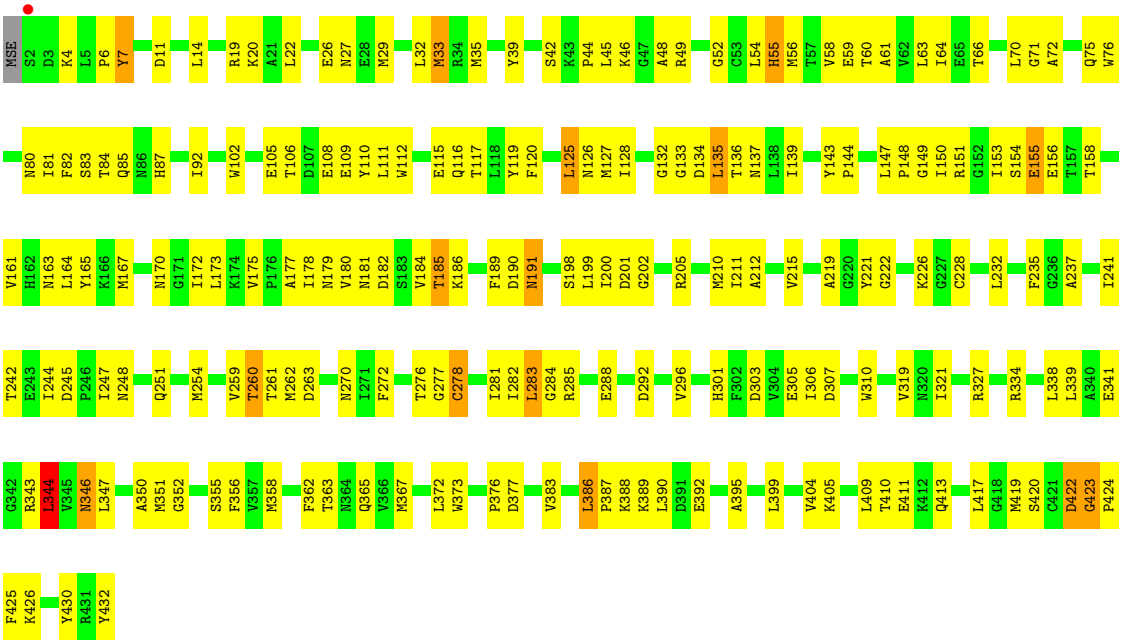
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

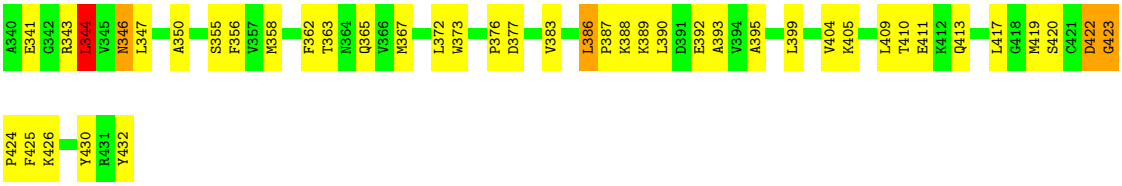
• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE

Chain A:



• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE

Chain B:


A340
E341
G342
R343
L344
V345
N346
L347
A350
S355
F356
V357
M358
F362
T363
N364
Q365
V366
M367
L372
W373
P376
D377
V383
L386
P387
K388
K389
L390
D391
E392
A393
V394
A395
L399
V404
K405
L409
T410
E411
K412
Q413
L417
G418
M419
S420
C421
D422
G423
P424
F425
K426
Y430
R431
Y432

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.93Å 168.02Å 137.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 45.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.80) 97.5 (45.97-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.90 (at 2.81Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.227 , 0.247 0.224 , 0.243	Depositor DCC
R_{free} test set	4829 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	1.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.036 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6834	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, ADC

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	0.44	0/3385	0.69	0/4556
1	B	0.43	0/3379	0.68	0/4548
All	All	0.43	0/6764	0.69	0/9104

There are no bond length outliers.

There are no bond angle outliers.

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	0	3350	212	0
1	B	3330	0	3345	221	1
2	A	44	0	26	2	0
2	B	44	0	25	2	0
3	A	17	0	8	3	0
3	B	17	0	9	3	0
4	A	27	0	0	4	0
4	B	19	0	0	0	2
All	All	6834	0	6763	417	2

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 31.

The worst 5 of 417 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:A:276:THR:HG22	1:A:278:CYS:H	1.16	1.07
1:B:276:THR:HG22	1:B:278:CYS:H	1.14	1.05
1:B:127:MSE:HE3	1:B:373:TRP:HB2	1.48	0.96
1:A:127:MSE:HE3	1:A:373:TRP:HB2	1.49	0.95
1:A:404:VAL:HG13	1:B:259:VAL:HB	1.51	0.90

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:446:HOH:O	4:B:446:HOH:O[6_555]	2.05	0.15
1:B:201:ASP:OD1	4:B:446:HOH:O[6_555]	2.19	0.01

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	429/432 (99%)	389 (91%)	35 (8%)	5 (1%)	13	39
1	B	428/432 (99%)	387 (90%)	35 (8%)	6 (1%)	11	34
All	All	857/864 (99%)	776 (90%)	70 (8%)	11 (1%)	12	36

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	B	7	TYR
1	B	55	HIS
1	A	55	HIS
1	A	185	THR

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	355/340 (104%)	338 (95%)	17 (5%)	25	58
1	B	354/340 (104%)	337 (95%)	17 (5%)	25	58
All	All	709/680 (104%)	675 (95%)	34 (5%)	25	58

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	346	ASN
1	B	377	ASP
1	B	422	ASP
1	A	377	ASP
1	A	346	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	ASN
1	B	413	GLN
1	B	324	GLN
1	B	360	ASN
1	A	346	ASN

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 monosaccharides 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	B	434	-	42,48,48	2.81	15 (35%)	50,73,73	2.87	22 (44%)
3	ADC	A	435	-	16,19,19	3.29	5 (31%)	11,28,28	1.72	1 (9%)
2	NAD	A	433	-	42,48,48	2.77	14 (33%)	50,73,73	2.86	23 (46%)
3	ADC	B	436	-	16,19,19	3.45	5 (31%)	11,28,28	2.13	2 (18%)

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	B	434	-	-	12/26/62/62	0/5/5/5
3	ADC	A	435	-	-	0/0/17/17	0/3/3/3
2	NAD	A	433	-	-	12/26/62/62	0/5/5/5
3	ADC	B	436	-	1/1/3/5	0/0/17/17	0/3/3/3

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	436	ADC	O3'-C3'	-12.09	1.20	1.43
3	A	435	ADC	O3'-C3'	-11.56	1.21	1.43
2	A	433	NAD	C3N-C7N	8.14	1.62	1.50
2	B	434	NAD	C3N-C7N	8.03	1.62	1.50
2	B	434	NAD	C2A-N3A	7.51	1.44	1.32

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	434	NAD	C2N-C3N-C4N	7.13	126.34	118.26
2	A	433	NAD	C2N-C3N-C4N	6.88	126.06	118.26
2	B	434	NAD	C3N-C2N-N1N	-6.58	114.00	120.43
2	A	433	NAD	C3N-C2N-N1N	-6.55	114.03	120.43
2	A	433	NAD	O5D-PN-O1N	-6.17	84.96	109.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	436	ADC	C3'

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	433	NAD	C5B-O5B-PA-O2A
2	A	433	NAD	C4B-C5B-O5B-PA
2	A	433	NAD	O4D-C4D-C5D-O5D
2	A	433	NAD	C3D-C4D-C5D-O5D
2	A	433	NAD	O4D-C1D-N1N-C2N

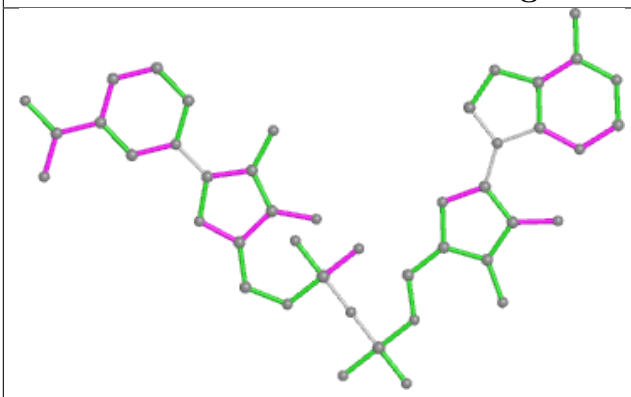
There are no ring outliers.

4 monomers are involved in 10 short contacts:

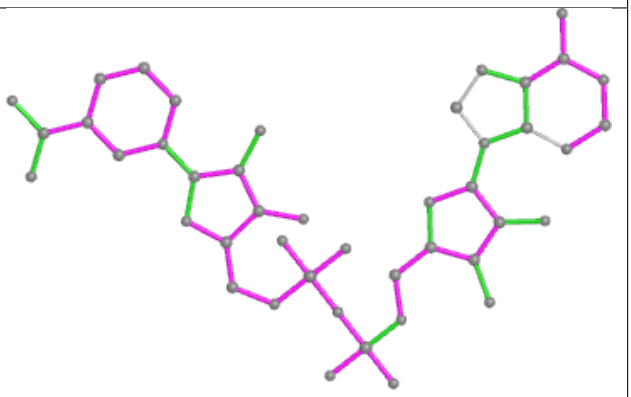
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	434	NAD	2	0
3	A	435	ADC	3	0
2	A	433	NAD	2	0
3	B	436	ADC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

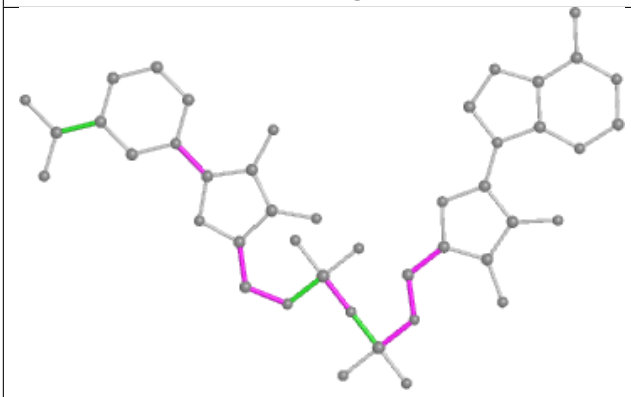
Ligand NAD B 434



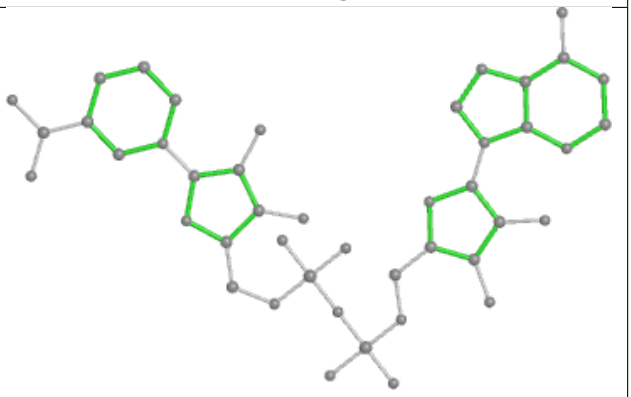
Bond lengths



Bond angles

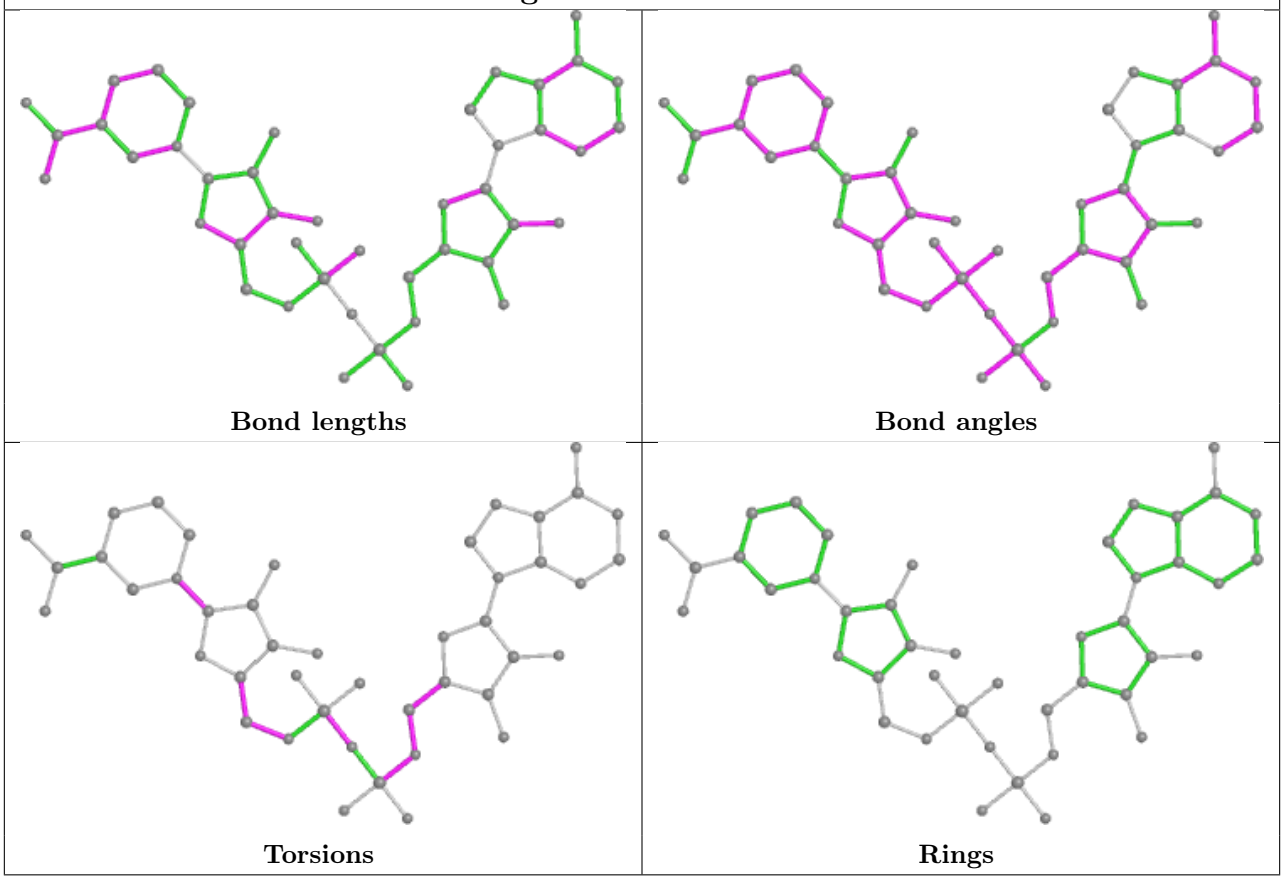


Torsions



Rings

Ligand NAD A 433



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	416/432 (96%)	-0.26	1 (0%)	95	94	2, 17, 27, 43	0
1	B	415/432 (96%)	-0.06	1 (0%)	95	94	7, 27, 39, 47	0
All	All	831/864 (96%)	-0.16	2 (0%)	95	94	2, 20, 36, 47	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.5
1	B	5	LEU	2.2

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	NAD	B	434	44/44	0.94	0.17	14,17,22,23	0
2	NAD	A	433	44/44	0.95	0.17	13,15,18,21	0
3	ADC	B	436	17/17	0.95	0.18	42,43,45,45	0

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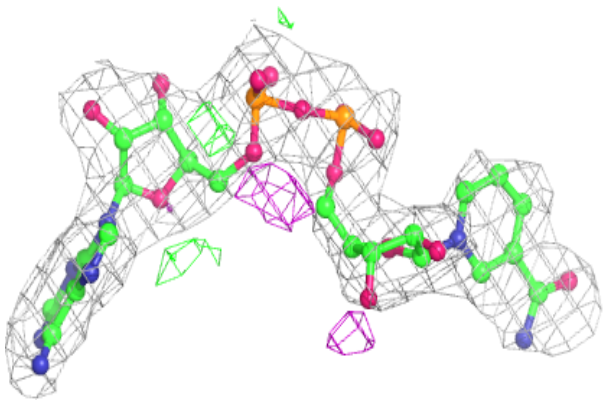
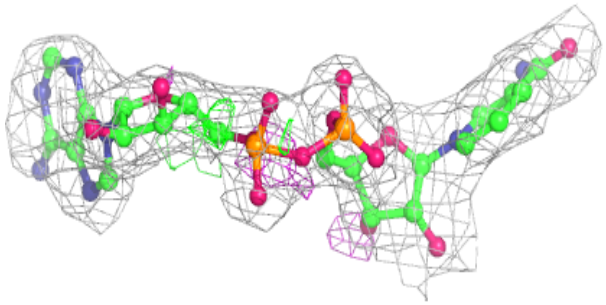
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADC	A	435	17/17	0.96	0.15	13,15,17,17	0

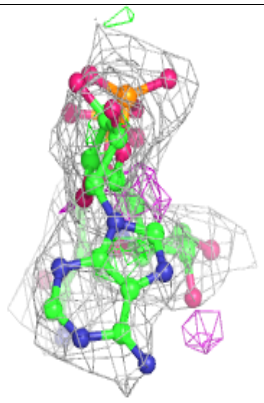
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD B 434:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

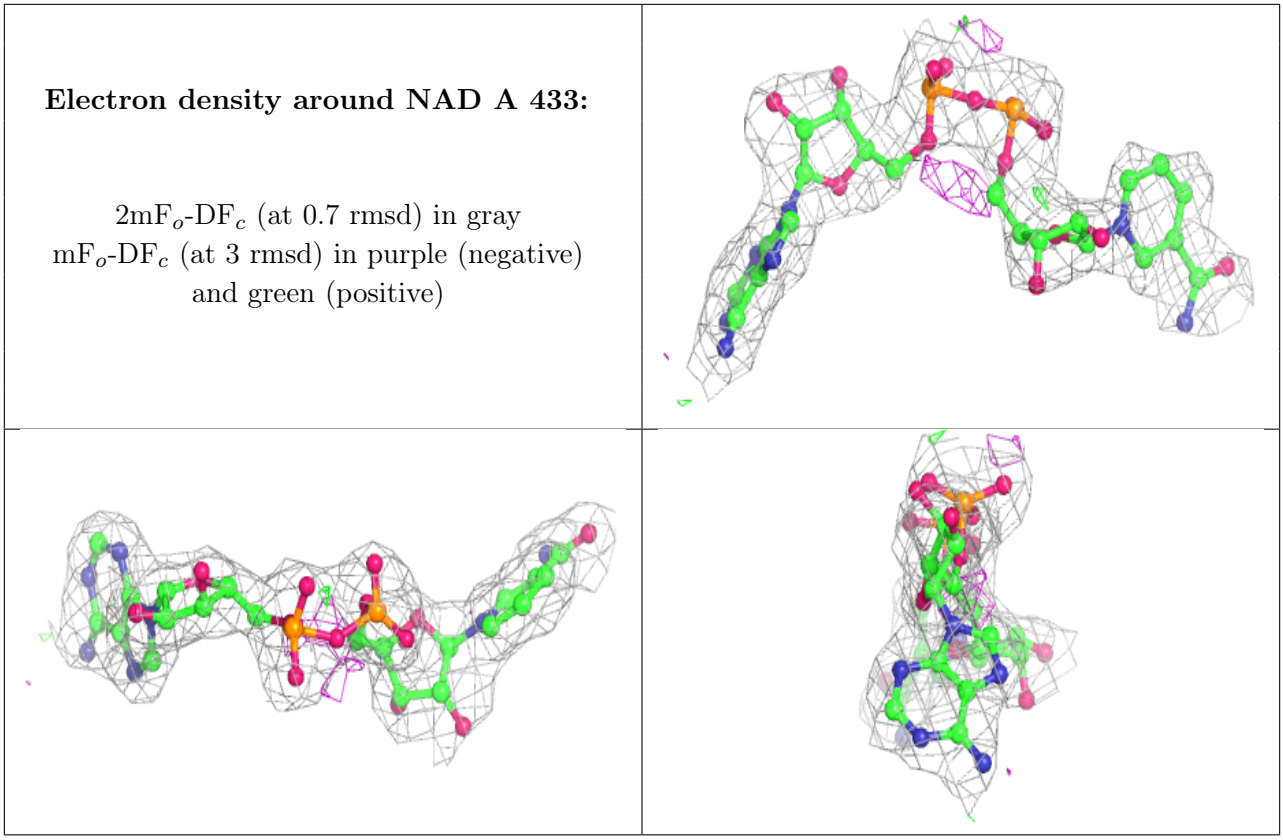






Electron density around NAD A 433:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.