



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 12:13 PM EDT

PDB ID : 1EFL  
Title : HUMAN MALIC ENZYME IN A QUATERNARY COMPLEX WITH NAD,  
MG, AND TARTRONATE  
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.  
Deposited on : 2000-02-09  
Resolution : 2.60 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

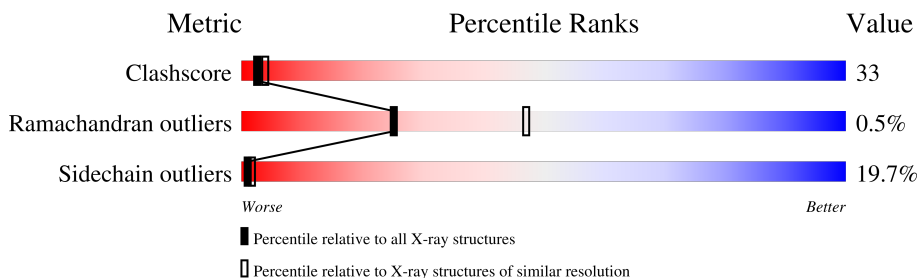
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (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 of 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	584	
1	B	584	
1	C	584	
1	D	584	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17947 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	29	MSE	MET	modified residue	UNP P23368
B	38	MSE	MET	modified residue	UNP P23368
B	47	MSE	MET	modified residue	UNP P23368
B	75	MSE	MET	modified residue	UNP P23368
B	86	MSE	MET	modified residue	UNP P23368
B	108	MSE	MET	modified residue	UNP P23368
B	177	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	modified residue	UNP P23368
B	239	MSE	MET	modified residue	UNP P23368
B	325	MSE	MET	modified residue	UNP P23368
B	327	MSE	MET	modified residue	UNP P23368
B	343	MSE	MET	modified residue	UNP P23368
B	407	MSE	MET	modified residue	UNP P23368
B	539	MSE	MET	modified residue	UNP P23368
C	29	MSE	MET	modified residue	UNP P23368
C	38	MSE	MET	modified residue	UNP P23368
C	47	MSE	MET	modified residue	UNP P23368
C	75	MSE	MET	modified residue	UNP P23368
C	86	MSE	MET	modified residue	UNP P23368
C	108	MSE	MET	modified residue	UNP P23368
C	177	MSE	MET	modified residue	UNP P23368
C	219	MSE	MET	modified residue	UNP P23368
C	239	MSE	MET	modified residue	UNP P23368
C	325	MSE	MET	modified residue	UNP P23368
C	327	MSE	MET	modified residue	UNP P23368
C	343	MSE	MET	modified residue	UNP P23368
C	407	MSE	MET	modified residue	UNP P23368
C	539	MSE	MET	modified residue	UNP P23368
D	29	MSE	MET	modified residue	UNP P23368
D	38	MSE	MET	modified residue	UNP P23368
D	47	MSE	MET	modified residue	UNP P23368
D	75	MSE	MET	modified residue	UNP P23368
D	86	MSE	MET	modified residue	UNP P23368
D	108	MSE	MET	modified residue	UNP P23368
D	177	MSE	MET	modified residue	UNP P23368
D	219	MSE	MET	modified residue	UNP P23368
D	239	MSE	MET	modified residue	UNP P23368
D	325	MSE	MET	modified residue	UNP P23368
D	327	MSE	MET	modified residue	UNP P23368
D	343	MSE	MET	modified residue	UNP P23368
D	407	MSE	MET	modified residue	UNP P23368
D	539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

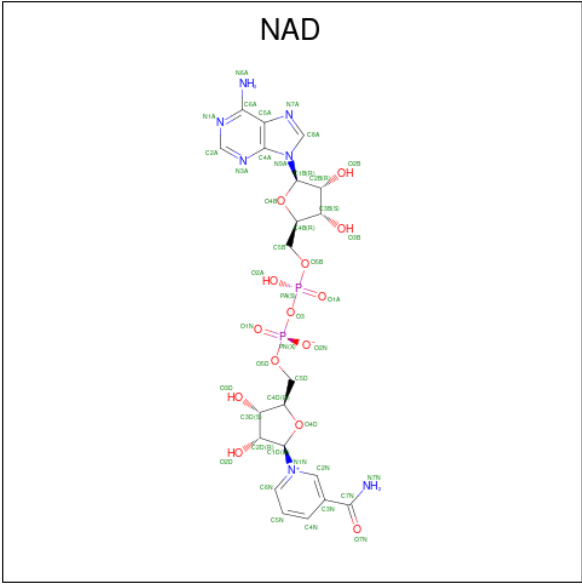
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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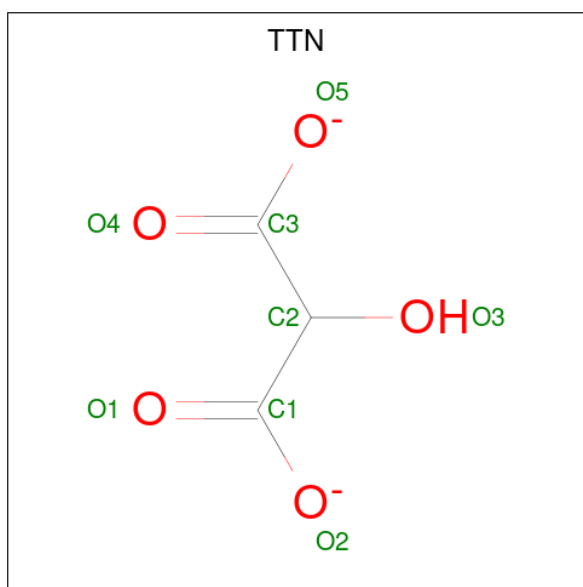
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 4 is TARTRONATE (three-letter code: TTN) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	3	5		
4	B	1	Total	C	O	0	0
			8	3	5		
4	C	1	Total	C	O	0	0
			8	3	5		
4	D	1	Total	C	O	0	0
			8	3	5		

- Molecule 5 is water.

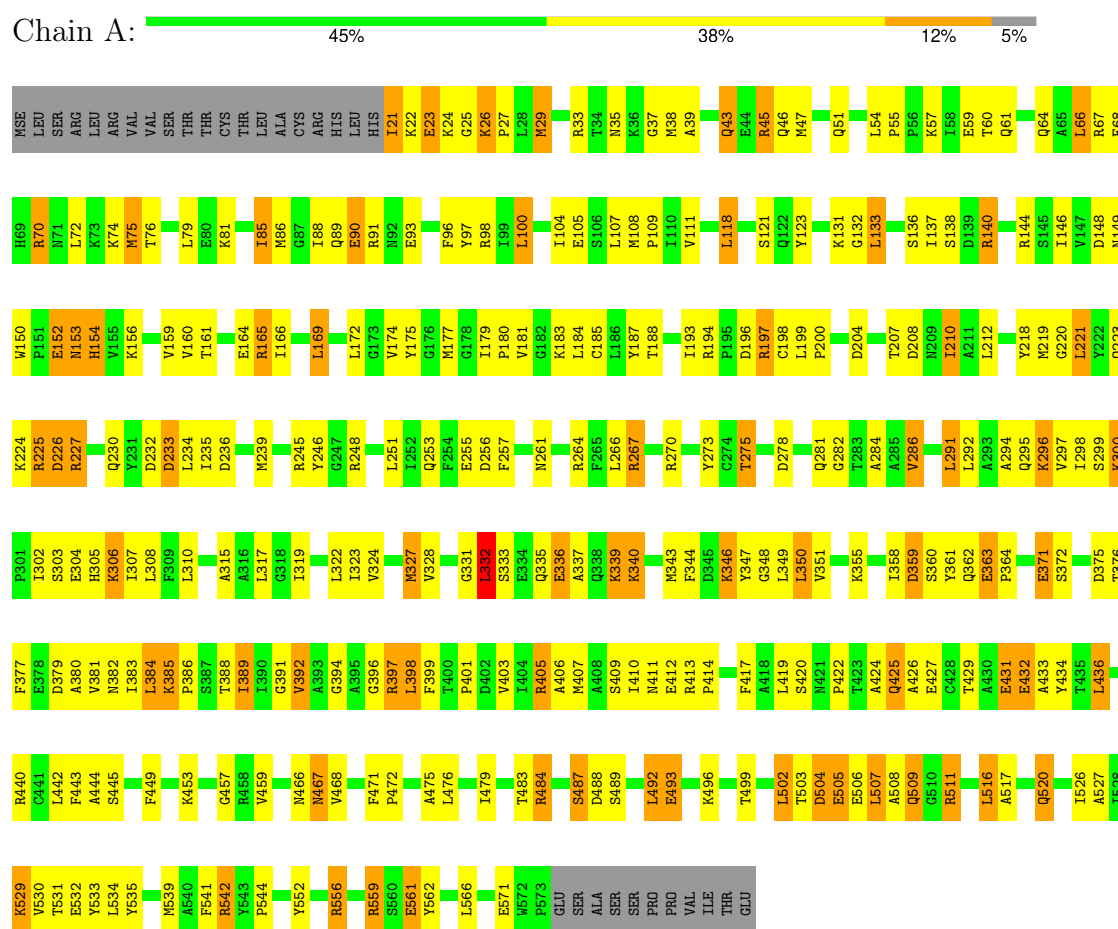
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	17	Total	O	0	0
			17	17		
5	C	23	Total	O	0	0
			23	23		
5	D	27	Total	O	0	0
			27	27		

### 3 Residue-property plots

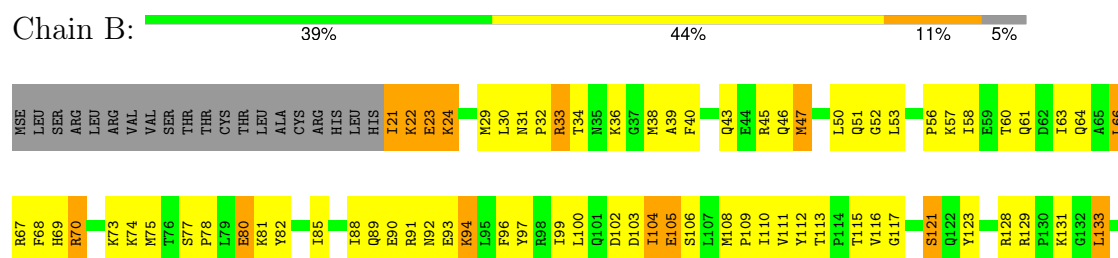
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

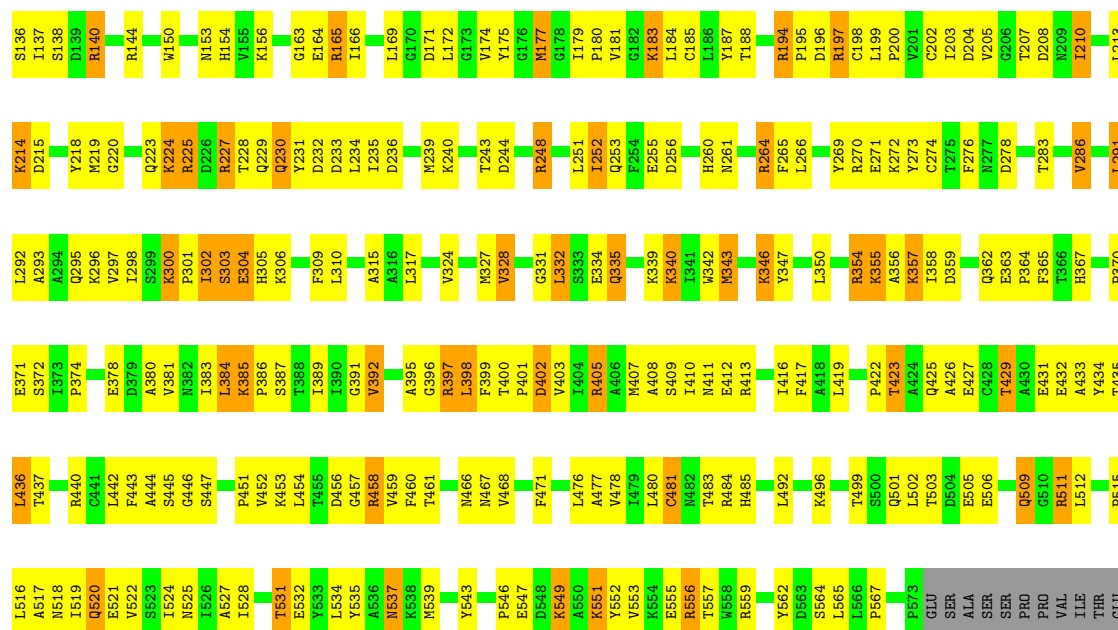
Note EDS was not executed.

#### • Molecule 1: MALIC ENZYME



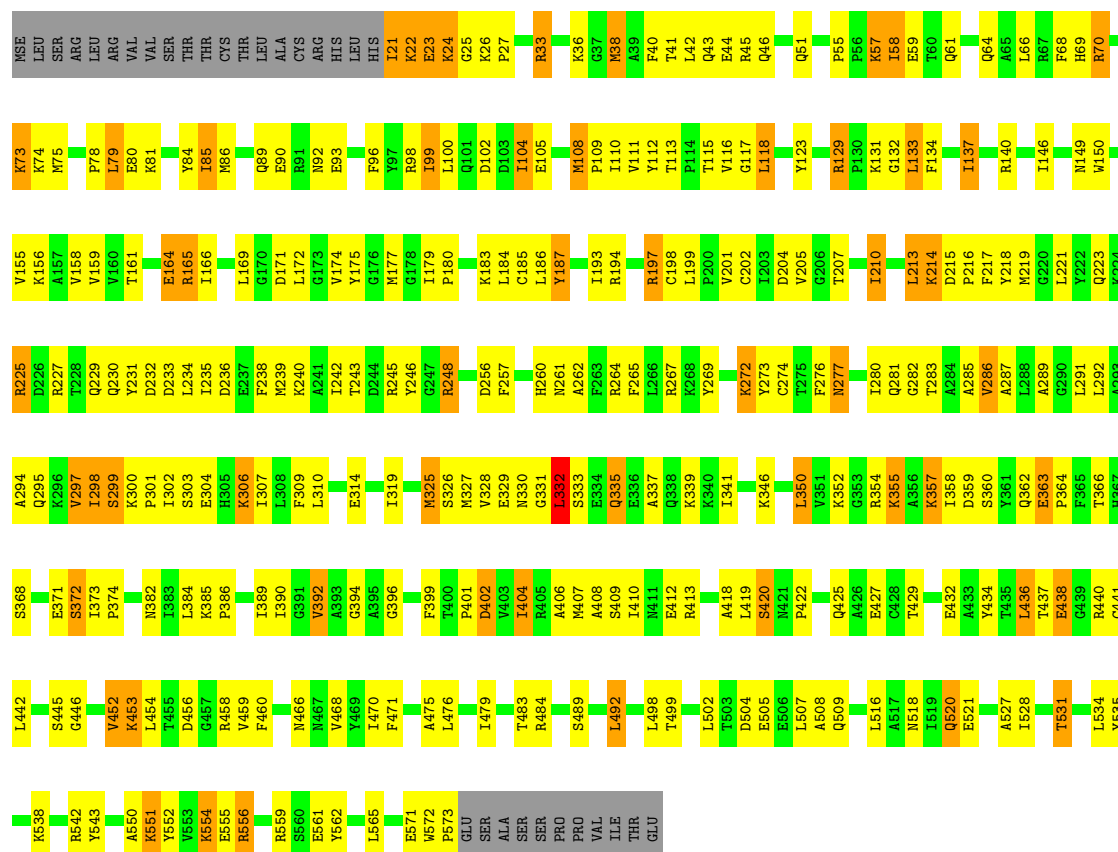
#### • Molecule 1: MALIC ENZYME





### • Molecule 1: MALIC ENZYME

Chain C:  45%  40%  10%  5%



### • Molecule 1: MALIC ENZYME



Chain D: 

HSE	L65	L221	A294	F377	G457	T531
LEU	L66	T222	Q295	E378	R458	E532
SER	R67	Q223	Q296	D379	F459	Y533
ARG	F68	K224	V297	A380	F460	L534
LEU	H69	R225	I298	V381		Y535
ARG	R70	D226	S299	N382	N466	A536
VAL	N71	R227	K300	L383	N467	N537
VAL	L72	T228	F301	L384	V468	A540
SER	K73	Q229	I302	K385	V469	F541
THR	K74	E152	S303	P386	L470	R542
THR	M75	Q230	E304	S387	F471	Y543
CYS	T76	D233	H305	T388	P472	Y544
THR	S77	L234	K306	L389	A475	P544
LEU	P78	I235	I307	L390	L476	E545
ALA	L79	D236	L308	G391	A477	D548
CYS	R81	E237	F309	V392	V478	K549
ARG	Y82	F238	L310	A393	L479	A550
HIS	I83	M239	E314	G394	L480	K551
LEU	I84	K240	A315		C481	
HIS	I85	L241	A316	R397	N482	R554
I21	I86	T242	I319	L398	T483	E555
K22	M86	T243	I319	F399	R484	R556
E23		D244		T400		
K24	R91	R245	V324	P401	H485	
G25	R92	Y246		D402	L486	R559
K26	E93		K327	V403		S560
P27	F94	T249	V328	L404	S489	E561
L28	L95	T250		R405		Y562
M29	F96	L251	G331	A406	L492	D563
L30	Y97	L252	G331	M407		S564
N31	R98	Q253	S333	A408	K496	L565
P32	I99	D256	E334	S409	L497	L566
R33	L100		E335	L410	L498	
T34	Q101		Q336	N411	T499	
N35		N261	E337	R413	S500	M572
K36	I104	A262	A337	P414	Q501	P573
G37		F263		P415	L502	GLU
K38	L107	R264	K342	V416	T503	SER
A39	M108	F265	K343	F417	D504	ALA
	P109	L266			E505	SER
Q43	I110	K267	K346		E506	SER
E44	V111	Y269	Y347	S420	L507	PRO
R45	Y112	R270	L350	T423	A508	VAL
Q46	T115	E271	K355	E427	Q509	THR
M47	H125	K272	A356		G510	GLU
Q51	R128	D208	K357	E432	R511	
L53	K131	N209	T275		P515	
L54	G132	I210	F276	L436	A517	
P55	L133	A211	A285	T437	N518	
P56	S136	L212	V286		I519	
I58	I137	L213	A287	R440	E520	
E59	S138	D215	K214	C441	E521	
T60	I137	P216	L288	L442		
Q61	D139	F217	A289	F443		
D62	R140	Y218	G290	S447		
T63		L292	L291			
Q64		G220	A293	D456		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.80Å 117.00Å 114.30Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.206 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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: MG, NAD, TTN

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	0.46	0/4447	0.65	0/5998
1	B	0.46	0/4447	0.66	0/5998
1	C	0.45	0/4447	0.65	1/5998 (0.0%)
1	D	0.46	0/4447	0.65	0/5998
All	All	0.46	0/17788	0.65	1/23992 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	LEU	N-CA-C	-5.09	97.27	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	4367	0	4407	333	0
1	B	4367	0	4407	331	0
1	C	4367	0	4407	252	0
1	D	4367	0	4407	314	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	88	0	52	6	0
3	B	88	0	52	2	0
3	C	88	0	52	5	0
3	D	88	0	52	4	0
4	A	8	0	1	0	0
4	B	8	0	1	1	0
4	C	8	0	1	2	0
4	D	8	0	2	1	0
5	A	24	0	0	5	0
5	B	17	0	0	9	0
5	C	23	0	0	5	0
5	D	27	0	0	3	0
All	All	17947	0	17841	1185	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 33.

The worst 5 of 1185 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:227:ARG:HH11	1:A:227:ARG:HG2	1.03	1.11
1:D:520:GLN:HE22	1:D:521:GLU:HG2	1.13	1.07
1:A:511:ARG:HH11	1:A:511:ARG:HB3	1.20	1.02
1:C:355:LYS:HA	1:C:355:LYS:HE2	1.42	1.01
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.24	1.00

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	551/584 (94%)	516 (94%)	33 (6%)	2 (0%)	30	52
1	B	551/584 (94%)	513 (93%)	35 (6%)	3 (0%)	25	47
1	C	551/584 (94%)	525 (95%)	23 (4%)	3 (0%)	25	47
1	D	551/584 (94%)	515 (94%)	32 (6%)	4 (1%)	19	38
All	All	2204/2336 (94%)	2069 (94%)	123 (6%)	12 (0%)	25	47

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	LEU
1	C	332	LEU
1	C	392	VAL
1	A	332	LEU
1	D	270	ARG

### 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	469/483 (97%)	371 (79%)	98 (21%)	1	1
1	B	469/483 (97%)	373 (80%)	96 (20%)	1	1
1	C	469/483 (97%)	379 (81%)	90 (19%)	1	2
1	D	469/483 (97%)	384 (82%)	85 (18%)	1	2
All	All	1876/1932 (97%)	1507 (80%)	369 (20%)	1	2

5 of 369 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	232	ASP
1	D	24	LYS
1	C	277	ASN
1	C	404	ILE
1	D	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	GLN
1	C	425	GLN
1	D	485	HIS
1	C	230	GLN
1	C	321	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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$
3	NAD	B	1601	-	42,48,48	1.99	10 (23%)	50,73,73	1.64	8 (16%)
3	NAD	D	3601	-	42,48,48	2.11	9 (21%)	50,73,73	1.62	7 (14%)
4	TTN	B	1603	2	5,7,7	1.40	1 (20%)	3,9,9	1.64	1 (33%)
3	NAD	B	1602	-	42,48,48	2.29	12 (28%)	50,73,73	1.41	5 (10%)
3	NAD	C	2602	-	42,48,48	2.65	13 (30%)	50,73,73	1.43	5 (10%)
4	TTN	D	3603	2	5,7,7	1.39	1 (20%)	3,9,9	1.65	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TTN	C	2603	2	5,7,7	1.43	2 (40%)	3,9,9	1.78	1 (33%)
3	NAD	A	601	-	42,48,48	1.97	10 (23%)	50,73,73	1.64	7 (14%)
3	NAD	C	2601	-	42,48,48	2.02	10 (23%)	50,73,73	1.62	6 (12%)
3	NAD	D	3602	-	42,48,48	2.41	11 (26%)	50,73,73	1.49	6 (12%)
4	TTN	A	603	2	5,7,7	1.40	1 (20%)	3,9,9	1.69	1 (33%)
3	NAD	A	602	-	42,48,48	2.33	10 (23%)	50,73,73	1.48	5 (10%)

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
3	NAD	B	1601	-	-	3/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	2/26/62/62	0/5/5/5
4	TTN	B	1603	2	-	2/8/8/8	-
3	NAD	B	1602	-	-	11/26/62/62	0/5/5/5
3	NAD	C	2602	-	-	9/26/62/62	0/5/5/5
4	TTN	D	3603	2	-	4/8/8/8	-
4	TTN	C	2603	2	-	2/8/8/8	-
3	NAD	A	601	-	-	2/26/62/62	0/5/5/5
3	NAD	C	2601	-	-	2/26/62/62	0/5/5/5
3	NAD	D	3602	-	-	11/26/62/62	0/5/5/5
4	TTN	A	603	2	-	2/8/8/8	-
3	NAD	A	602	-	-	11/26/62/62	0/5/5/5

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3602	NAD	C2N-N1N	8.38	1.44	1.35
3	C	2602	NAD	C2N-N1N	8.31	1.44	1.35
3	B	1602	NAD	C2N-N1N	8.18	1.44	1.35
3	A	602	NAD	C2N-N1N	8.13	1.43	1.35
3	C	2602	NAD	O4D-C1D	7.37	1.50	1.40

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2601	NAD	N3A-C2A-N1A	-6.15	120.32	128.67
3	A	602	NAD	N3A-C2A-N1A	-5.97	120.57	128.67
3	A	601	NAD	N3A-C2A-N1A	-5.92	120.64	128.67
3	B	1601	NAD	N3A-C2A-N1A	-5.84	120.75	128.67
3	D	3601	NAD	N3A-C2A-N1A	-5.82	120.78	128.67

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAD	O4D-C1D-N1N-C6N
3	A	602	NAD	C5B-O5B-PA-O1A
3	A	602	NAD	C5B-O5B-PA-O3
3	A	602	NAD	PA-O3-PN-O5D
3	A	602	NAD	C5D-O5D-PN-O3

There are no ring outliers.

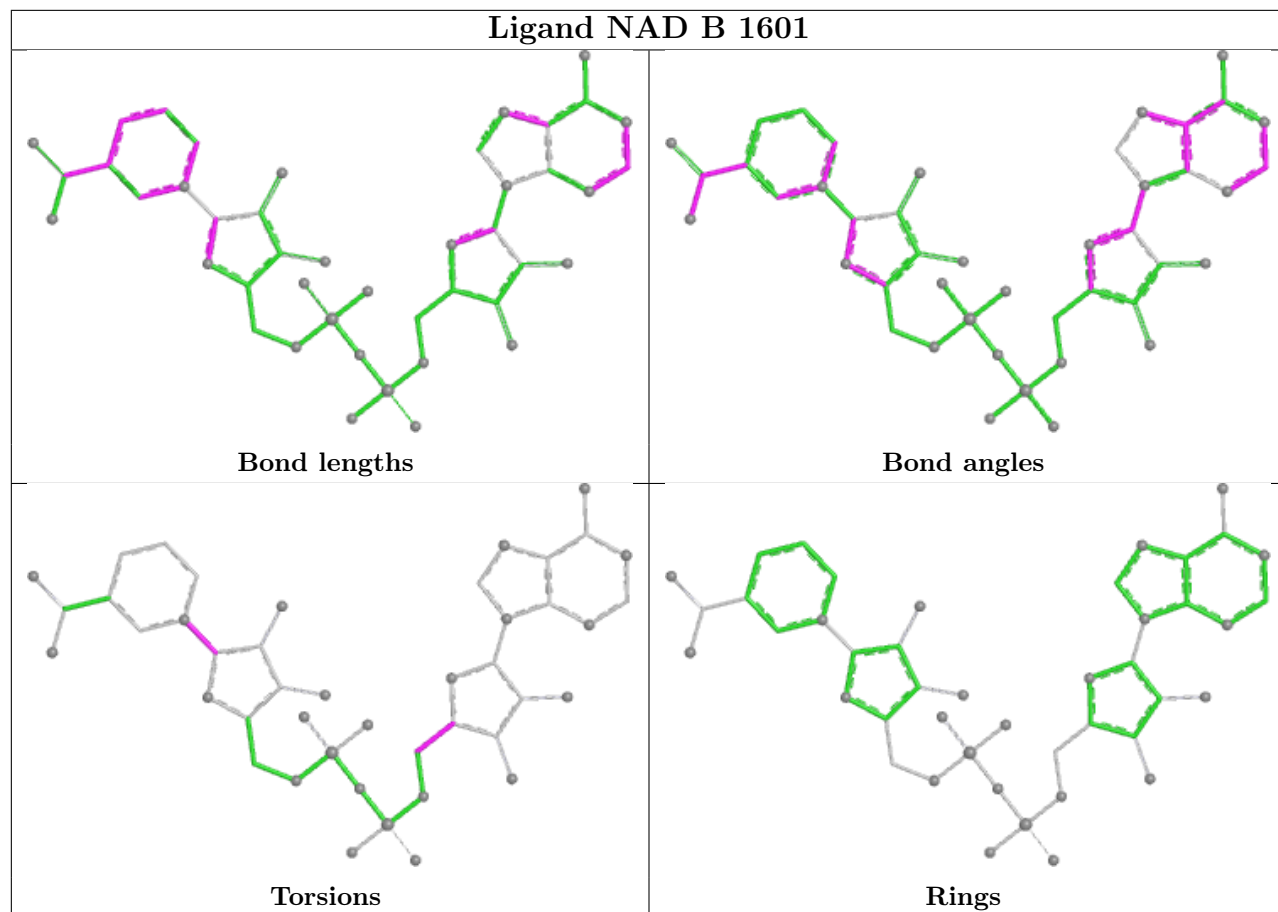
11 monomers are involved in 21 short contacts:

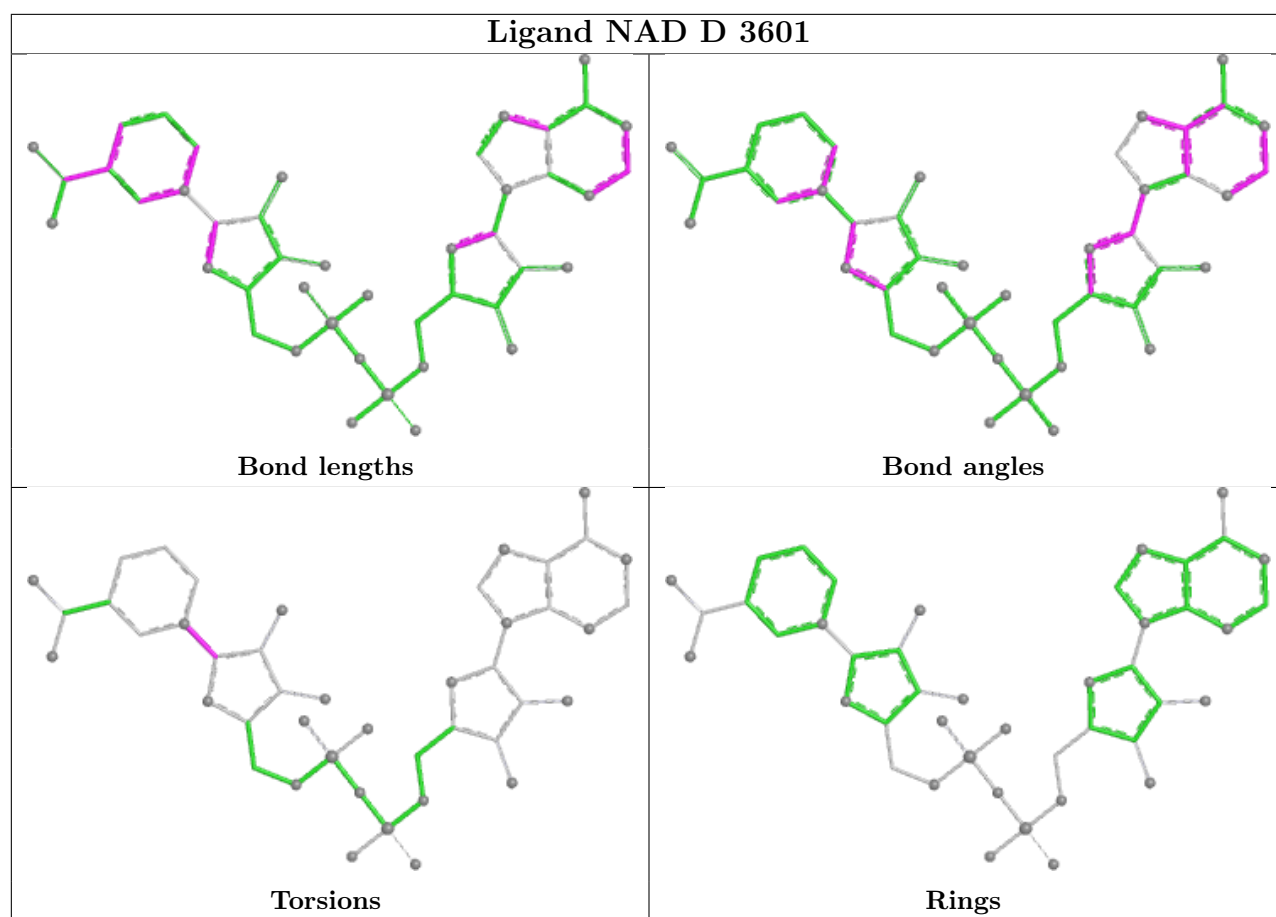
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1601	NAD	1	0
3	D	3601	NAD	1	0
4	B	1603	TTN	1	0
3	B	1602	NAD	1	0
3	C	2602	NAD	1	0
4	D	3603	TTN	1	0
4	C	2603	TTN	2	0
3	A	601	NAD	4	0
3	C	2601	NAD	4	0
3	D	3602	NAD	3	0
3	A	602	NAD	2	0

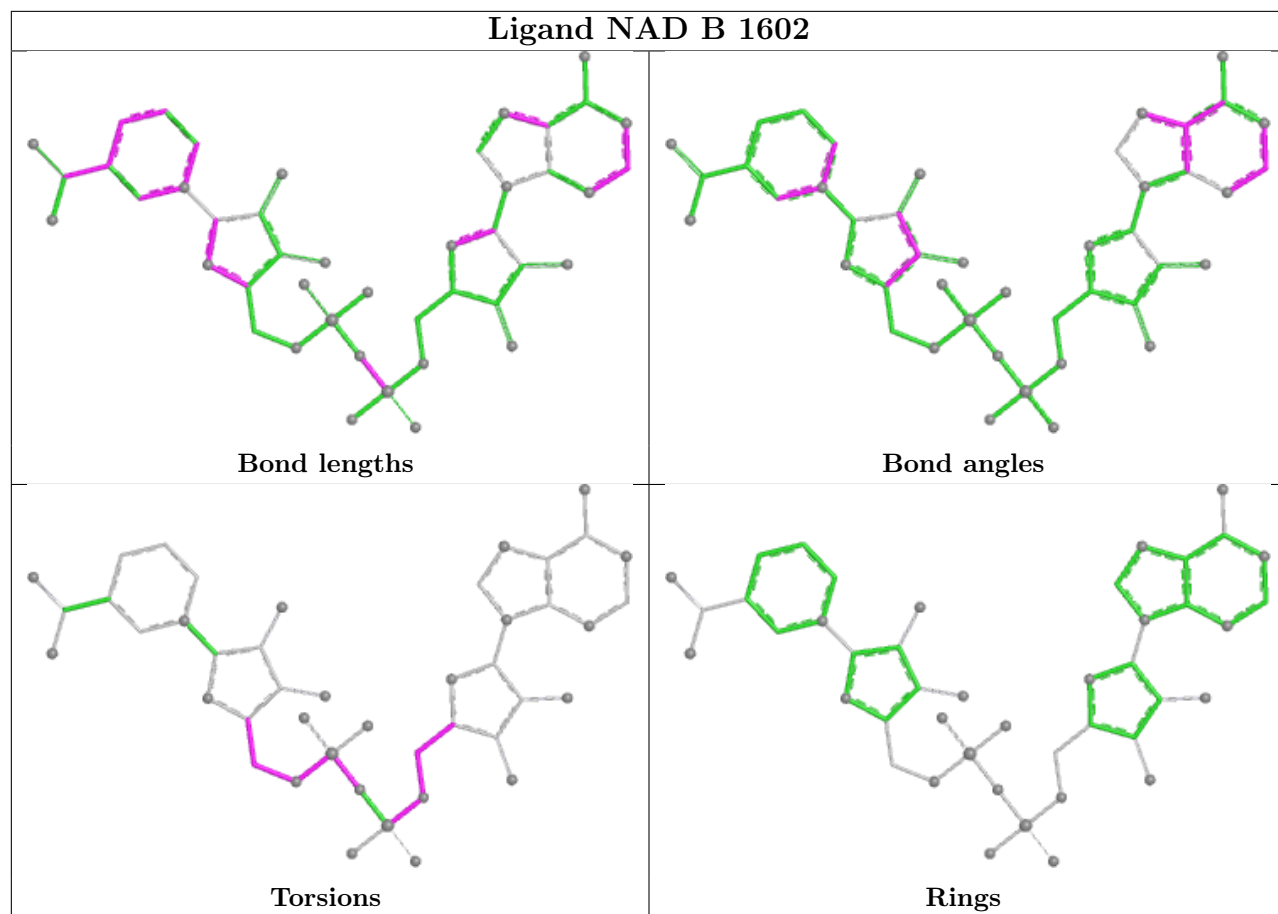
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

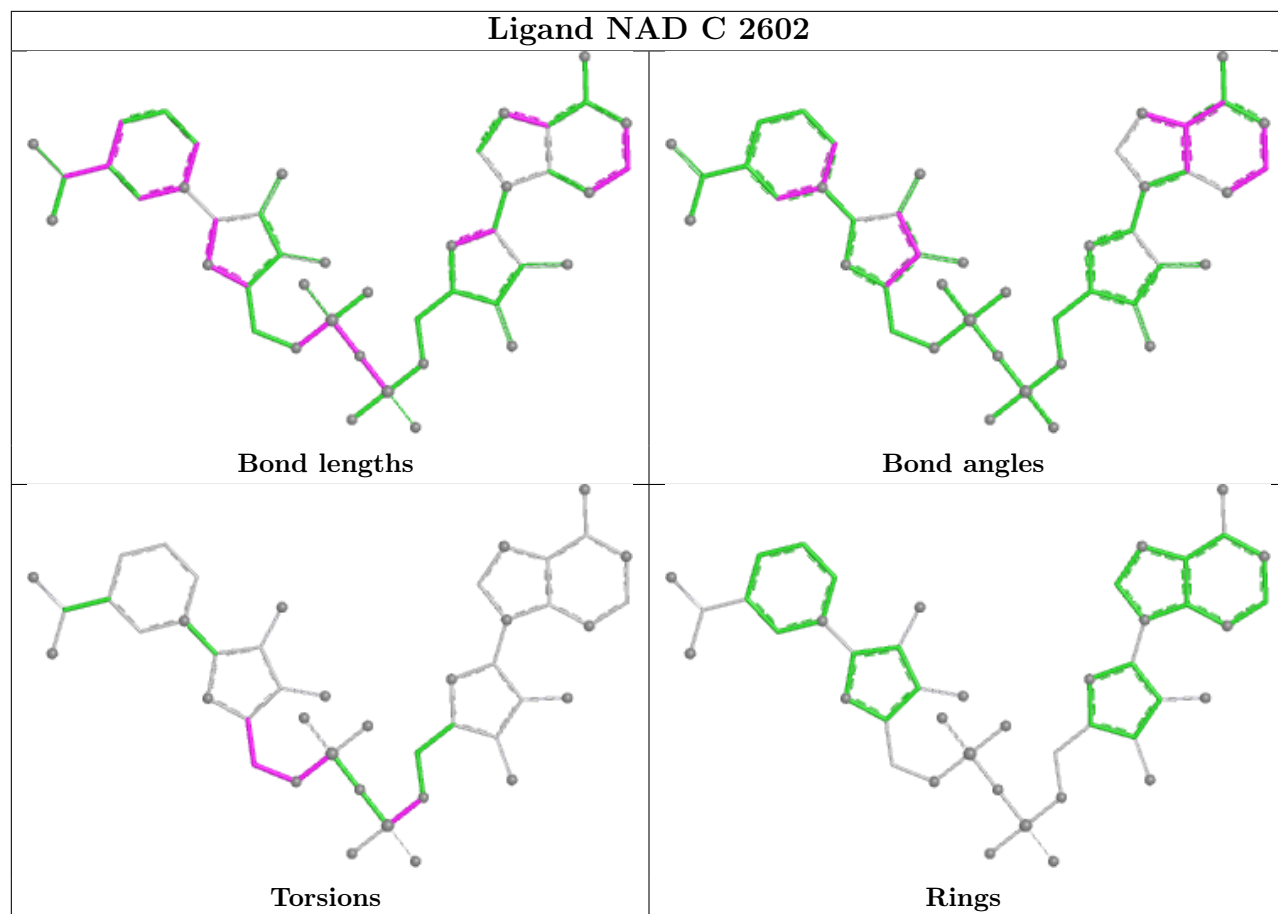


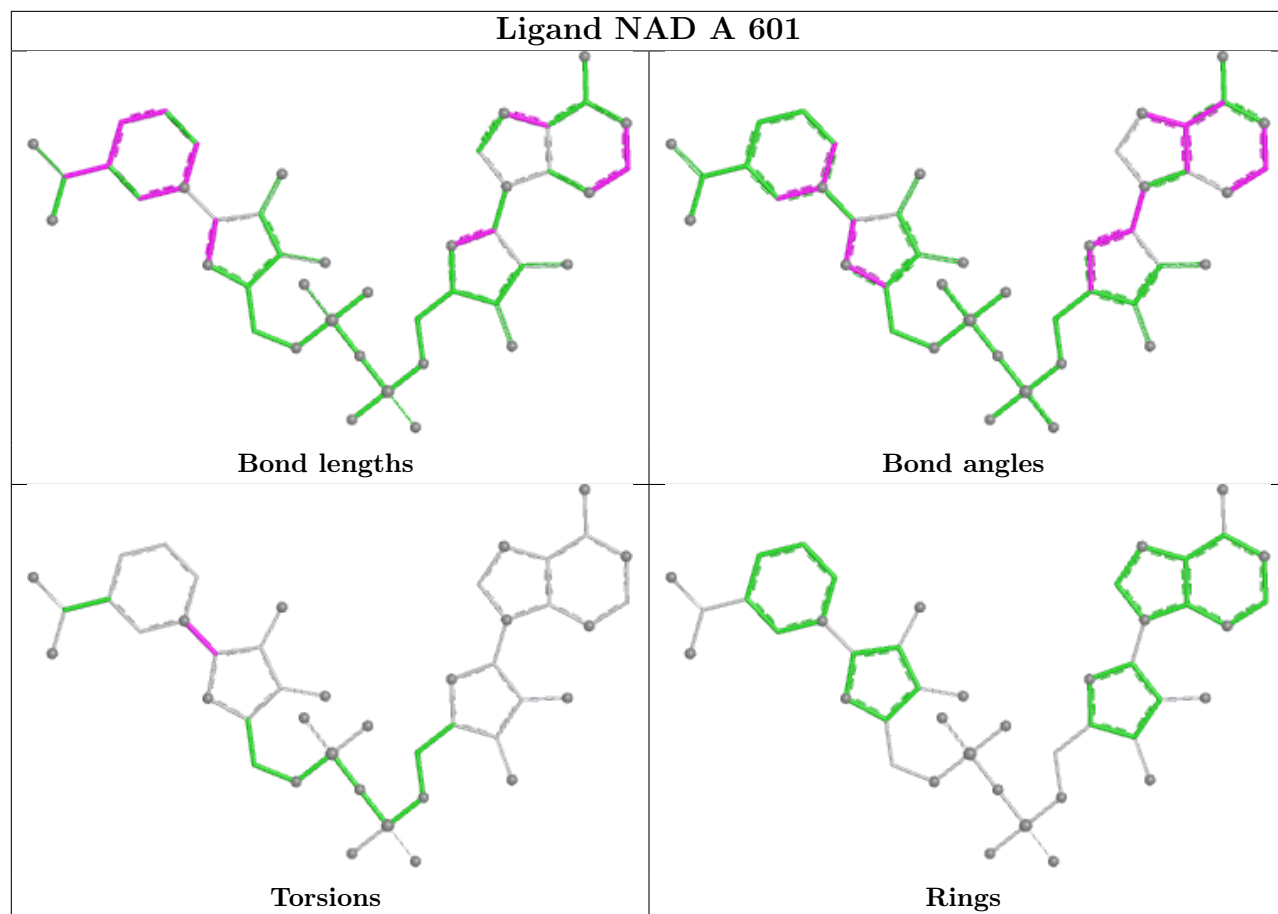
equivalents in the CSD to analyse the geometry.

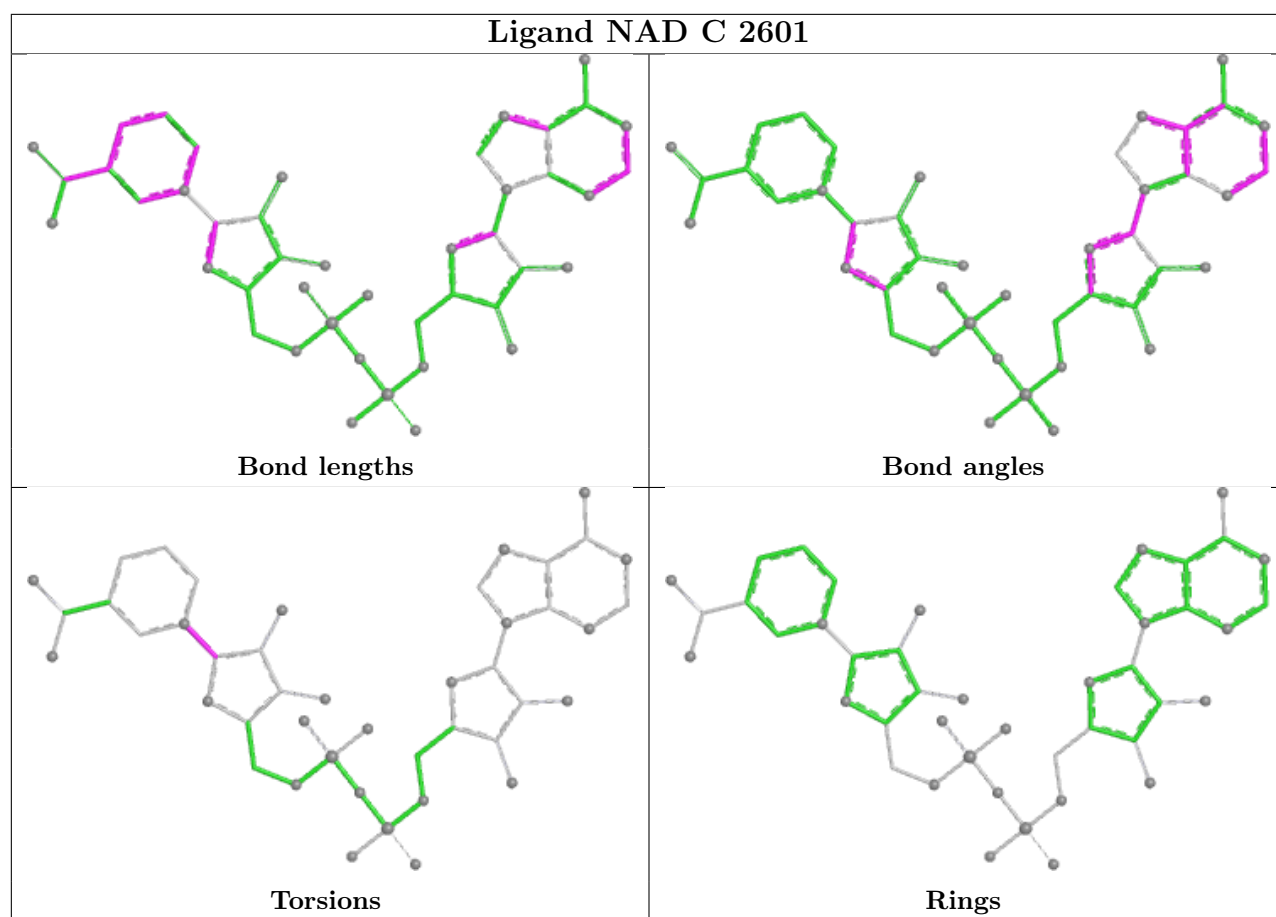


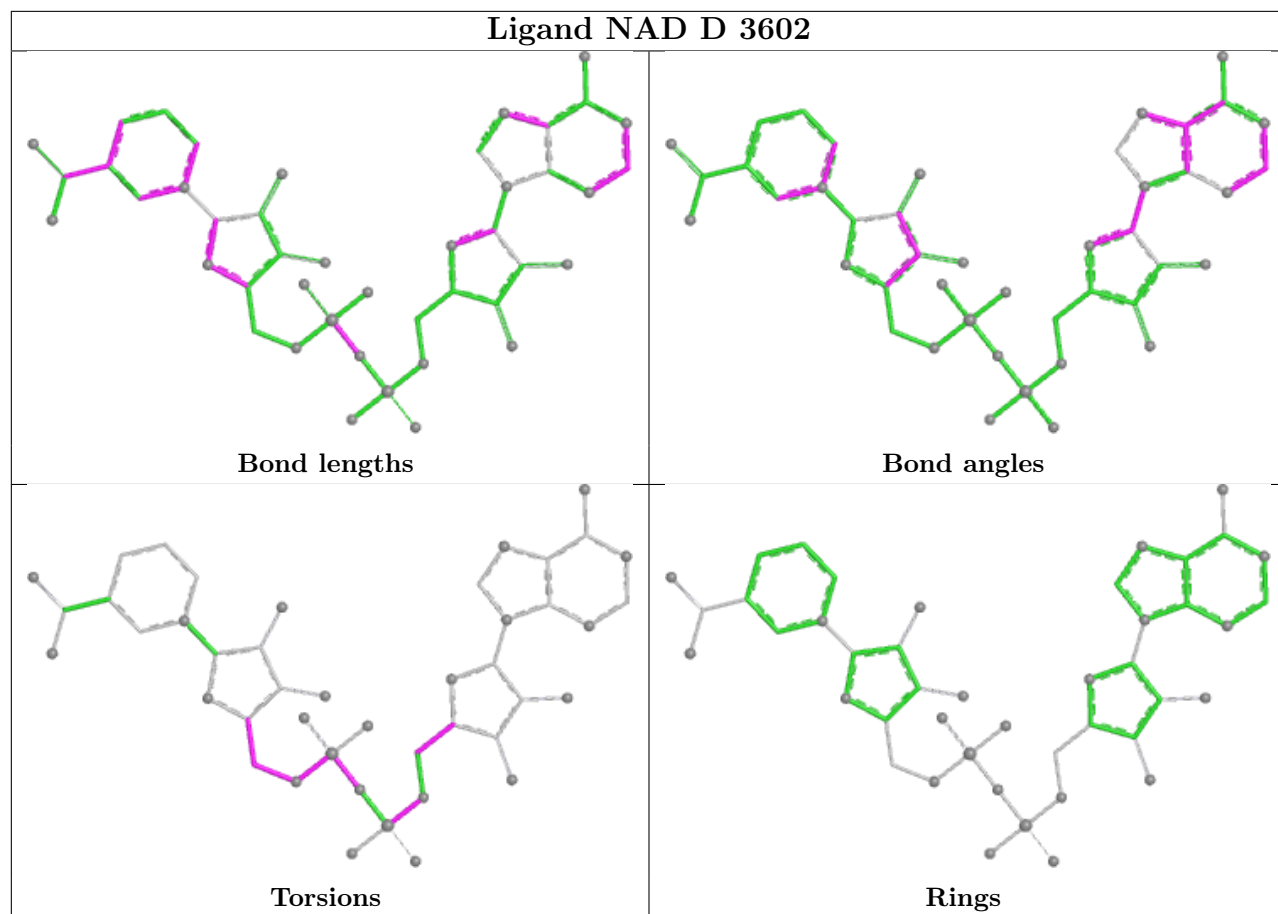


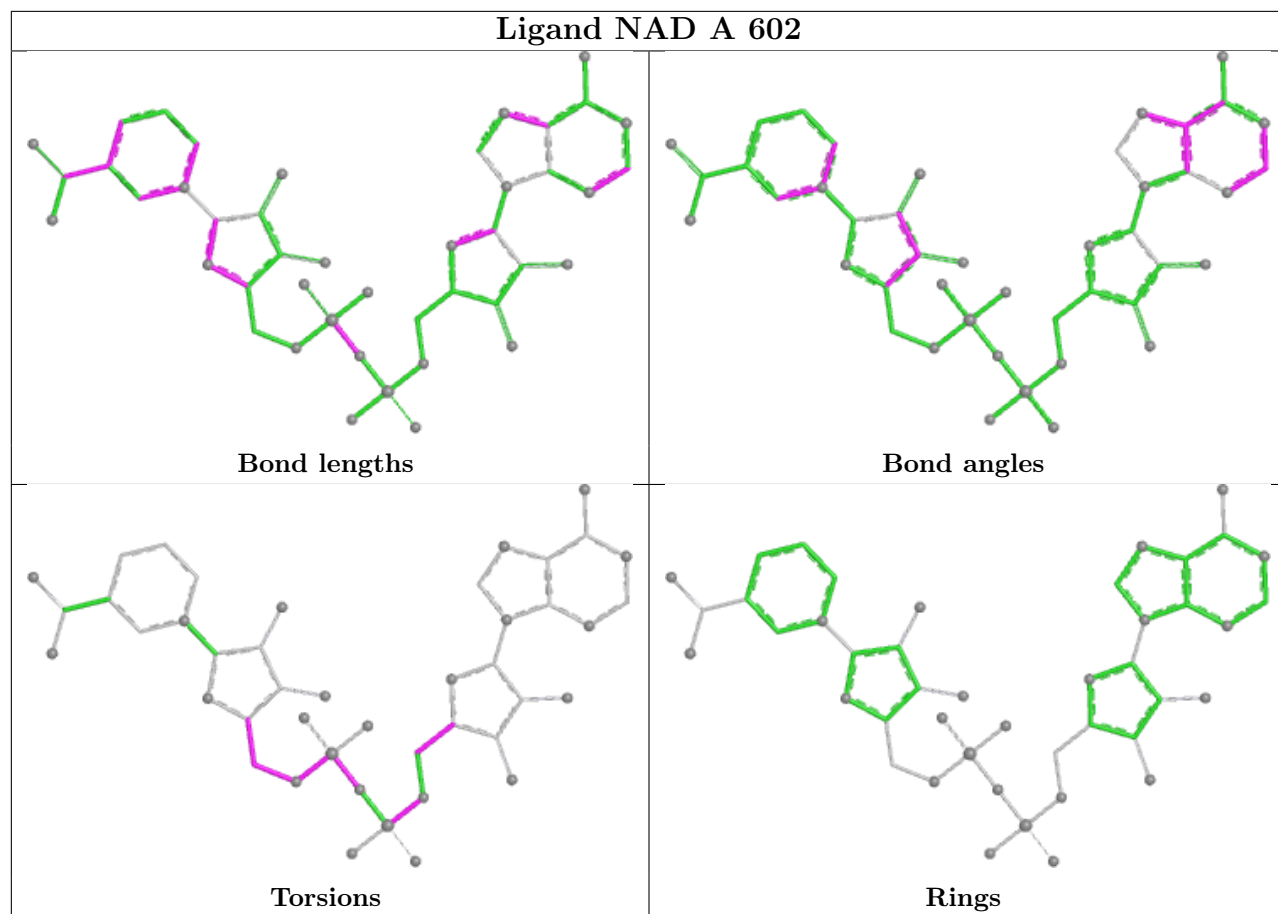












## 5.7 Other polymers [i](#)

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.