



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:51 AM UTC

PDB ID : 1KY5 / pdb_00001ky5
Title : D244E mutant 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

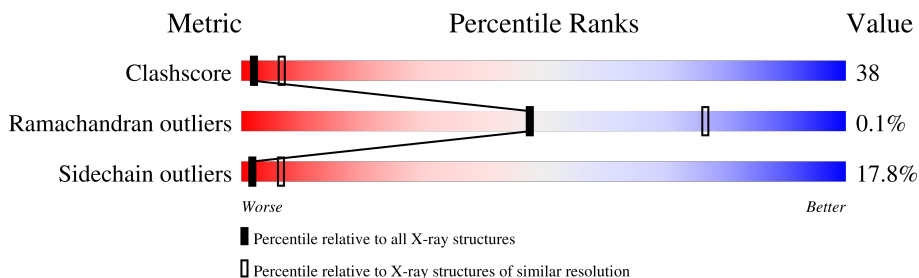
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	48% 41% 11%
1	B	431	45% 42% 13%
1	C	431	46% 41% 13%
1	D	431	47% 40% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13784 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.

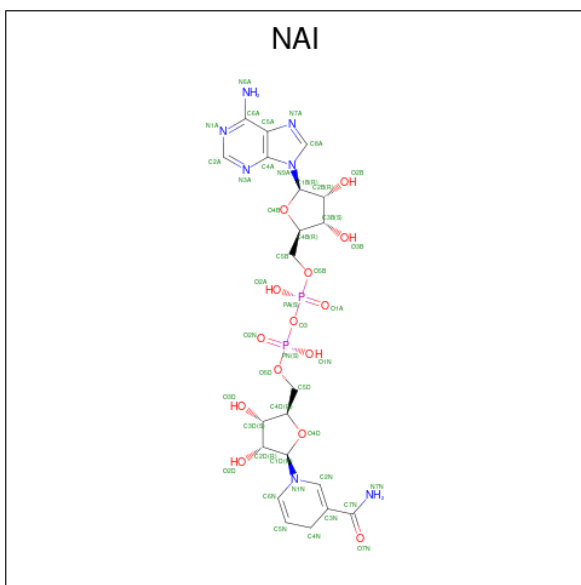
- Molecule 1 is a protein called S-adenosylhomocysteine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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:

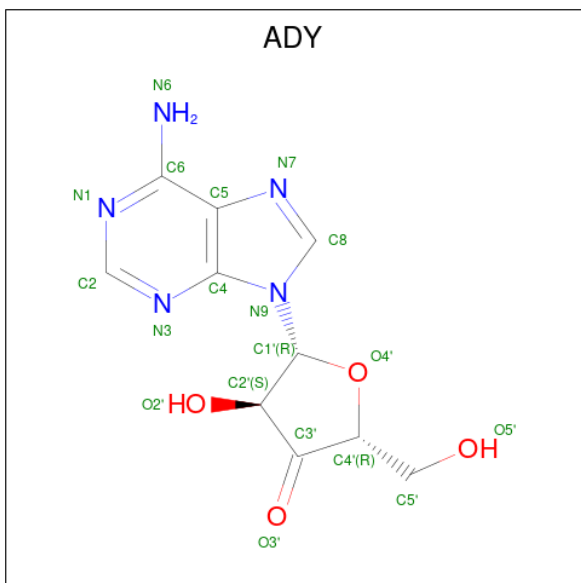
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	engineered mutation	UNP P10760
B	1244	GLU	ASP	engineered mutation	UNP P10760
C	2244	GLU	ASP	engineered mutation	UNP P10760
D	3244	GLU	ASP	engineered mutation	UNP P10760

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

- Molecule 3 is 3'-OXO-ADENOSINE (CCD ID: ADY) (formula: $\text{C}_{10}\text{H}_{11}\text{N}_5\text{O}_4$).



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.

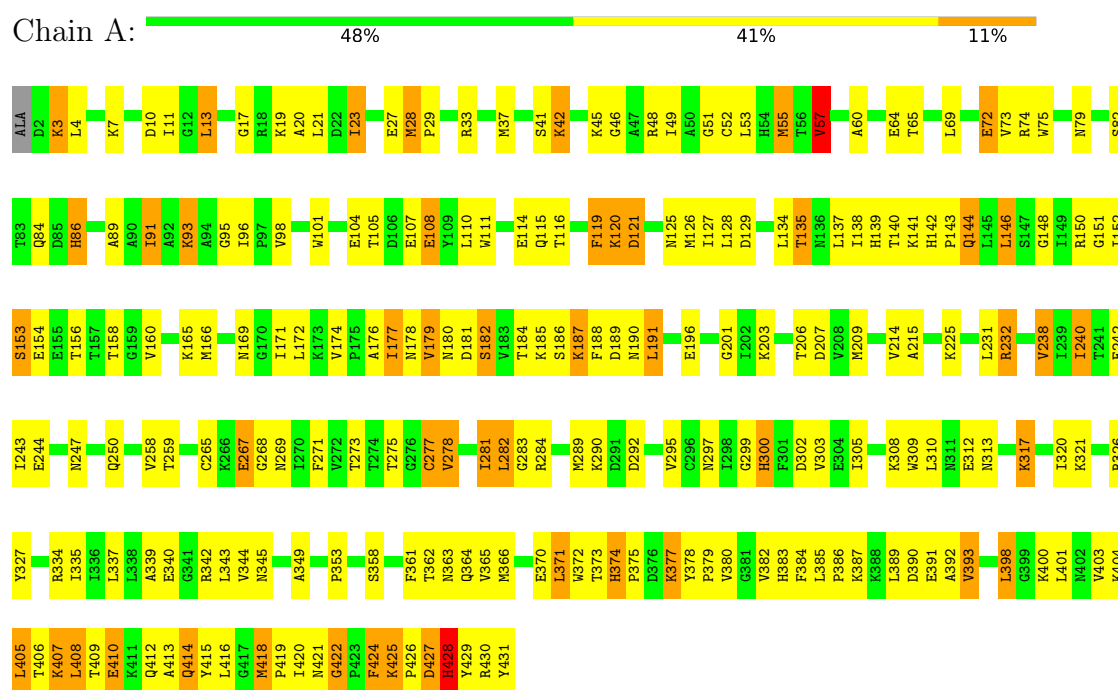
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	68	Total	O	0	0
			68	68		
4	C	54	Total	O	0	0
			54	54		
4	D	51	Total	O	0	0
			51	51		

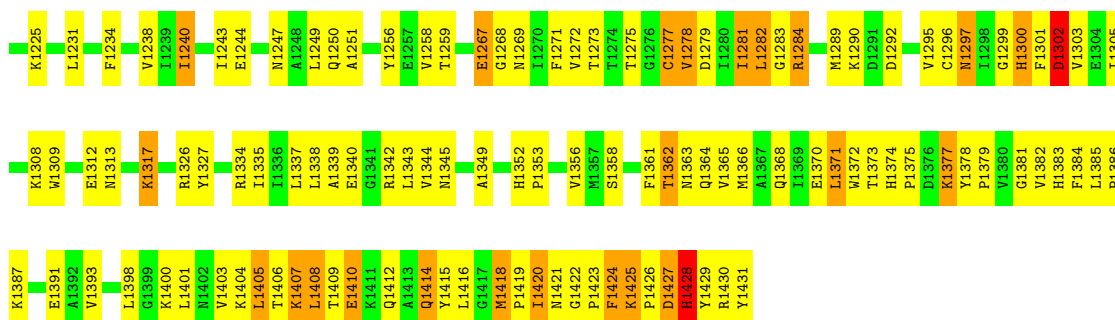
3 Residue-property plots

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. 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.

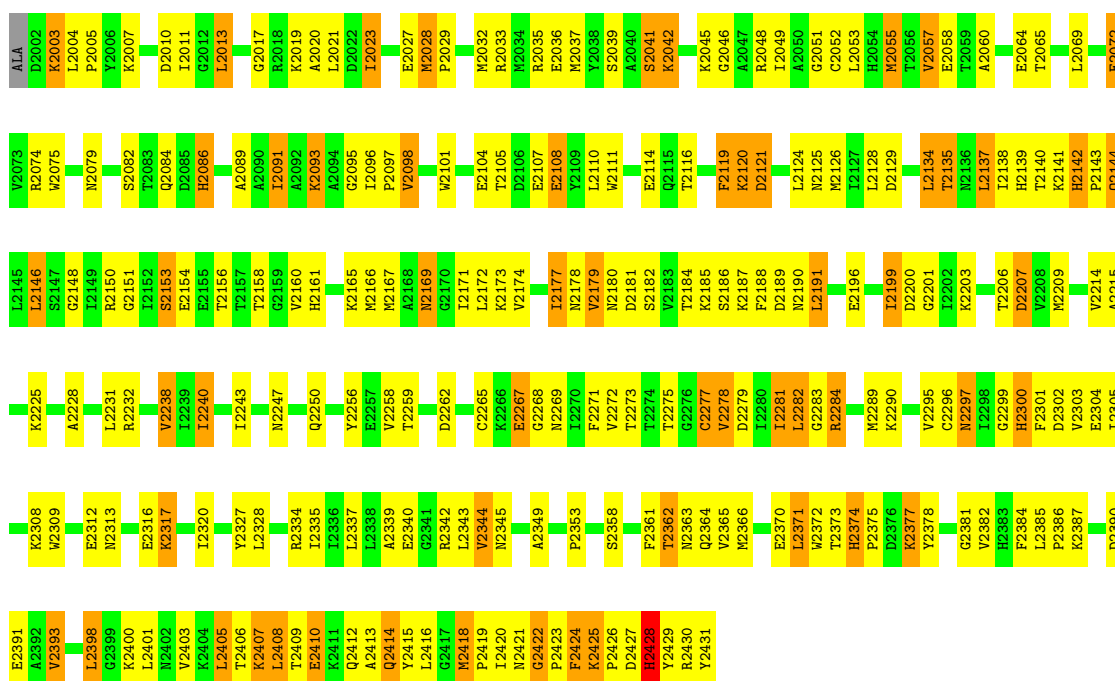
• Molecule 1: S-adenosylhomocysteine hydrolase





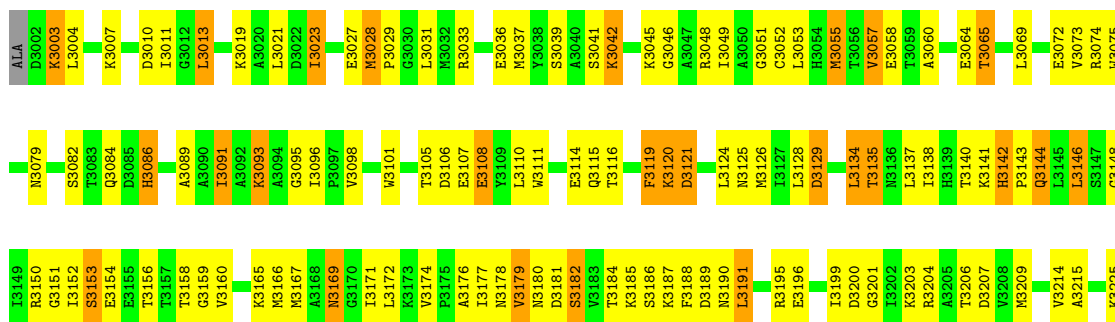
• Molecule 1: S-adenosylhomocysteine hydrolase

Chain C: 46% 41% 13%



• Molecule 1: S-adenosylhomocysteine hydrolase

Chain D: 47% 40% 13%



F3402	N3313		L3231
F3403	K3317		V3238
K3404			I3239
L3405	Y3327		I3240
K3407			
L3408	R3334		
T3409	I3335		I3243
E3410	L3336		E3244
K3411	L3337		P3245
Q3412	L3338		I3246
A3413	A3339		N3247
Q3414	E3340		A3248
Y3415	G3341		L3249
L3416	R3342		Q3250
G3417	L3343		
K3418	Y3344		E3257
F3419	N3345		V3258
L3420			
N3421	A3349		D3262
G3422			
P3423	H3352		C3265
F3424	P3353		K3266
K3425			E3267
P3426	M3357		Q3268
D3427	S3358		N3269
K3428			
Y3429	F3361		V3272
R3430	T3362		T3273
F3431	N3363		T3274
	Q3364		T3275
	V3365		G3276
	M3366		C3277
			V3278
	E3370		D3279
	L3371		I3280
	K3372		I3281
	T3373		L3282
	H3374		G3283
	P3375		R3284
	D3376		H3285
	K3377		
	Y3378		K3290
	V3379		
	V3380		V3295
	G3381		C3296
	V3382		N3297
	H3383		I3298
	P3384		G3299
			H3300
	K3387		F3301
			D3302
	E3391		V3303
	A3392		E3304
	V3393		I3305
	L3398		K3308
	G3399		V3309
	K3400		
	L3401		F3212

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 223.00Å 91.20Å 90.00° 90.00° 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}	0.215 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13784	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: NAI, ADY

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	0.52	0/3385	0.98	15/4580 (0.3%)
1	B	0.52	0/3385	0.99	17/4580 (0.4%)
1	C	0.54	0/3385	0.98	17/4580 (0.4%)
1	D	0.53	0/3385	0.98	17/4580 (0.4%)
All	All	0.53	0/13540	0.98	66/18320 (0.4%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3278	VAL	N-CA-C	8.15	118.94	110.05
1	A	278	VAL	N-CA-C	8.12	118.90	110.05
1	B	1302	ASP	N-CA-C	7.82	123.36	112.72
1	B	1278	VAL	N-CA-C	7.78	118.53	110.05
1	D	3302	ASP	N-CA-C	7.65	122.65	112.25

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	3320	0	3343	273	0
1	B	3320	0	3343	275	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3320	0	3343	284	0
1	D	3320	0	3343	284	1
2	A	44	0	27	2	0
2	B	44	0	27	2	0
2	C	44	0	27	2	0
2	D	44	0	27	2	0
3	A	19	0	11	0	0
3	B	19	0	11	0	0
3	C	19	0	10	0	0
3	D	19	0	10	0	0
4	A	79	0	0	2	0
4	B	68	0	0	2	0
4	C	54	0	0	1	0
4	D	51	0	0	2	0
All	All	13784	0	13522	1021	1

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 38.

The worst 5 of 1021 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:2120:LYS:H	1:C:2120:LYS:HD2	1.13	1.10
1:C:2060:ALA:HB1	1:C:2091:ILE:HD11	1.34	1.08
1:D:3420:ILE:HG23	1:D:3421:ASN:OD1	1.56	1.05
1:A:430:ARG:HA	1:B:1430:ARG:HG2	1.38	1.03
1:D:3120:LYS:H	1:D:3120:LYS:HD2	1.20	1.02

All (1) 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)
1:D:3317:LYS:O	1:D:3317:LYS:O[2_555]	2.12	0.08

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%)	398 (93%)	30 (7%)	0	100	100
1	B	428/431 (99%)	401 (94%)	26 (6%)	1 (0%)	43	72
1	C	428/431 (99%)	396 (92%)	32 (8%)	0	100	100
1	D	428/431 (99%)	400 (94%)	28 (6%)	0	100	100
All	All	1712/1724 (99%)	1595 (93%)	116 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1420	ILE

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%)	291 (82%)	62 (18%)	2	7
1	B	353/353 (100%)	291 (82%)	62 (18%)	2	7
1	C	353/353 (100%)	288 (82%)	65 (18%)	1	6
1	D	353/353 (100%)	291 (82%)	62 (18%)	2	7
All	All	1412/1412 (100%)	1161 (82%)	251 (18%)	2	6

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1407	LYS
1	D	3191	LEU
1	C	2121	ASP
1	D	3179	VAL
1	D	3377	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2269	ASN
1	D	3084	GLN
1	C	2313	ASN
1	C	2412	GLN
1	D	3169	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	NAI	D	3432	-	47,48,48	1.19	4 (8%)	64,73,73	1.16	7 (10%)
2	NAI	C	2432	-	47,48,48	1.16	4 (8%)	64,73,73	1.13	6 (9%)
3	ADY	C	2433	-	19,21,21	1.99	2 (10%)	22,31,31	1.21	3 (13%)
3	ADY	A	433	-	19,21,21	1.05	1 (5%)	22,31,31	1.30	4 (18%)
2	NAI	A	432	-	47,48,48	1.30	4 (8%)	64,73,73	1.23	7 (10%)
3	ADY	B	1433	-	19,21,21	1.20	2 (10%)	22,31,31	1.35	4 (18%)
3	ADY	D	3433	-	19,21,21	1.78	3 (15%)	22,31,31	1.32	3 (13%)
2	NAI	B	1432	-	47,48,48	1.19	4 (8%)	64,73,73	1.14	5 (7%)

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	NAI	D	3432	-	-	8/29/72/72	0/5/5/5
2	NAI	C	2432	-	-	8/29/72/72	0/5/5/5
3	ADY	C	2433	-	-	0/6/22/22	0/3/3/3
3	ADY	A	433	-	-	0/6/22/22	0/3/3/3
2	NAI	A	432	-	-	8/29/72/72	0/5/5/5
3	ADY	B	1433	-	-	0/6/22/22	0/3/3/3
3	ADY	D	3433	-	-	0/6/22/22	0/3/3/3
2	NAI	B	1432	-	-	9/29/72/72	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2433	ADY	O3'-C3'	7.05	1.32	1.21
3	D	3433	ADY	O3'-C3'	5.61	1.30	1.21
2	A	432	NAI	PN-O3	4.51	1.64	1.59
2	A	432	NAI	C2N-C3N	4.19	1.46	1.35
2	D	3432	NAI	C2N-C3N	3.97	1.46	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1432	NAI	O7N-C7N-C3N	-4.30	112.79	120.90
3	D	3433	ADY	O5'-C5'-C4'	-4.18	101.11	111.73
2	D	3432	NAI	O7N-C7N-C3N	-4.14	113.11	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	NAI	O7N-C7N-C3N	-4.05	113.28	120.90
2	A	432	NAI	C3N-C7N-N7N	3.92	124.63	117.67

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

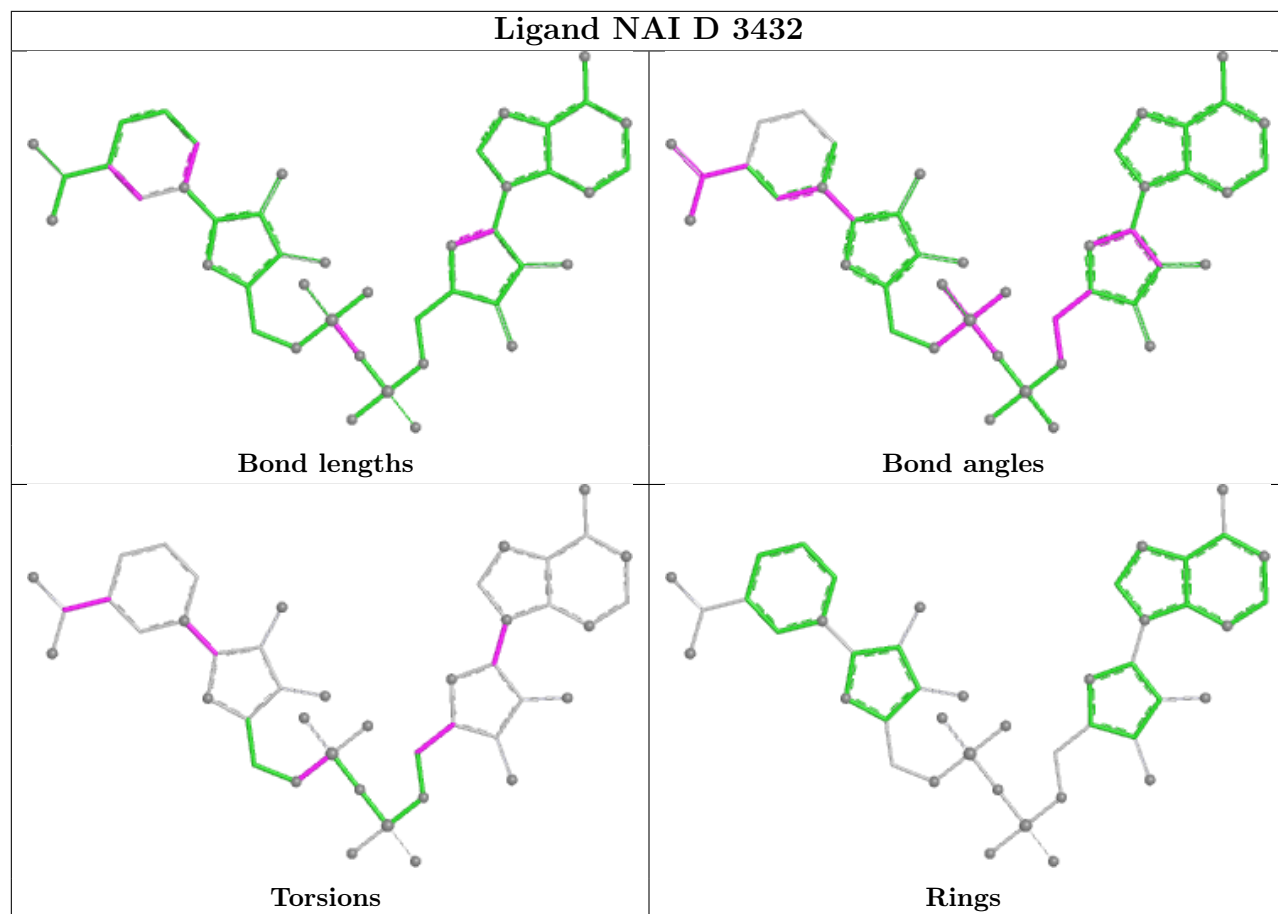
Mol	Chain	Res	Type	Atoms
2	B	1432	NAI	C2B-C1B-N9A-C8A
2	A	432	NAI	C2D-C1D-N1N-C2N
2	A	432	NAI	C2D-C1D-N1N-C6N
2	B	1432	NAI	C2D-C1D-N1N-C2N
2	D	3432	NAI	C2D-C1D-N1N-C2N

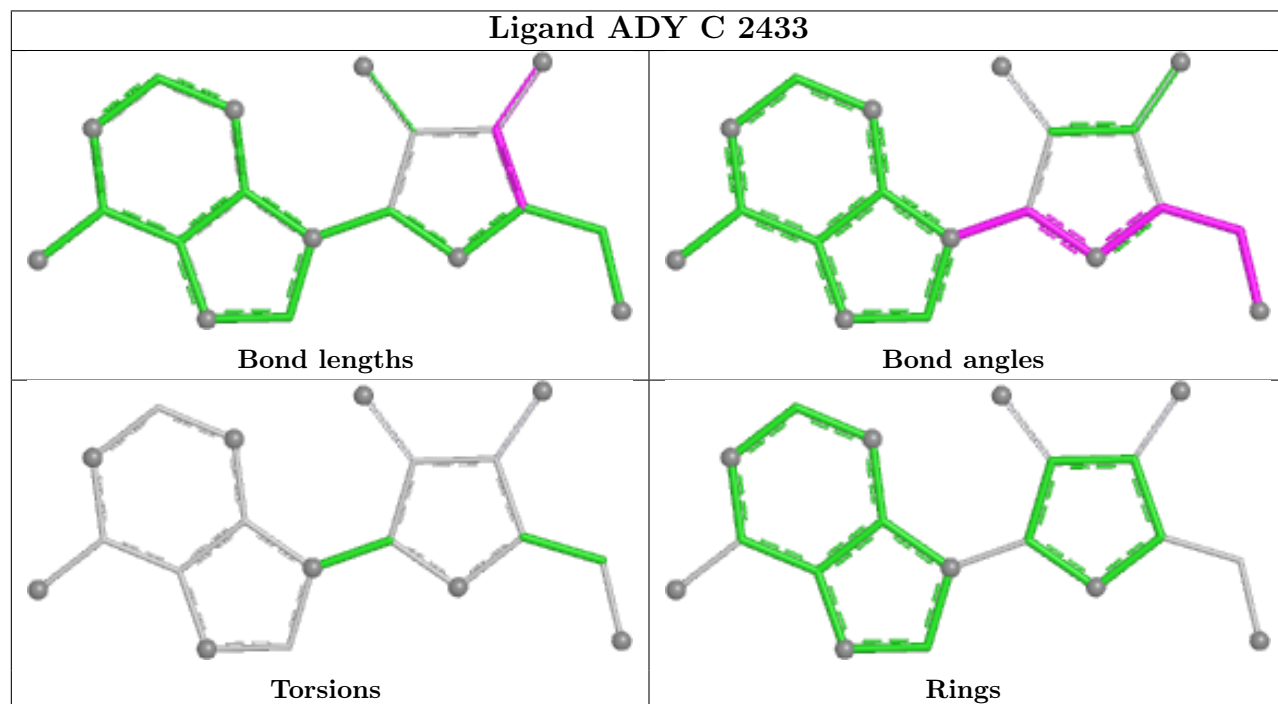
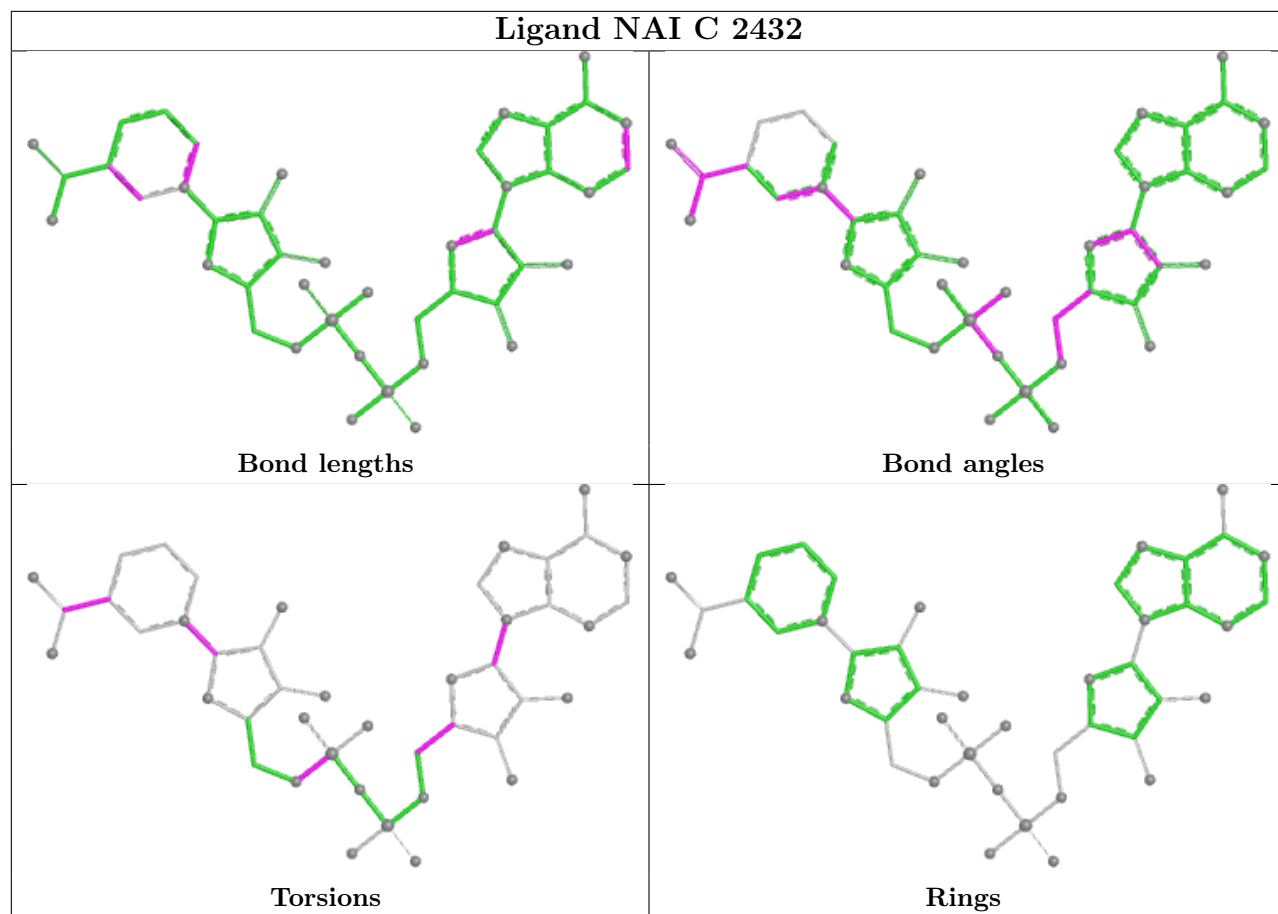
There are no ring outliers.

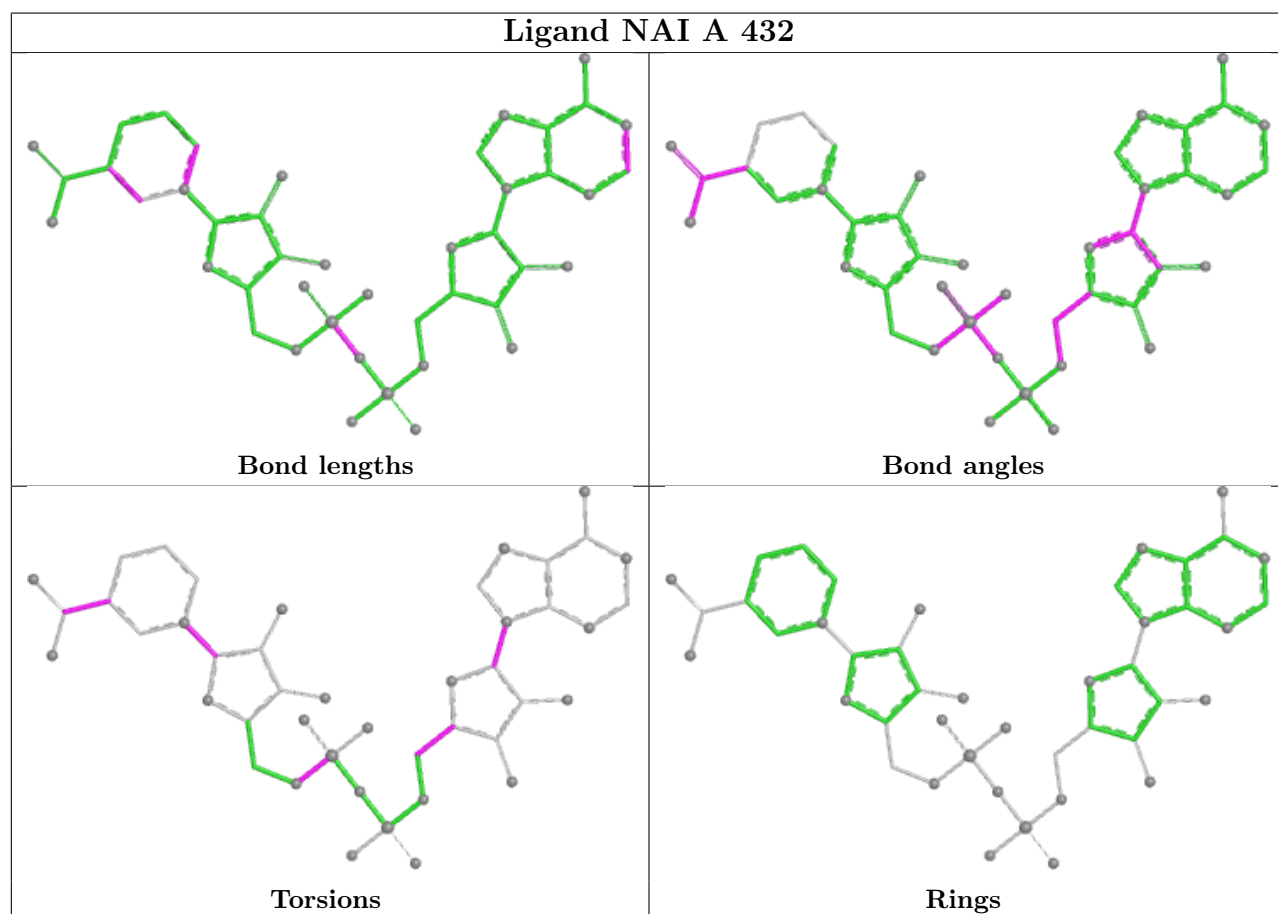
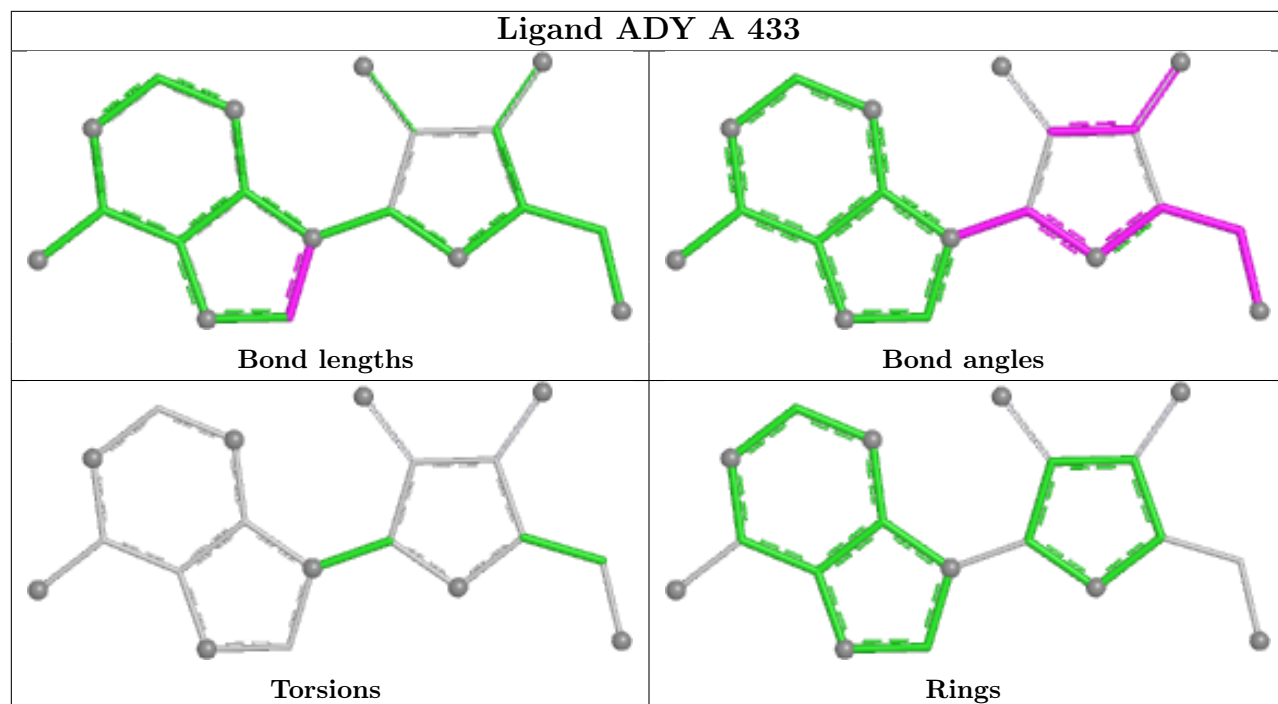
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3432	NAI	2	0
2	C	2432	NAI	2	0
2	A	432	NAI	2	0
2	B	1432	NAI	2	0

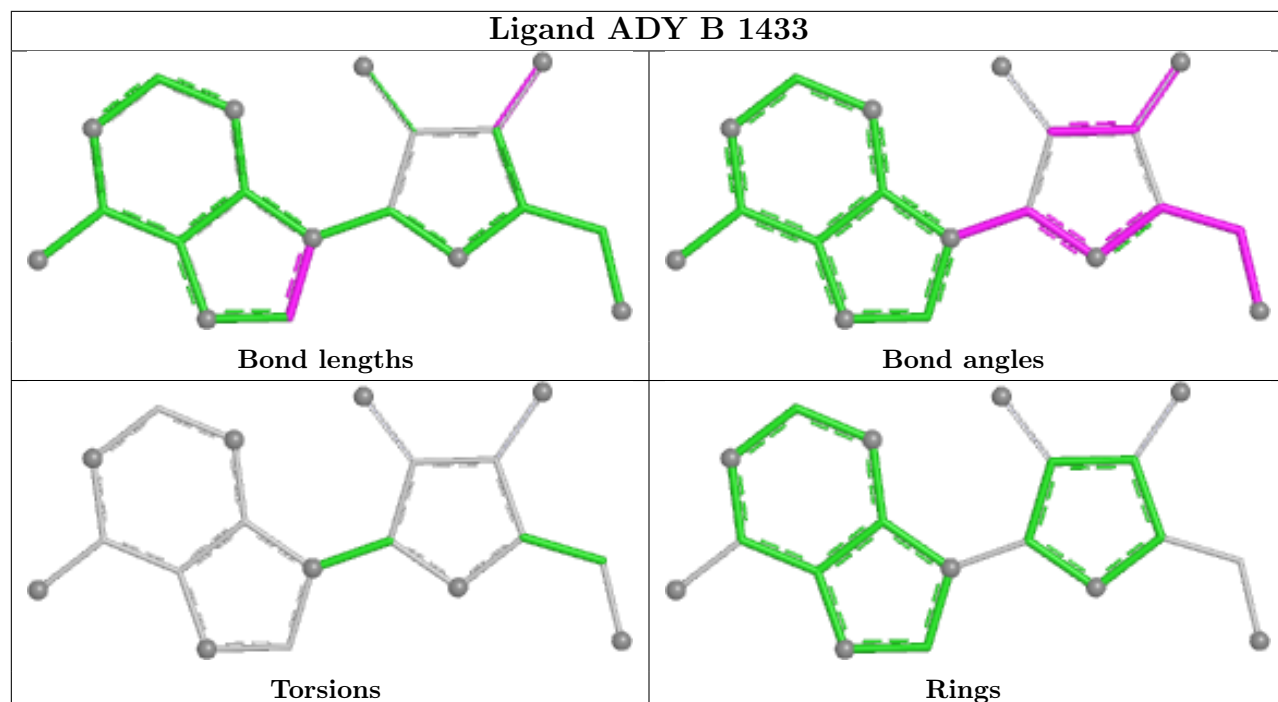
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



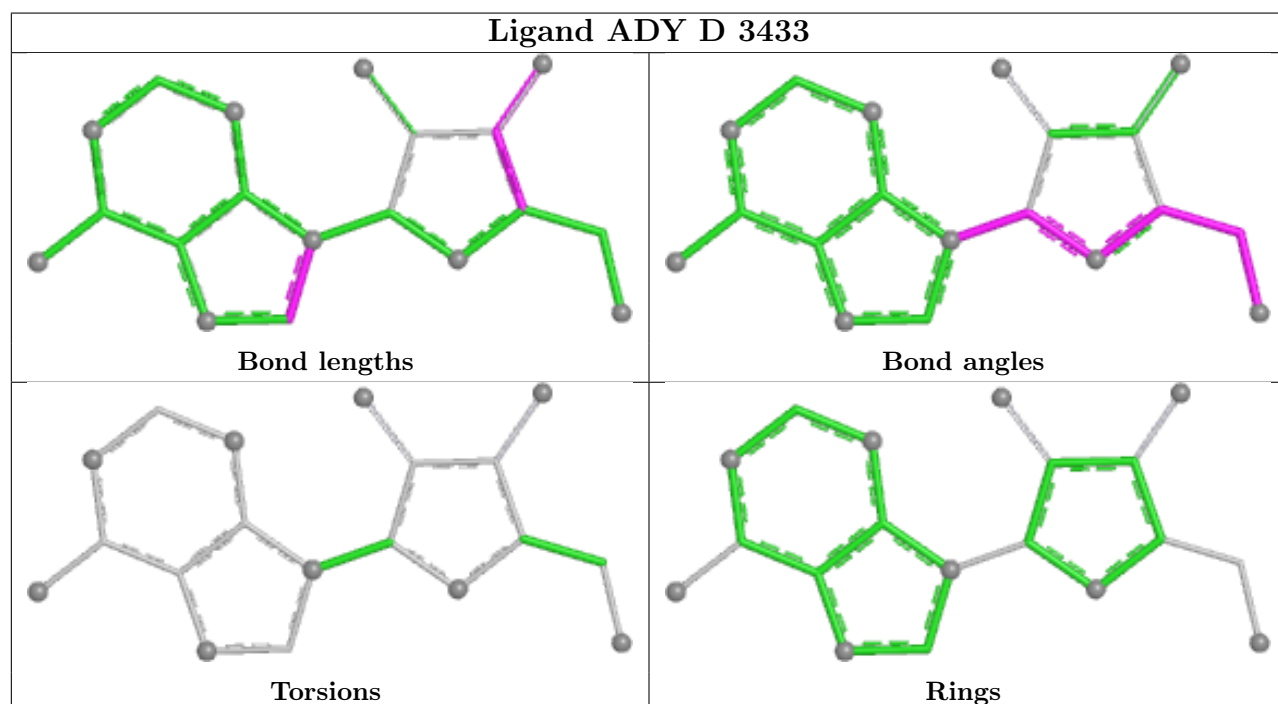


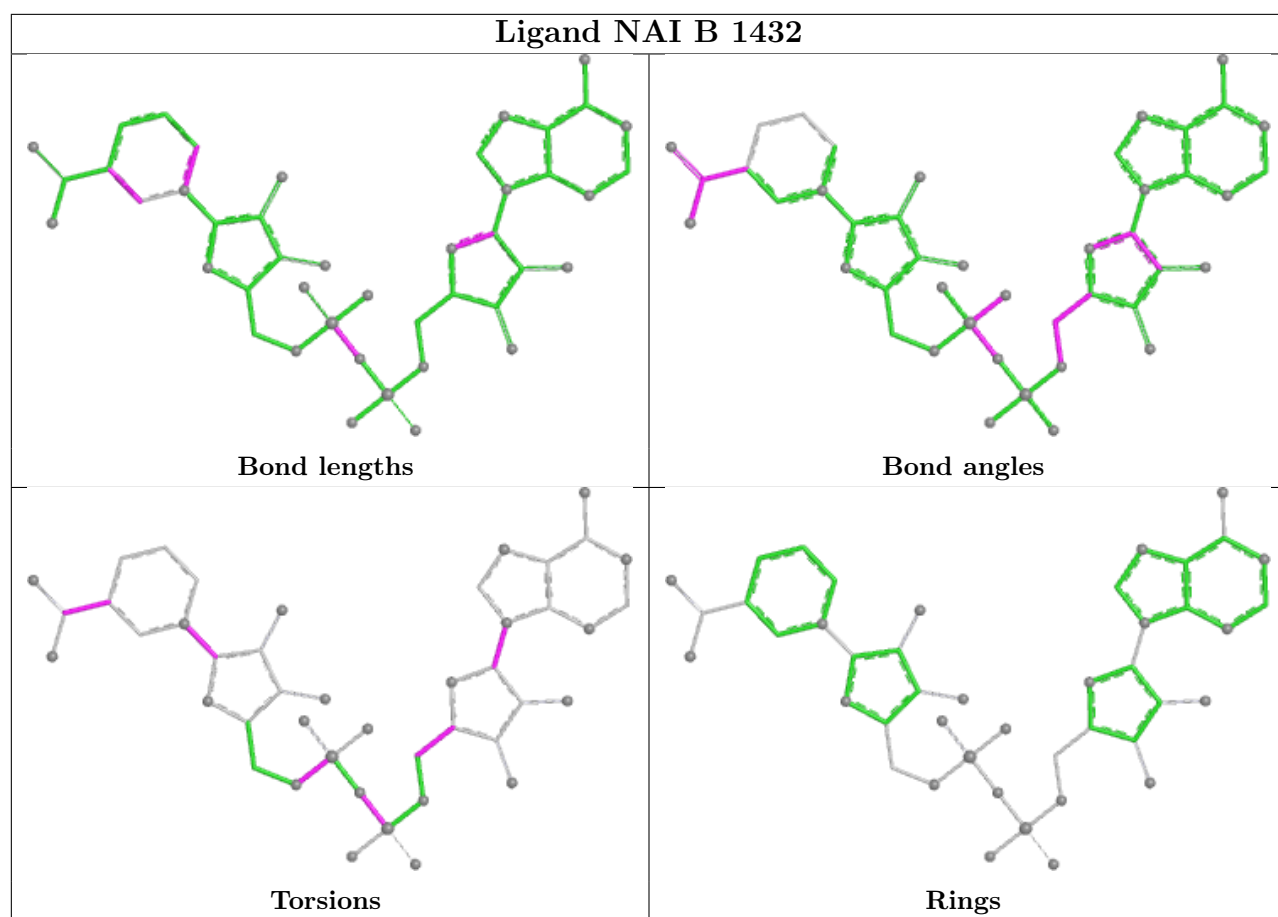


Ligand ADY B 1433



Ligand ADY D 3433





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.