



# wwPDB X-ray Structure Validation Summary Report

Jun 14, 2020 – 04:32 am BST

PDB ID : 1KY4  
Title : S-Adenosylhomocysteine hydrolase refined with noncrystallographic restraints  
Authors : Takata, Y.; Takusagawa, F.  
Deposited on : 2002-02-03  
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](mailto: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  symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

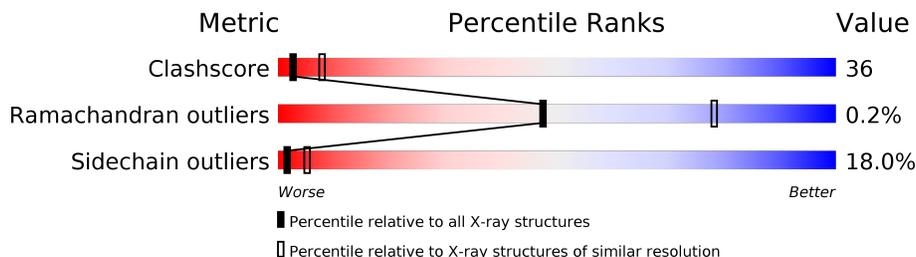
# 1 Overall quality at a glance i

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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></span> 48% 42% 10% .
1	B	431	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></span> 46% 44% 9% .
1	C	431	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></span> 47% 42% 10% .
1	D	431	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, green, yellow, orange, red, grey);"></span> 45% 44% 10% .



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 water.

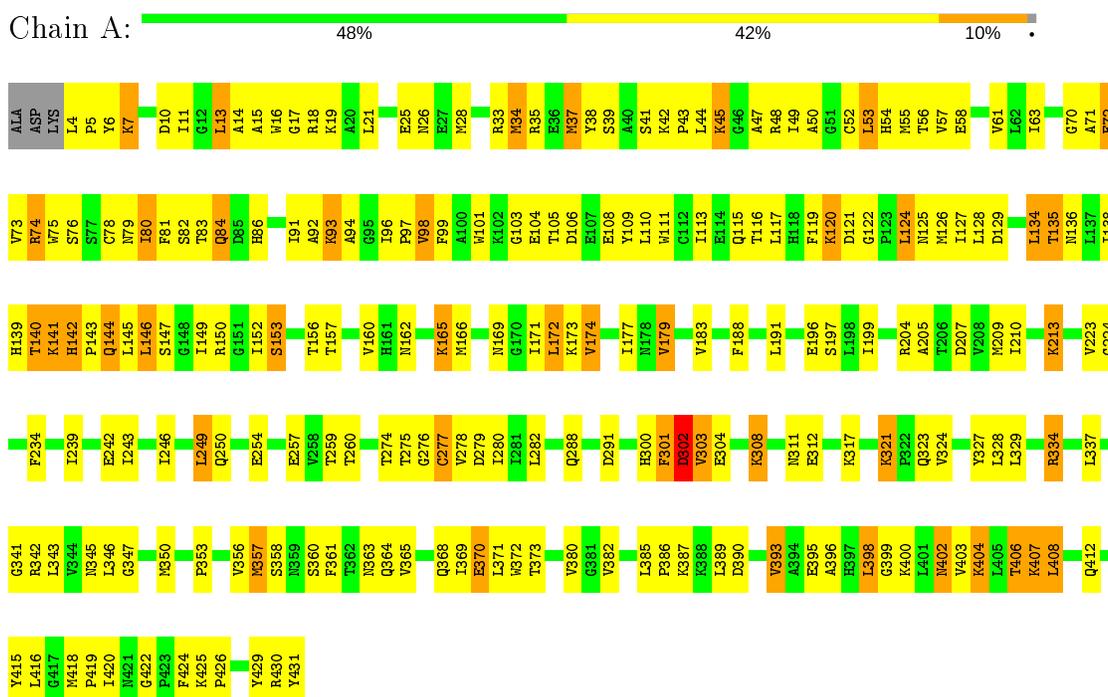
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	75	Total	O	0	0
			75	75		
3	C	60	Total	O	0	0
			60	60		
3	D	63	Total	O	0	0
			63	63		

### 3 Residue-property plots

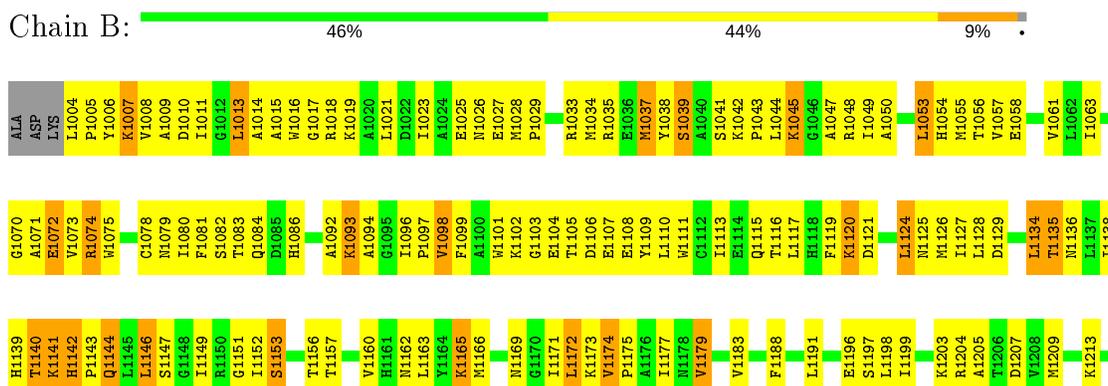
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

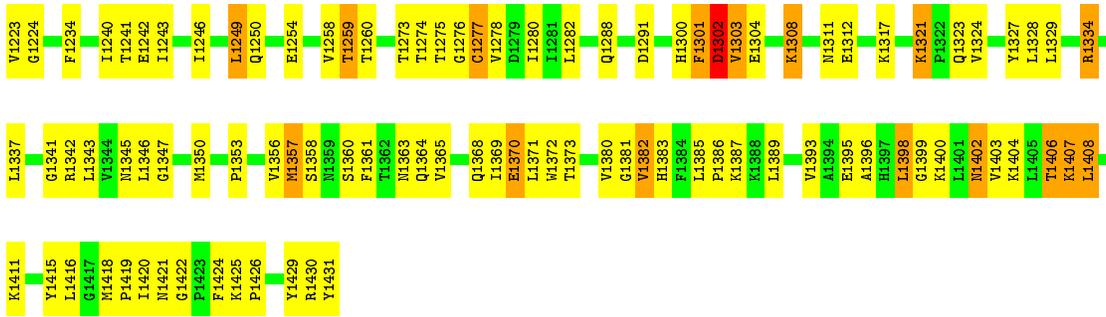
Note EDS was not executed.

- Molecule 1: S-adenosylhomocysteine hydrolase



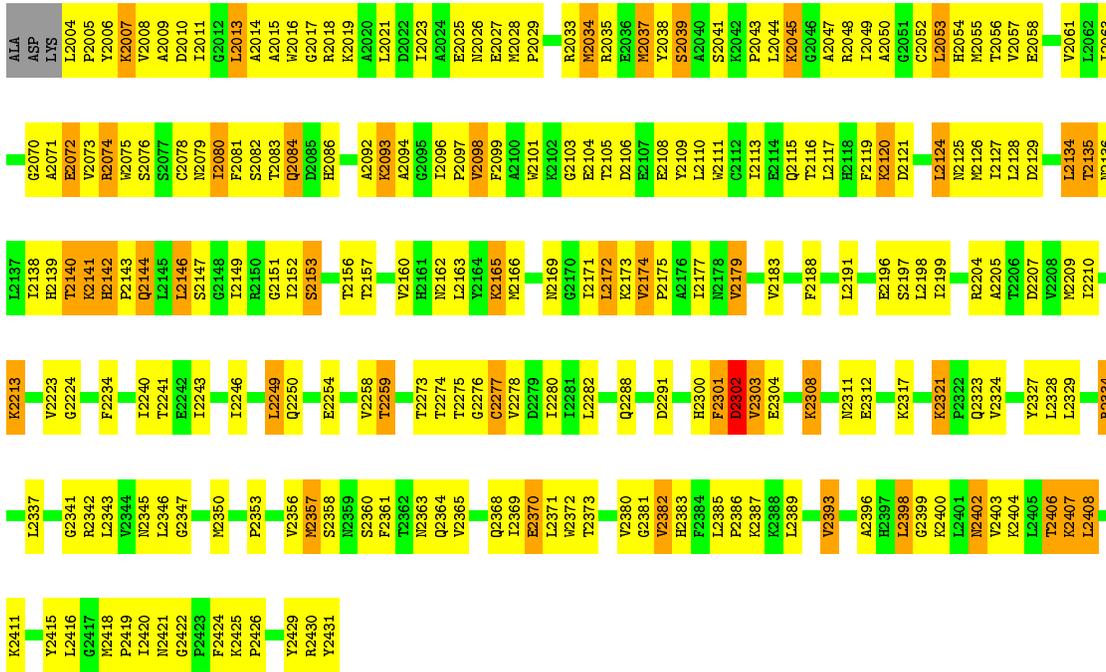
- Molecule 1: S-adenosylhomocysteine hydrolase





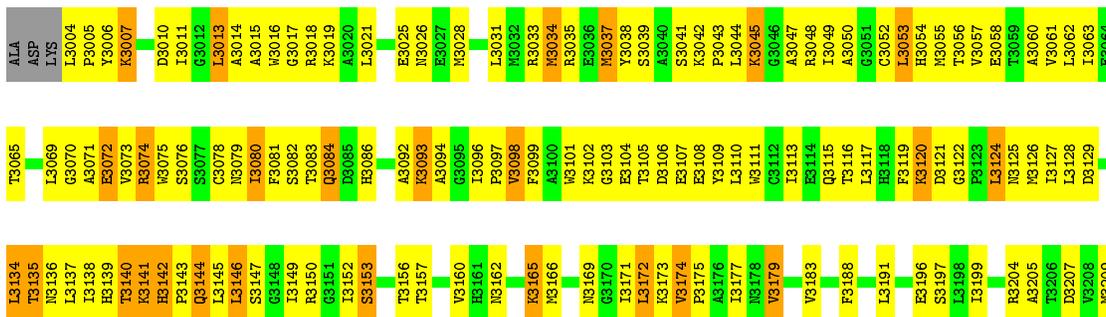
• Molecule 1: S-adenosylhomocysteine hydrolase

Chain C: 47% 42% 10%



• Molecule 1: S-adenosylhomocysteine hydrolase

Chain D: 45% 44% 10%



I3210	Q8323	R3402
R3213	V3324	V3403
V3223	R3325	R3404
G3224	R3326	L3405
R3232	V3327	T3406
G3233	L3328	K3407
F3234	L3329	L3408
I3239	R3334	T3409
E3242	L3337	Q3412
I3243	L3342	Y3415
I3246	L3343	L3416
L3249	V3344	G3417
Q3250	R3345	R3418
E3254	L3346	P3419
E3257	G3347	I3420
V3258	M3350	N3421
T3259	P3353	G3422
T3260	V3356	F3423
T3274	M3357	F3424
T3275	S3358	K3425
G3276	R3359	P3426
G3277	S3360	Y3429
V3278	F3361	R3430
D3279	T3362	Y3431
I3280	N3363	
I3281	Q3364	
L3282	V3365	
Q3288	Q3368	
D3291	I3369	
H3300	E3370	
F3301	L3371	
D3302	M3372	
V3303	T3373	
E3304	V3380	
K3308	G3381	
N3311	V3382	
E3312	I3385	
N3313	P3386	
K3317	K3387	
N3318	K3388	
N3319	L3389	
I3320	V3393	
K3321	A3394	
P3322	E3395	
	A3396	
	R3397	
	L3398	
	G3399	
	K3400	
	I3401	

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.76Å 134.48Å 102.26Å 90.00° 114.35° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.228 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/3367	0.63	1/4557 (0.0%)
1	B	0.37	0/3367	0.62	1/4557 (0.0%)
1	C	0.37	0/3367	0.62	1/4557 (0.0%)
1	D	0.37	0/3367	0.62	1/4557 (0.0%)
All	All	0.37	0/13468	0.62	4/18228 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3302	ASP	N-CA-C	5.47	125.76	111.00
1	A	302	ASP	N-CA-C	5.31	125.33	111.00
1	C	2302	ASP	N-CA-C	5.06	124.67	111.00
1	B	1302	ASP	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3302	0	3324	253	0
1	B	3302	0	3324	268	0
1	C	3302	0	3324	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3302	0	3324	266	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	68	0	0	2	0
3	B	75	0	0	8	0
3	C	60	0	0	2	0
3	D	63	0	0	10	0
All	All	13650	0	13400	968	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 36.

The worst 5 of 968 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:C:2430:ARG:HB3	1:D:3430:ARG:HB3	1.25	1.15
1:A:430:ARG:HB3	1:B:1430:ARG:HB3	1.29	1.15
1:A:370:GLU:HG3	1:A:389:LEU:HD11	1.41	1.03
1:D:3370:GLU:HG3	1:D:3389:LEU:HD11	1.41	1.03
1:C:2370:GLU:HG3	1:C:2389:LEU:HD11	1.39	1.01

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	426/431 (99%)	409 (96%)	16 (4%)	1 (0%)	47 78
1	B	426/431 (99%)	407 (96%)	18 (4%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	426/431 (99%)	410 (96%)	15 (4%)	1 (0%)	47	78
1	D	426/431 (99%)	408 (96%)	17 (4%)	1 (0%)	47	78
All	All	1704/1724 (99%)	1634 (96%)	66 (4%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	1302	ASP
1	C	2302	ASP
1	D	3302	ASP

### 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	351/353 (99%)	288 (82%)	63 (18%)	2	5
1	B	351/353 (99%)	288 (82%)	63 (18%)	2	5
1	C	351/353 (99%)	287 (82%)	64 (18%)	1	5
1	D	351/353 (99%)	288 (82%)	63 (18%)	2	5
All	All	1404/1412 (99%)	1151 (82%)	253 (18%)	1	5

5 of 253 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1370	GLU
1	C	2098	VAL
1	D	3301	PHE
1	B	1393	VAL
1	C	2026	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1169	ASN
1	C	2084	GLN
1	D	3169	ASN
1	B	1300	HIS
1	C	2115	GLN

### 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](#)

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	1432	-	42,48,48	2.17	9 (21%)	50,73,73	2.16	12 (24%)
2	NAD	A	432	-	42,48,48	2.09	9 (21%)	50,73,73	2.12	12 (24%)
2	NAD	D	3432	-	42,48,48	2.18	8 (19%)	50,73,73	2.12	12 (24%)
2	NAD	C	2432	-	42,48,48	2.18	8 (19%)	50,73,73	2.13	13 (26%)

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	1432	-	-	7/26/62/62	0/5/5/5
2	NAD	A	432	-	-	7/26/62/62	0/5/5/5
2	NAD	D	3432	-	-	7/26/62/62	0/5/5/5
2	NAD	C	2432	-	-	7/26/62/62	0/5/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2432	NAD	C5N-C4N	6.63	1.52	1.38
2	B	1432	NAD	C5N-C4N	6.55	1.52	1.38
2	D	3432	NAD	C2N-N1N	6.11	1.42	1.35
2	D	3432	NAD	C5N-C4N	6.07	1.51	1.38
2	A	432	NAD	C5N-C4N	6.04	1.51	1.38

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	NAD	O5D-PN-O1N	-6.89	82.16	109.07
2	C	2432	NAD	O5D-PN-O1N	-6.85	82.29	109.07
2	D	3432	NAD	O5D-PN-O1N	-6.78	82.59	109.07
2	B	1432	NAD	O5D-PN-O1N	-6.68	82.97	109.07
2	A	432	NAD	C3N-C7N-N7N	5.72	124.61	117.75

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1432	NAD	O4D-C1D-N1N-C2N
2	B	1432	NAD	O4D-C1D-N1N-C6N
2	B	1432	NAD	C2D-C1D-N1N-C2N
2	B	1432	NAD	C2D-C1D-N1N-C6N
2	A	432	NAD	O4D-C1D-N1N-C2N

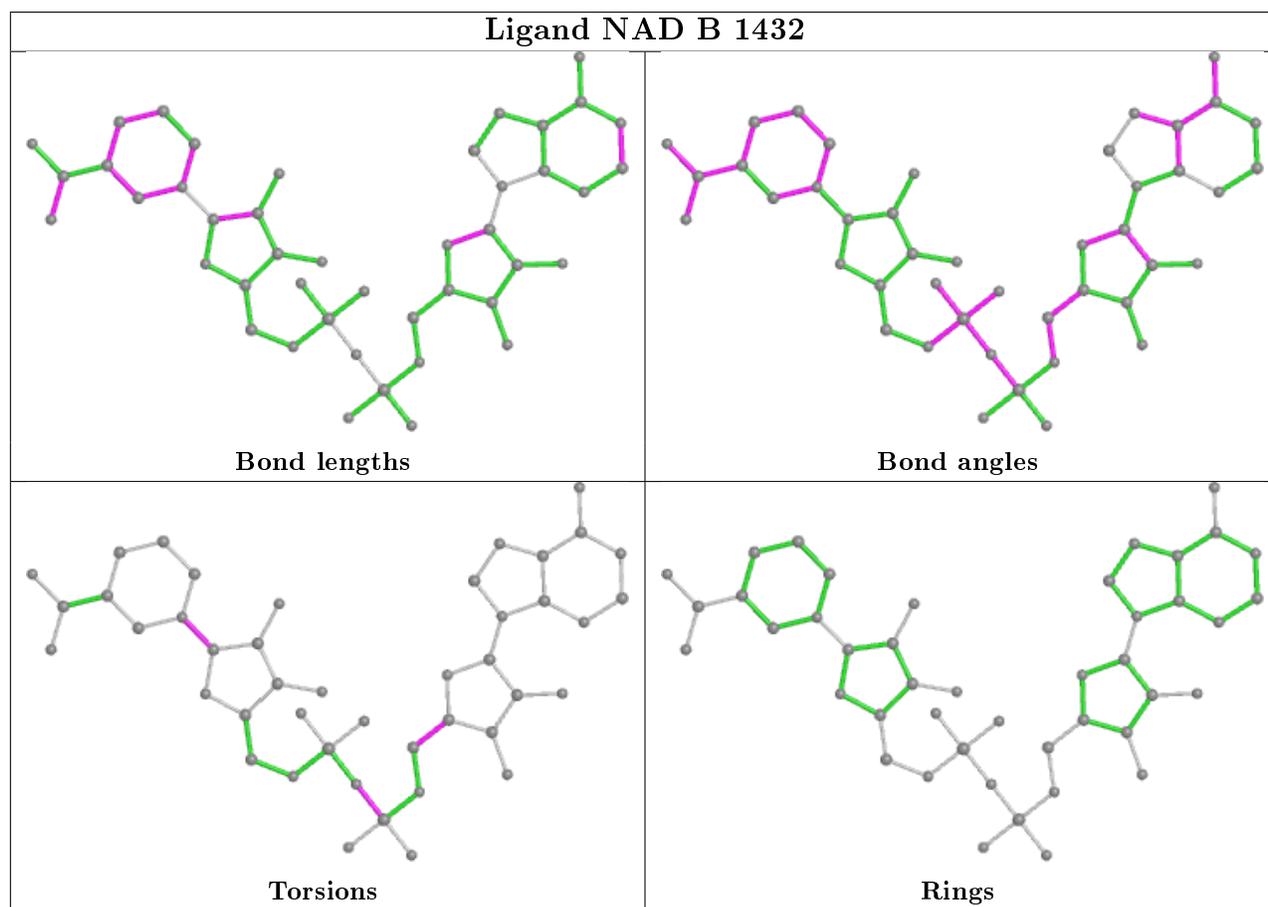
There are no ring outliers.

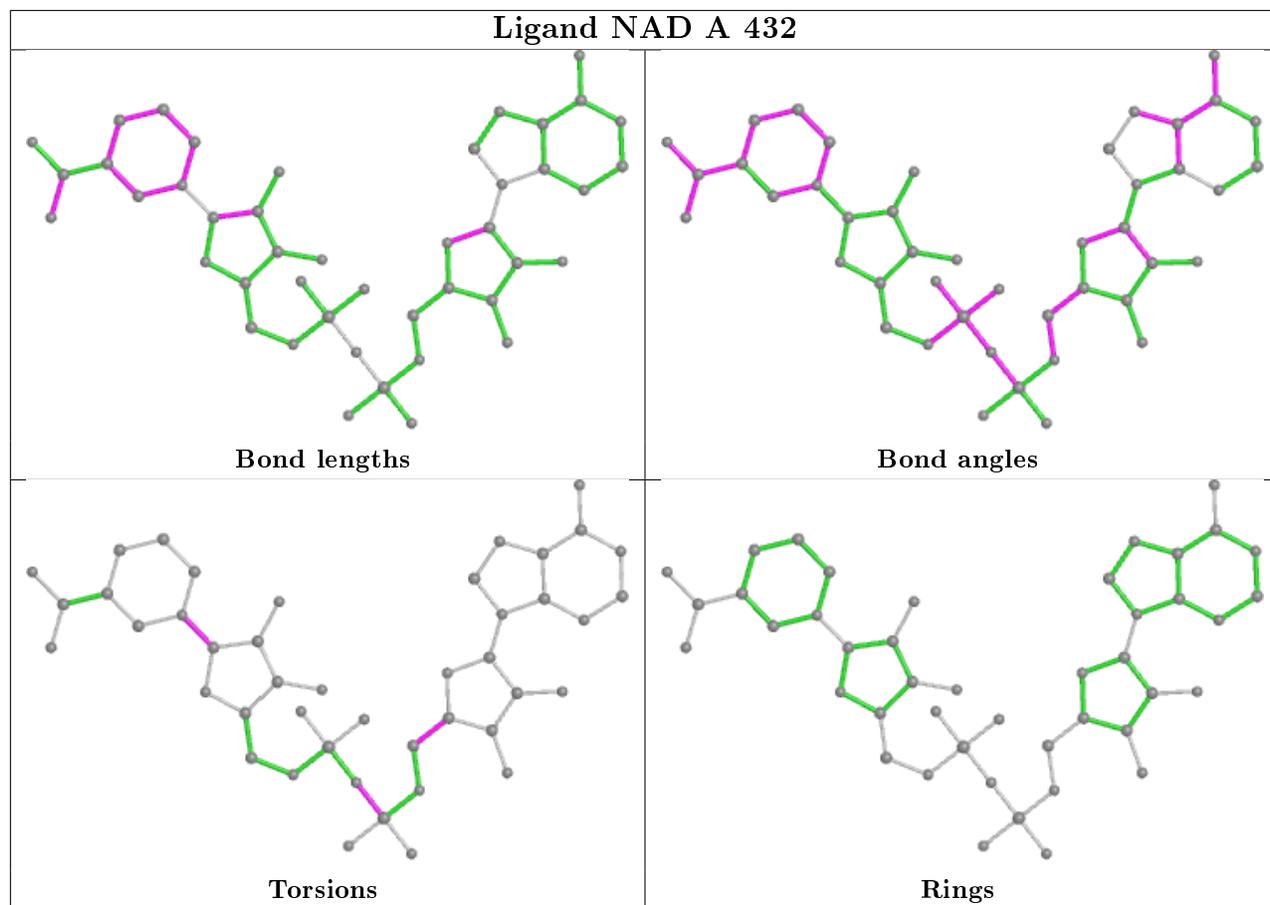
2 monomers are involved in 2 short contacts:

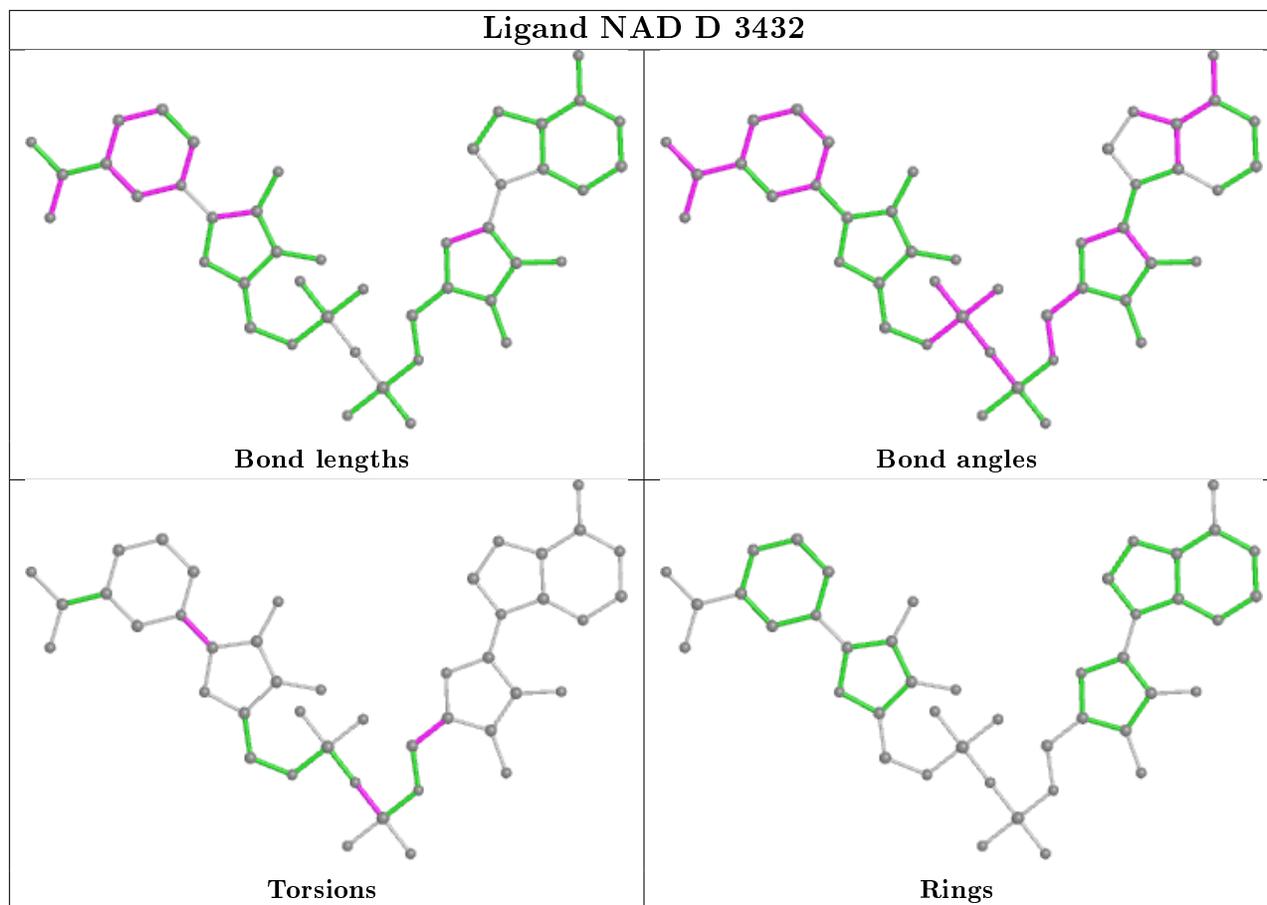
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	NAD	1	0
2	C	2432	NAD	1	0

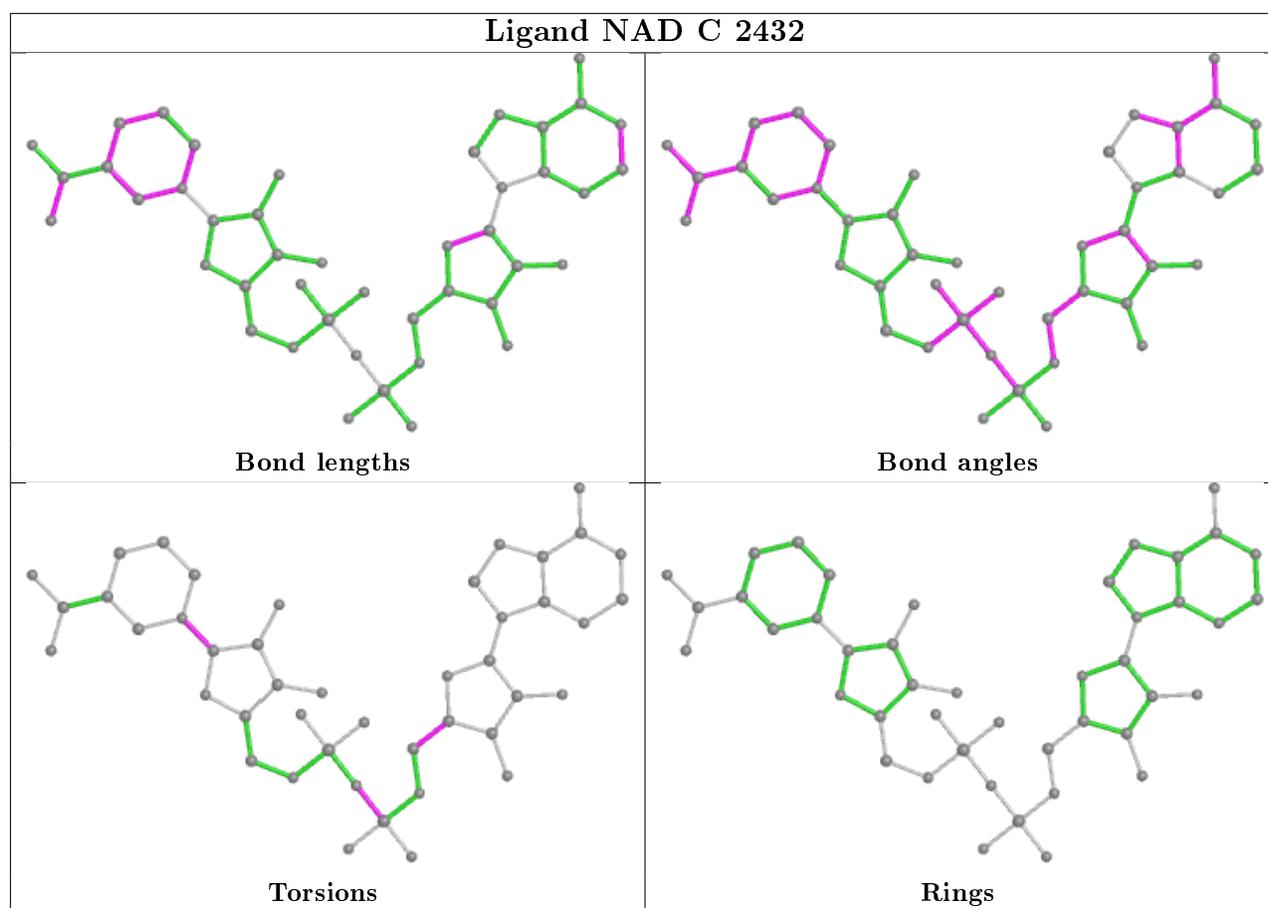
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 than 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.









## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.