



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2023 – 10:35 AM EDT

PDB ID : 1LLU  
Title : THE TERNARY COMPLEX OF PSEUDOMONAS AERUGINOSA ALCOHOL DEHYDROGENASE WITH ITS COENZYME AND WEAK SUBSTRATE  
Authors : Levin, I.; Meiri, G.; Peretz, M.; Frolow, F.; Burstein, Y.  
Deposited on : 2002-04-30  
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

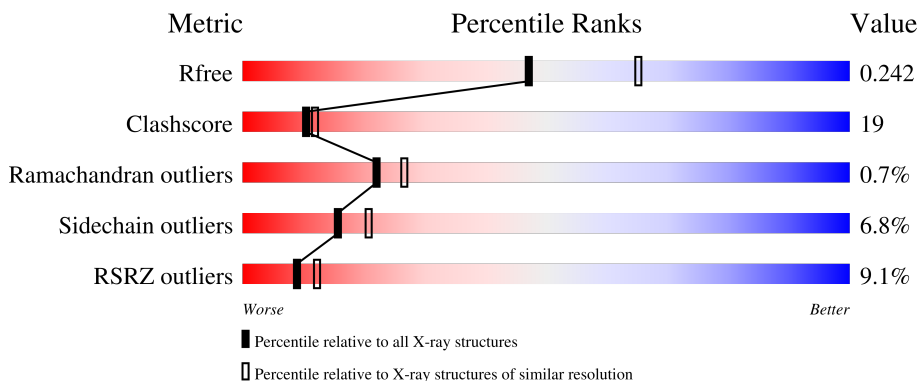
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


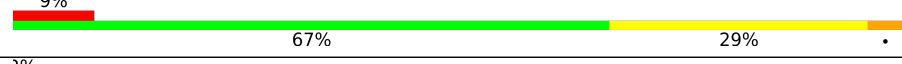


The reported resolution of this entry is 2.30 Å.

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.



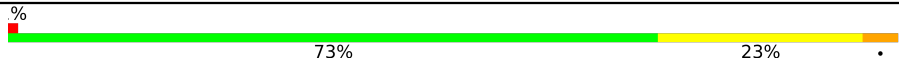


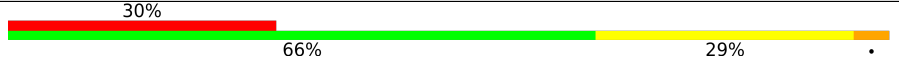
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\leq 5\%$ . 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	342	
1	B	342	
1	C	342	
1	D	342	

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Mol	Chain	Length	Quality of chain
1	E	342	 <p>% 73% 23% .</p>
1	F	342	 <p>10% 65% 30% .</p>
1	G	342	 <p>% 73% 23% .</p>
1	H	342	 <p>30% 66% 29% .</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21580 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 Alcohol Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2515	1596	439	468	12	0	0	0
1	B	341	2515	1596	439	468	12	0	0	0
1	C	341	2515	1596	439	468	12	0	0	0
1	D	341	2515	1596	439	468	12	0	0	0
1	E	341	2515	1596	439	468	12	0	0	0
1	F	341	2515	1596	439	468	12	0	0	0
1	G	341	2515	1596	439	468	12	0	0	0
1	H	341	2515	1596	439	468	12	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
A	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
B	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
B	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
C	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
C	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
D	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
D	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
E	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
E	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
F	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
F	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
G	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9

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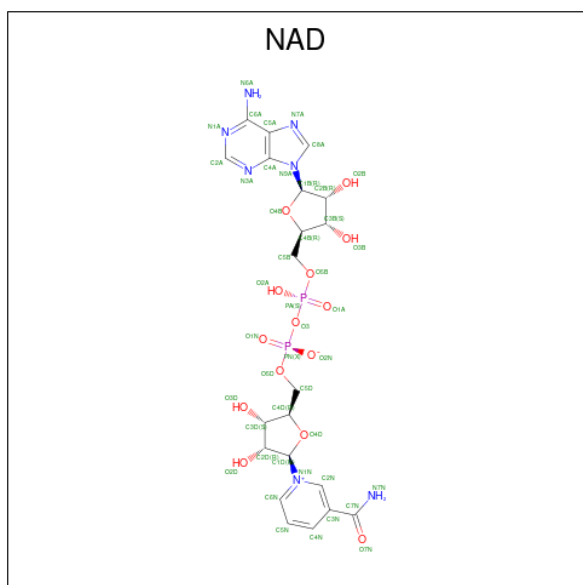
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Chain	Residue	Modelled	Actual	Comment	Reference
G	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9
H	229	ALA	VAL	SEE REMARK 999	UNP Q9HTD9
H	230	ILE	LEU	SEE REMARK 999	UNP Q9HTD9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

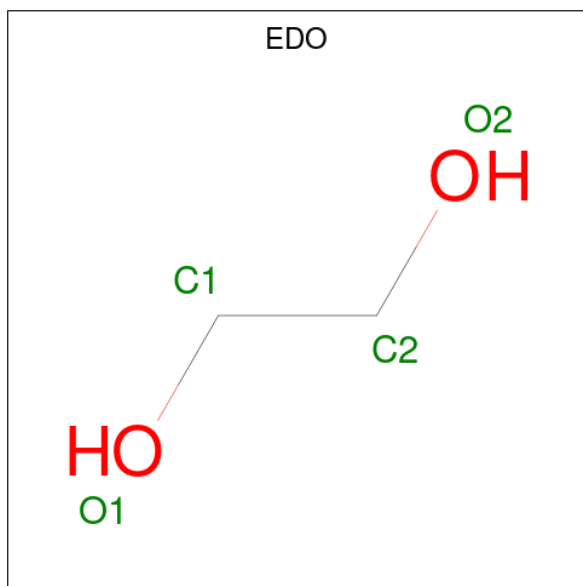
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

- 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
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
3	B	1	44	21	7	14	2	0	0
3	C	1	44	21	7	14	2	0	0
3	D	1	44	21	7	14	2	0	0
3	E	1	44	21	7	14	2	0	0
3	F	1	44	21	7	14	2	0	0
3	G	1	44	21	7	14	2	0	0
3	H	1	44	21	7	14	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	C	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

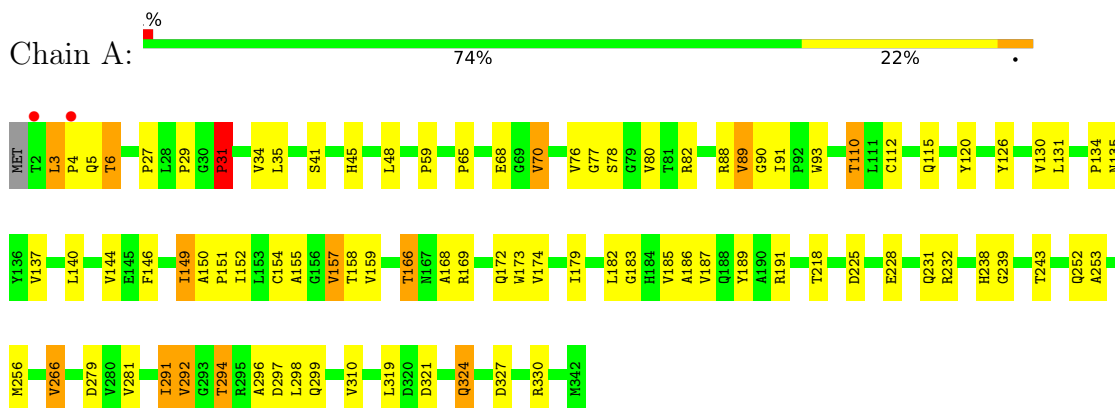
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	173	Total O 173 173	0	0
5	B	88	Total O 88 88	0	0
5	C	173	Total O 173 173	0	0
5	D	88	Total O 88 88	0	0
5	E	173	Total O 173 173	0	0
5	F	88	Total O 88 88	0	0
5	G	173	Total O 173 173	0	0
5	H	88	Total O 88 88	0	0

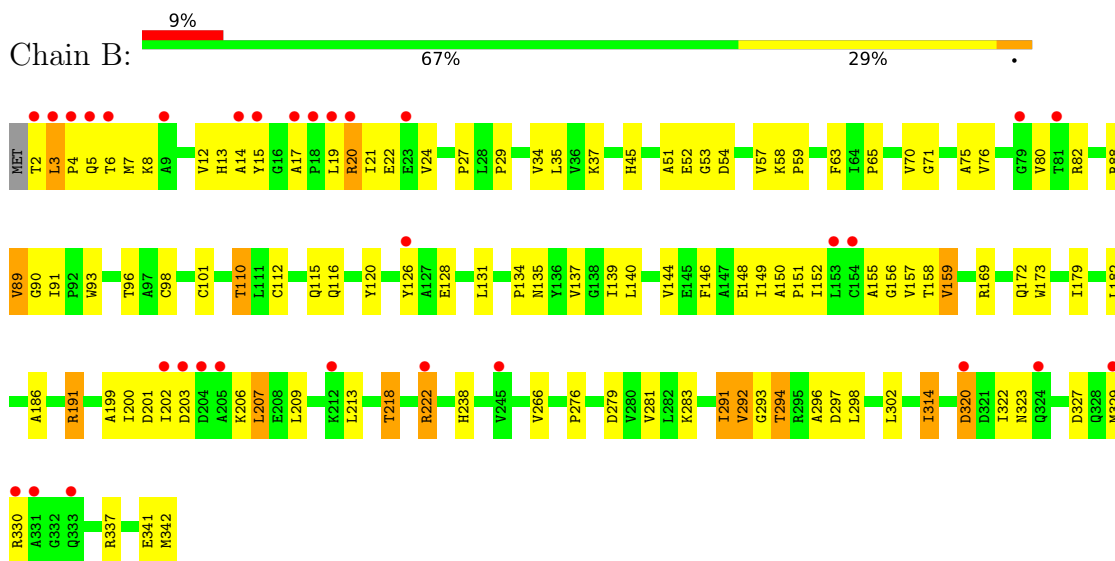
### 3 Residue-property plots [i](#)

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.

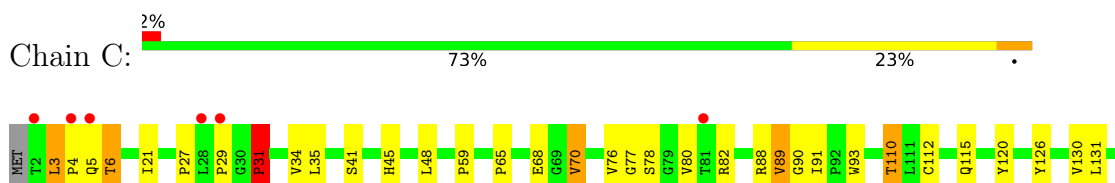
- Molecule 1: Alcohol Dehydrogenase



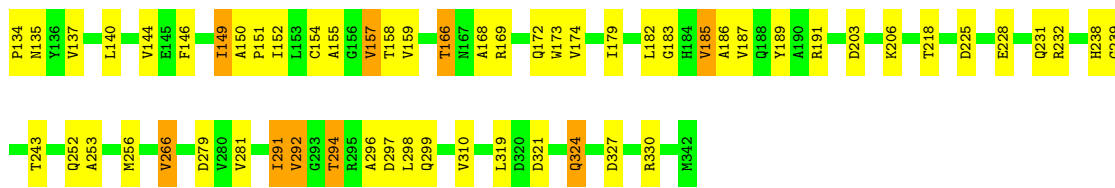
- Molecule 1: Alcohol Dehydrogenase



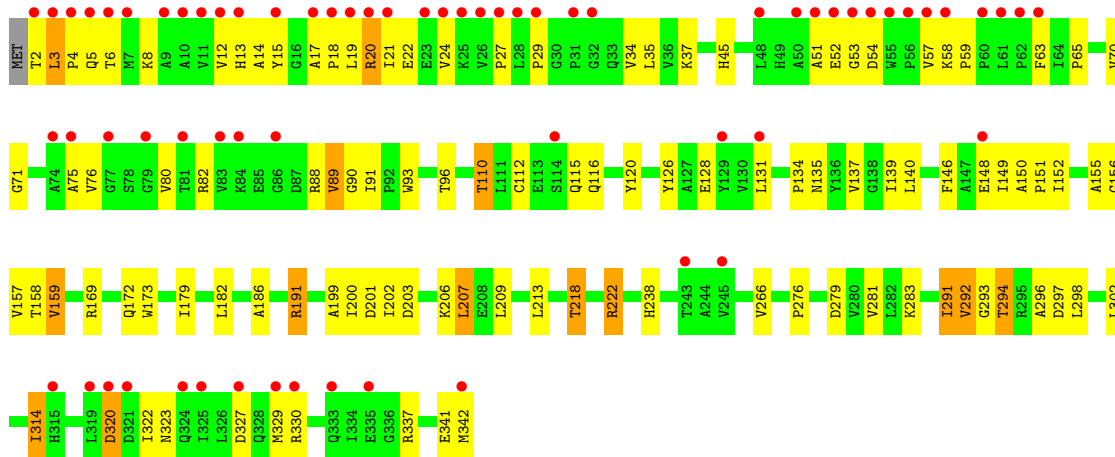
- Molecule 1: Alcohol Dehydrogenase



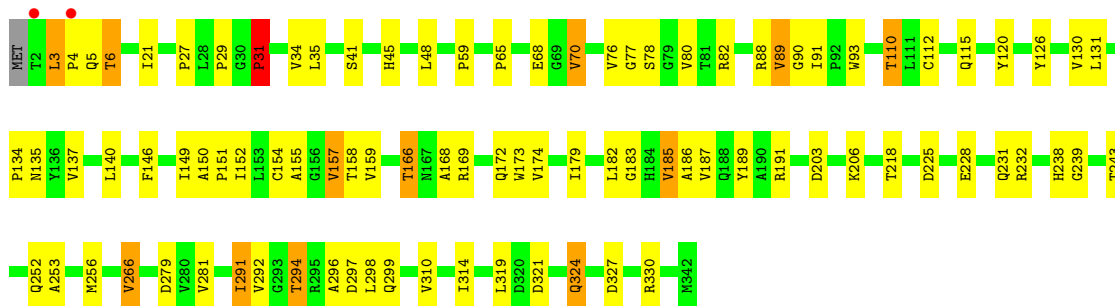
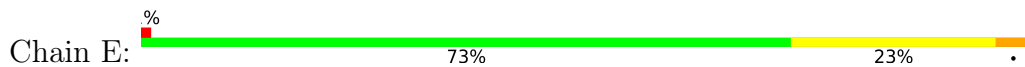




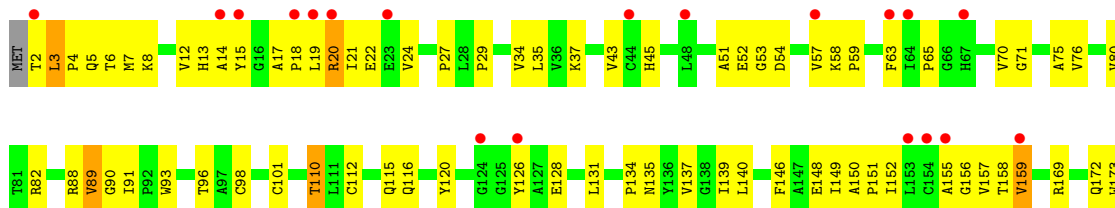
• Molecule 1: Alcohol Dehydrogenase

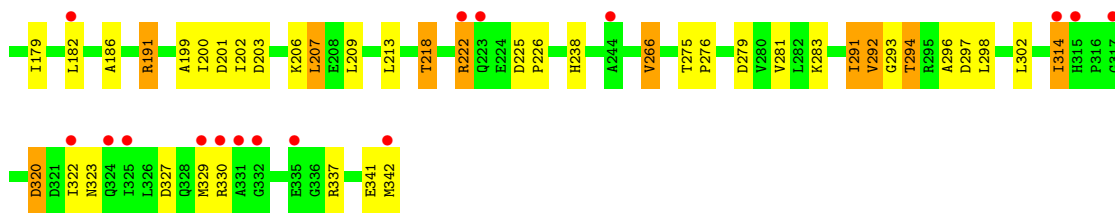


• Molecule 1: Alcohol Dehydrogenase

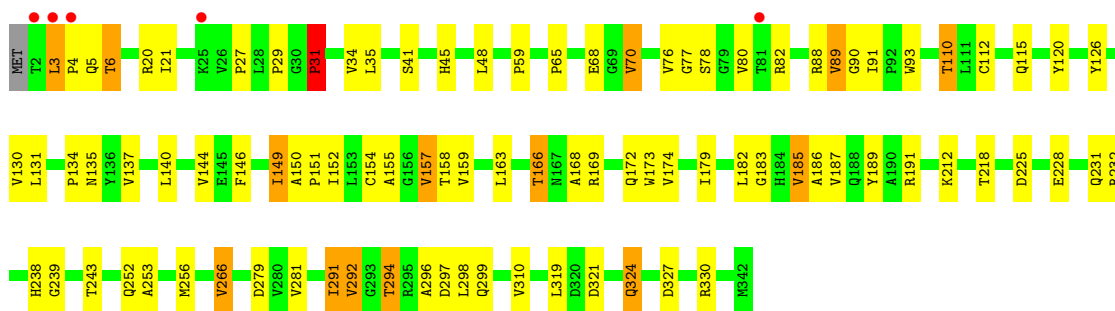
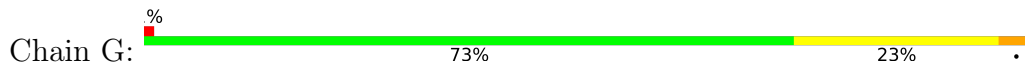


• Molecule 1: Alcohol Dehydrogenase

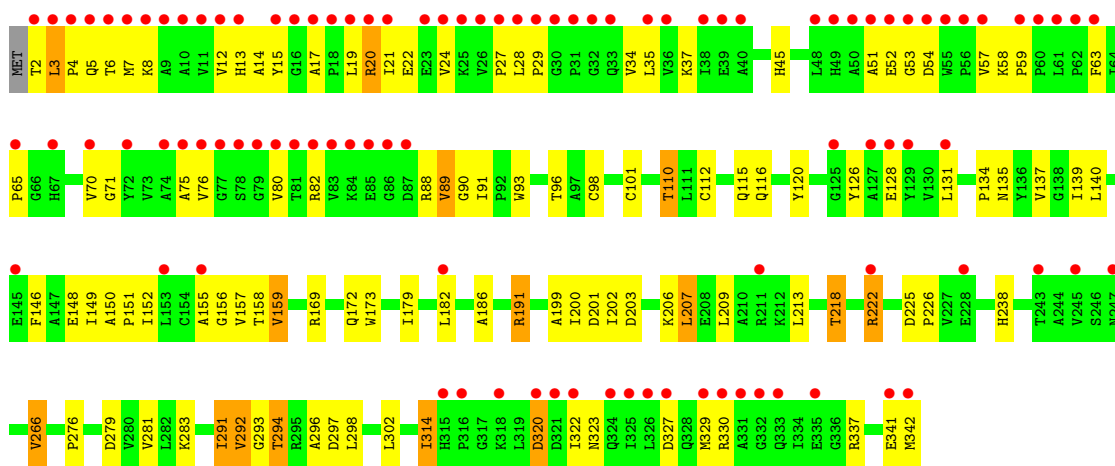




● Molecule 1: Alcohol Dehydrogenase



● Molecule 1: Alcohol Dehydrogenase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.17Å 86.33Å 125.70Å 79.34° 78.66° 71.58°	Depositor
Resolution (Å)	19.99 – 2.30 29.92 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.4 (19.99-2.30) 95.4 (29.92-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.12Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.246 0.228 , 0.242	Depositor DCC
$R_{free}$ test set	12264 reflections (7.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0768e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: EDO, NAD, ZN

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	0.40	0/2568	0.67	0/3498
1	B	0.35	0/2568	0.61	0/3498
1	C	0.40	0/2568	0.67	0/3498
1	D	0.35	0/2568	0.61	0/3498
1	E	0.40	0/2568	0.67	0/3498
1	F	0.35	0/2568	0.61	0/3498
1	G	0.40	0/2568	0.67	0/3498
1	H	0.35	0/2568	0.61	0/3498
All	All	0.37	0/20544	0.64	0/27984

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 [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	2515	0	2523	76	1
1	B	2515	0	2523	112	0
1	C	2515	0	2523	79	0
1	D	2515	0	2523	111	0
1	E	2515	0	2523	77	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2515	0	2523	118	0
1	G	2515	0	2523	80	4
1	H	2515	0	2523	117	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
3	C	44	0	26	3	0
3	D	44	0	26	1	0
3	E	44	0	26	3	0
3	F	44	0	26	1	0
3	G	44	0	26	3	0
3	H	44	0	26	1	0
4	A	8	0	11	2	0
4	B	4	0	5	1	0
4	C	8	0	11	2	0
4	D	4	0	5	1	0
4	E	8	0	11	2	0
4	F	4	0	5	1	0
4	G	8	0	11	2	0
4	H	4	0	5	1	0
5	A	173	0	0	6	11
5	B	88	0	0	2	0
5	C	173	0	0	6	12
5	D	88	0	0	2	0
5	E	173	0	0	6	14
5	F	88	0	0	2	0
5	G	173	0	0	6	11
5	H	88	0	0	2	0
All	All	21580	0	20456	762	27

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 19.

The worst 5 of 762 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:H:70:VAL:HG23	1:H:140:LEU:HD11	1.50	0.94
1:B:70:VAL:HG23	1:B:140:LEU:HD11	1.50	0.92
1:D:70:VAL:HG23	1:D:140:LEU:HD11	1.50	0.92
1:F:70:VAL:HG23	1:F:140:LEU:HD11	1.50	0.91
1:A:70:VAL:HG22	1:A:140:LEU:HD11	1.55	0.89

The worst 5 of 27 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)
5:A:1270:HOH:O	5:G:881:HOH:O[1_655]	1.05	1.15
5:C:1275:HOH:O	5:E:613:HOH:O[1_556]	1.11	1.09
1:G:212:LYS:NZ	5:E:839:HOH:O[1_455]	1.23	0.97
5:C:1318:HOH:O	5:E:640:HOH:O[1_556]	1.31	0.89
5:C:1297:HOH:O	5:E:668:HOH:O[1_556]	1.41	0.79

## 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	339/342 (99%)	323 (95%)	13 (4%)	3 (1%)	17 20
1	B	339/342 (99%)	320 (94%)	17 (5%)	2 (1%)	25 31
1	C	339/342 (99%)	323 (95%)	13 (4%)	3 (1%)	17 20
1	D	339/342 (99%)	320 (94%)	17 (5%)	2 (1%)	25 31
1	E	339/342 (99%)	323 (95%)	13 (4%)	3 (1%)	17 20
1	F	339/342 (99%)	321 (95%)	16 (5%)	2 (1%)	25 31
1	G	339/342 (99%)	323 (95%)	13 (4%)	3 (1%)	17 20
1	H	339/342 (99%)	320 (94%)	17 (5%)	2 (1%)	25 31
All	All	2712/2736 (99%)	2573 (95%)	119 (4%)	20 (1%)	22 26

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LEU
1	D	3	LEU
1	F	3	LEU
1	H	3	LEU
1	A	292	VAL

### 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	258/259 (100%)	239 (93%)	19 (7%)	13	17
1	B	258/259 (100%)	242 (94%)	16 (6%)	18	25
1	C	258/259 (100%)	239 (93%)	19 (7%)	13	17
1	D	258/259 (100%)	242 (94%)	16 (6%)	18	25
1	E	258/259 (100%)	239 (93%)	19 (7%)	13	17
1	F	258/259 (100%)	242 (94%)	16 (6%)	18	25
1	G	258/259 (100%)	239 (93%)	19 (7%)	13	17
1	H	258/259 (100%)	242 (94%)	16 (6%)	18	25
All	All	2064/2072 (100%)	1924 (93%)	140 (7%)	16	21

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	185	VAL
1	G	279	ASP
1	H	159	VAL
1	C	266	VAL
1	C	231	GLN

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	G	231	GLN
1	H	286	HIS
1	G	238	HIS
1	H	135	ASN
1	C	324	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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$
4	EDO	F	1268	2	3,3,3	0.35	0	2,2,2	0.41	0
3	NAD	F	1255	-	42,48,48	2.75	14 (33%)	50,73,73	2.61	14 (28%)
4	EDO	E	1266	2	3,3,3	0.43	0	2,2,2	0.45	0
4	EDO	D	1265	2	3,3,3	0.36	0	2,2,2	0.41	0
3	NAD	B	1251	-	42,48,48	2.75	14 (33%)	50,73,73	2.61	14 (28%)
3	NAD	A	1250	-	42,48,48	2.66	10 (23%)	50,73,73	2.56	16 (32%)
4	EDO	H	1271	2	3,3,3	0.36	0	2,2,2	0.41	0
4	EDO	G	1269	2	3,3,3	0.42	0	2,2,2	0.44	0
3	NAD	C	1252	-	42,48,48	2.65	10 (23%)	50,73,73	2.56	16 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAD	G	1256	-	42,48,48	2.65	10 (23%)	50,73,73	2.56	16 (32%)
4	EDO	G	1270	-	3,3,3	0.61	0	2,2,2	0.40	0
4	EDO	B	1262	2	3,3,3	0.36	0	2,2,2	0.41	0
3	NAD	H	1258	-	42,48,48	2.76	14 (33%)	50,73,73	2.61	14 (28%)
4	EDO	A	1260	2	3,3,3	0.42	0	2,2,2	0.45	0
4	EDO	A	1261	-	3,3,3	0.61	0	2,2,2	0.40	0
4	EDO	E	1267	-	3,3,3	0.62	0	2,2,2	0.40	0
4	EDO	C	1263	2	3,3,3	0.42	0	2,2,2	0.44	0
3	NAD	D	1253	-	42,48,48	2.75	14 (33%)	50,73,73	2.61	14 (28%)
4	EDO	C	1264	-	3,3,3	0.61	0	2,2,2	0.41	0
3	NAD	E	1254	-	42,48,48	2.66	10 (23%)	50,73,73	2.56	16 (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
4	EDO	F	1268	2	-	0/1/1/1	-
3	NAD	F	1255	-	-	3/26/62/62	0/5/5/5
4	EDO	E	1266	2	-	0/1/1/1	-
4	EDO	D	1265	2	-	0/1/1/1	-
3	NAD	B	1251	-	-	3/26/62/62	0/5/5/5
3	NAD	A	1250	-	-	6/26/62/62	0/5/5/5
4	EDO	H	1271	2	-	0/1/1/1	-
4	EDO	G	1269	2	-	0/1/1/1	-
3	NAD	C	1252	-	-	6/26/62/62	0/5/5/5
3	NAD	G	1256	-	-	6/26/62/62	0/5/5/5
4	EDO	G	1270	-	-	0/1/1/1	-
4	EDO	B	1262	2	-	0/1/1/1	-
3	NAD	H	1258	-	-	3/26/62/62	0/5/5/5
4	EDO	A	1260	2	-	0/1/1/1	-
4	EDO	A	1261	-	-	0/1/1/1	-
4	EDO	E	1267	-	-	0/1/1/1	-
4	EDO	C	1263	2	-	0/1/1/1	-
3	NAD	D	1253	-	-	3/26/62/62	0/5/5/5
4	EDO	C	1264	-	-	0/1/1/1	-
3	NAD	E	1254	-	-	6/26/62/62	0/5/5/5

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1253	NAD	C2N-N1N	8.87	1.45	1.35
3	H	1258	NAD	C2N-N1N	8.85	1.45	1.35
3	B	1251	NAD	C2N-N1N	8.84	1.45	1.35
3	F	1255	NAD	C2N-N1N	8.83	1.45	1.35
3	E	1254	NAD	C4N-C3N	8.37	1.53	1.39

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1255	NAD	C5N-C4N-C3N	-8.84	109.89	120.34
3	D	1253	NAD	C5N-C4N-C3N	-8.83	109.89	120.34
3	B	1251	NAD	C5N-C4N-C3N	-8.83	109.90	120.34
3	H	1258	NAD	C5N-C4N-C3N	-8.80	109.93	120.34
3	E	1254	NAD	C5N-C4N-C3N	-8.45	110.35	120.34

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1250	NAD	O4D-C1D-N1N-C2N
3	A	1250	NAD	C2D-C1D-N1N-C2N
3	B	1251	NAD	O4D-C1D-N1N-C2N
3	B	1251	NAD	C2D-C1D-N1N-C2N
3	C	1252	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

20 monomers are involved in 28 short contacts:

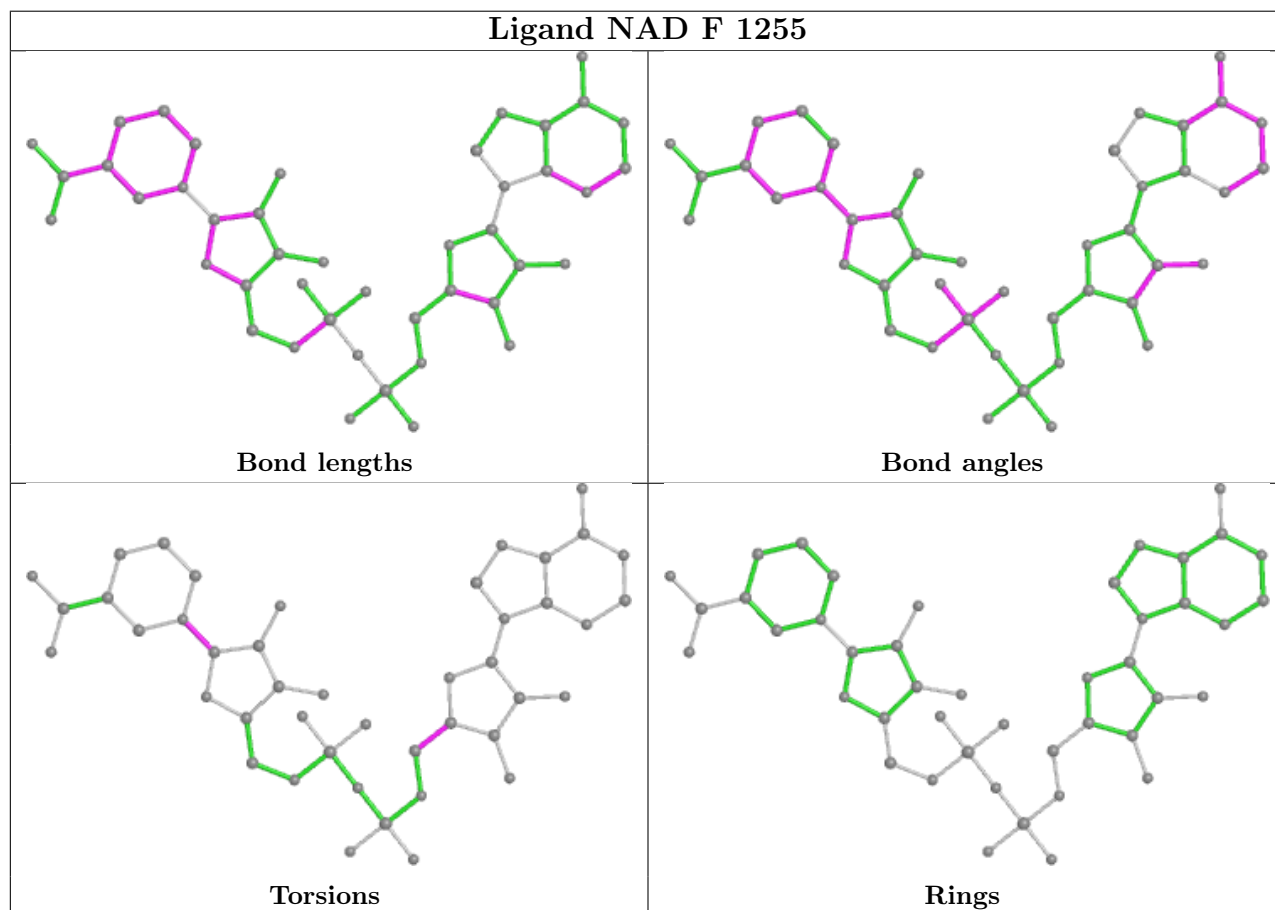
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1268	EDO	1	0
3	F	1255	NAD	1	0
4	E	1266	EDO	1	0
4	D	1265	EDO	1	0
3	B	1251	NAD	1	0
3	A	1250	NAD	3	0
4	H	1271	EDO	1	0
4	G	1269	EDO	1	0
3	C	1252	NAD	3	0
3	G	1256	NAD	3	0
4	G	1270	EDO	1	0
4	B	1262	EDO	1	0
3	H	1258	NAD	1	0

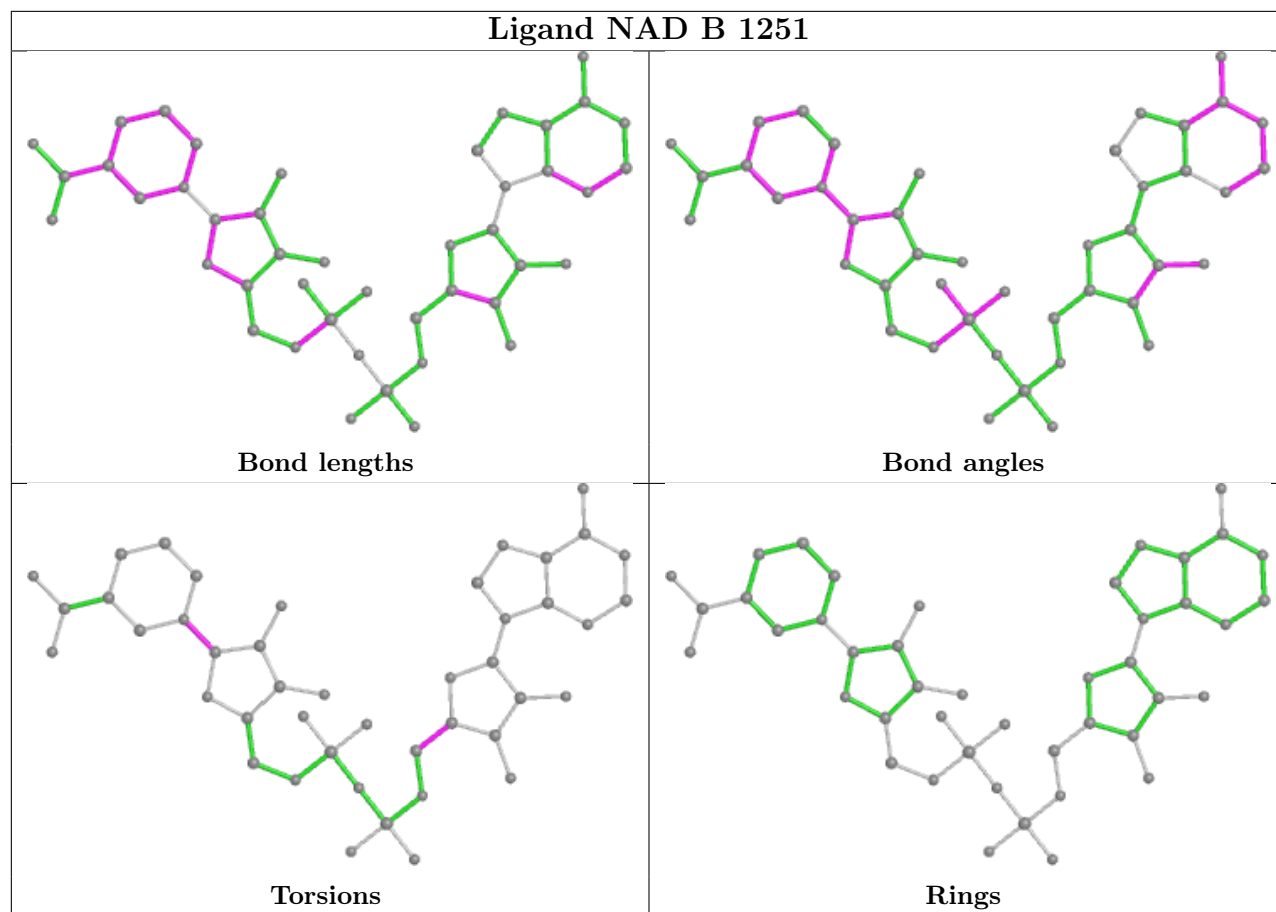
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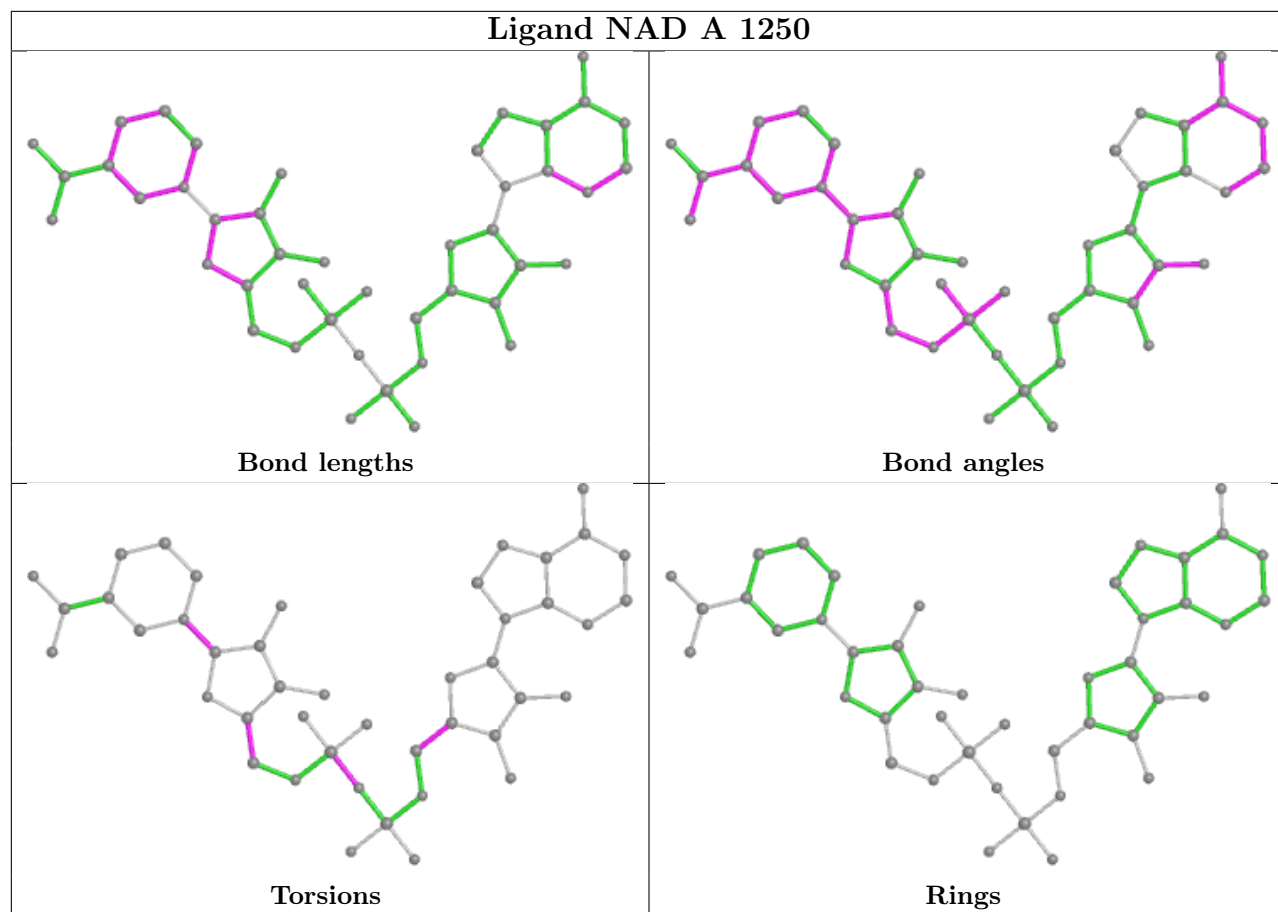
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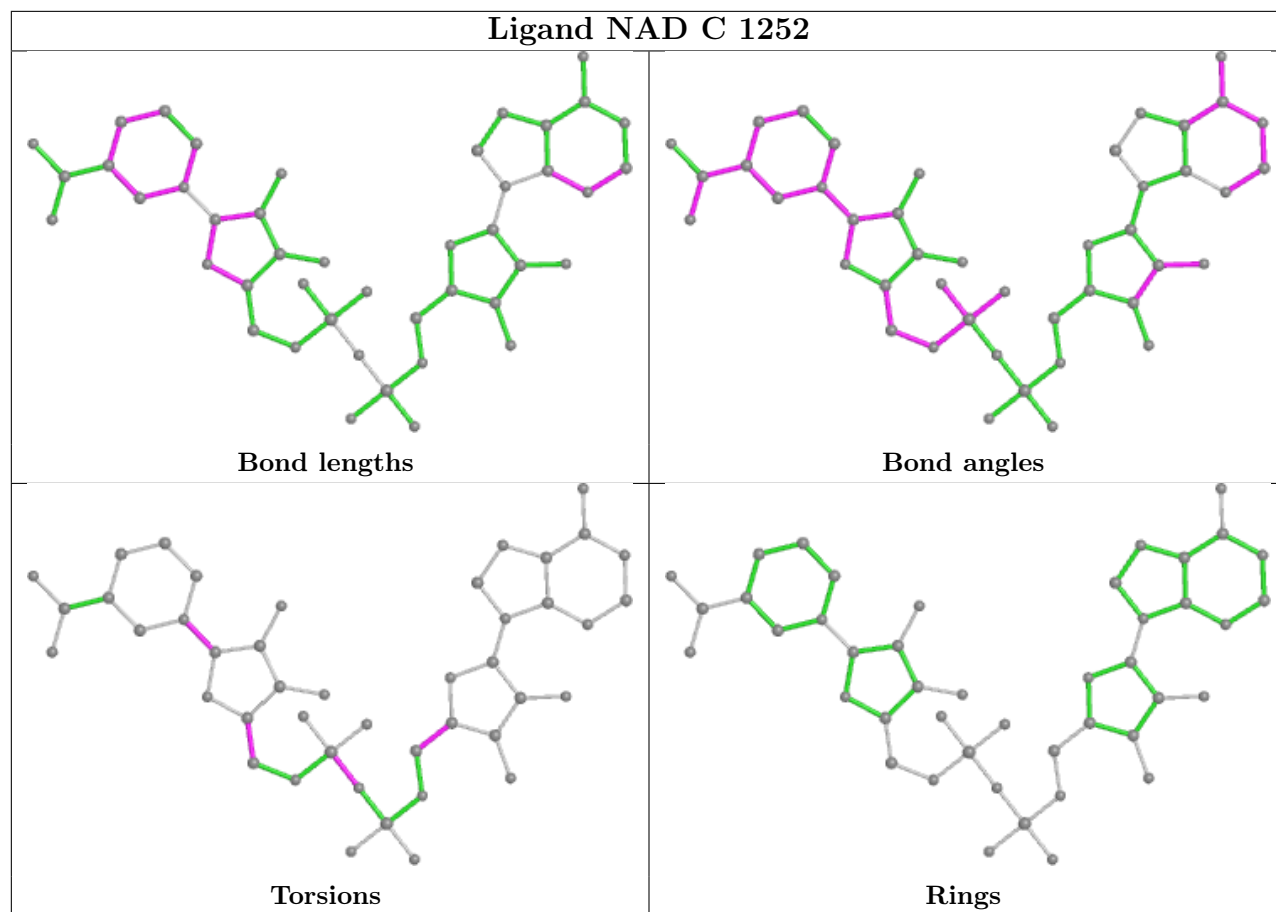
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1260	EDO	1	0
4	A	1261	EDO	1	0
4	E	1267	EDO	1	0
4	C	1263	EDO	1	0
3	D	1253	NAD	1	0
4	C	1264	EDO	1	0
3	E	1254	NAD	3	0

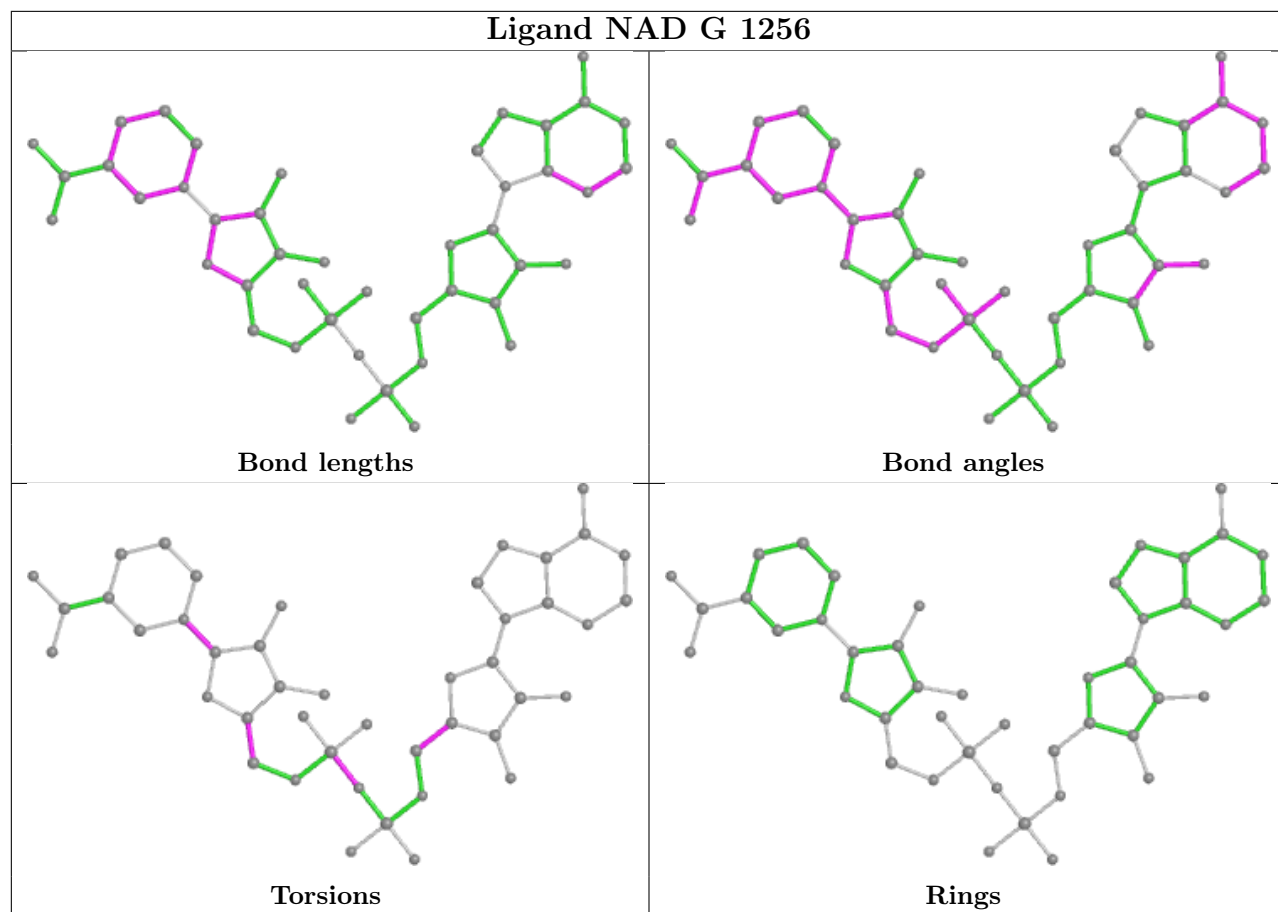
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

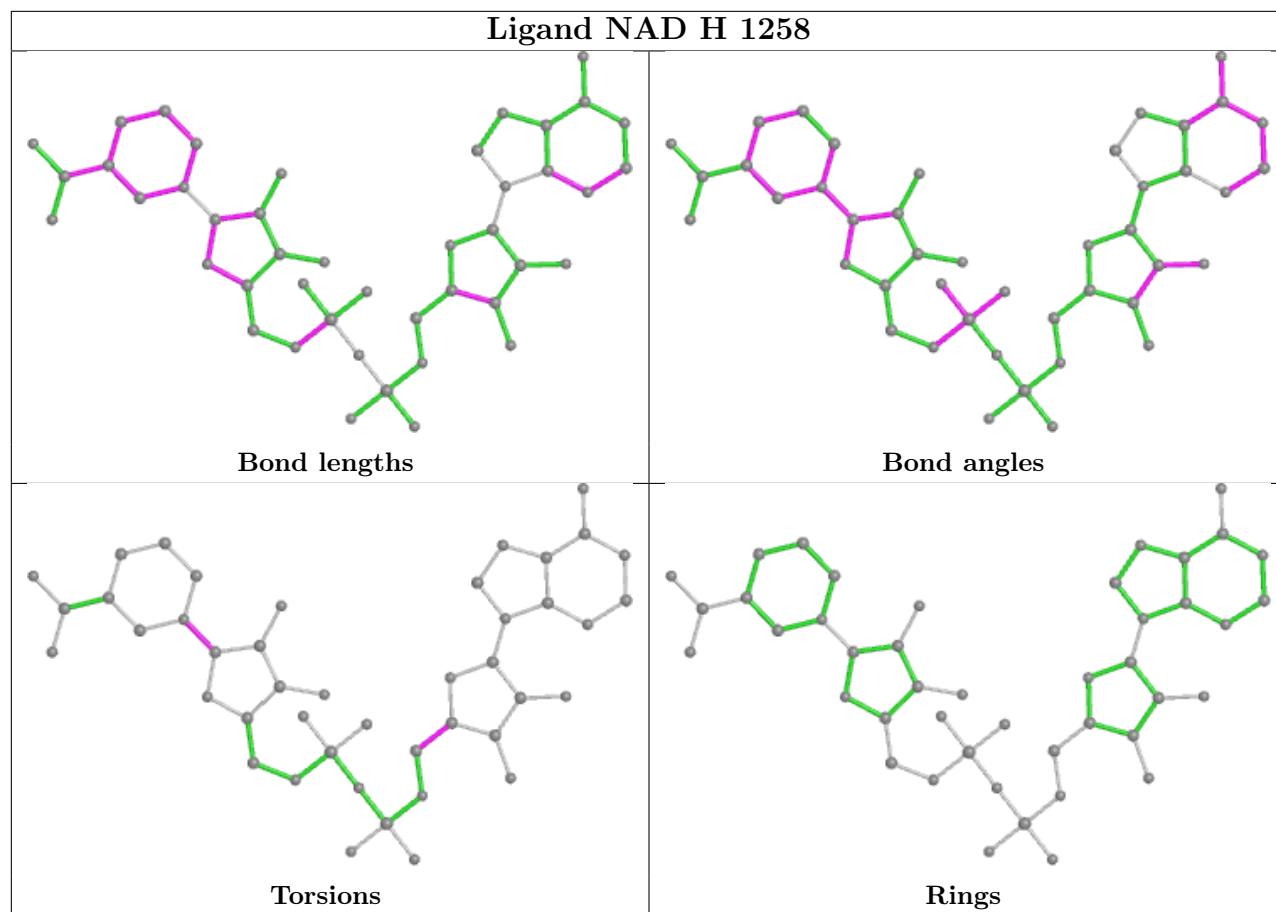




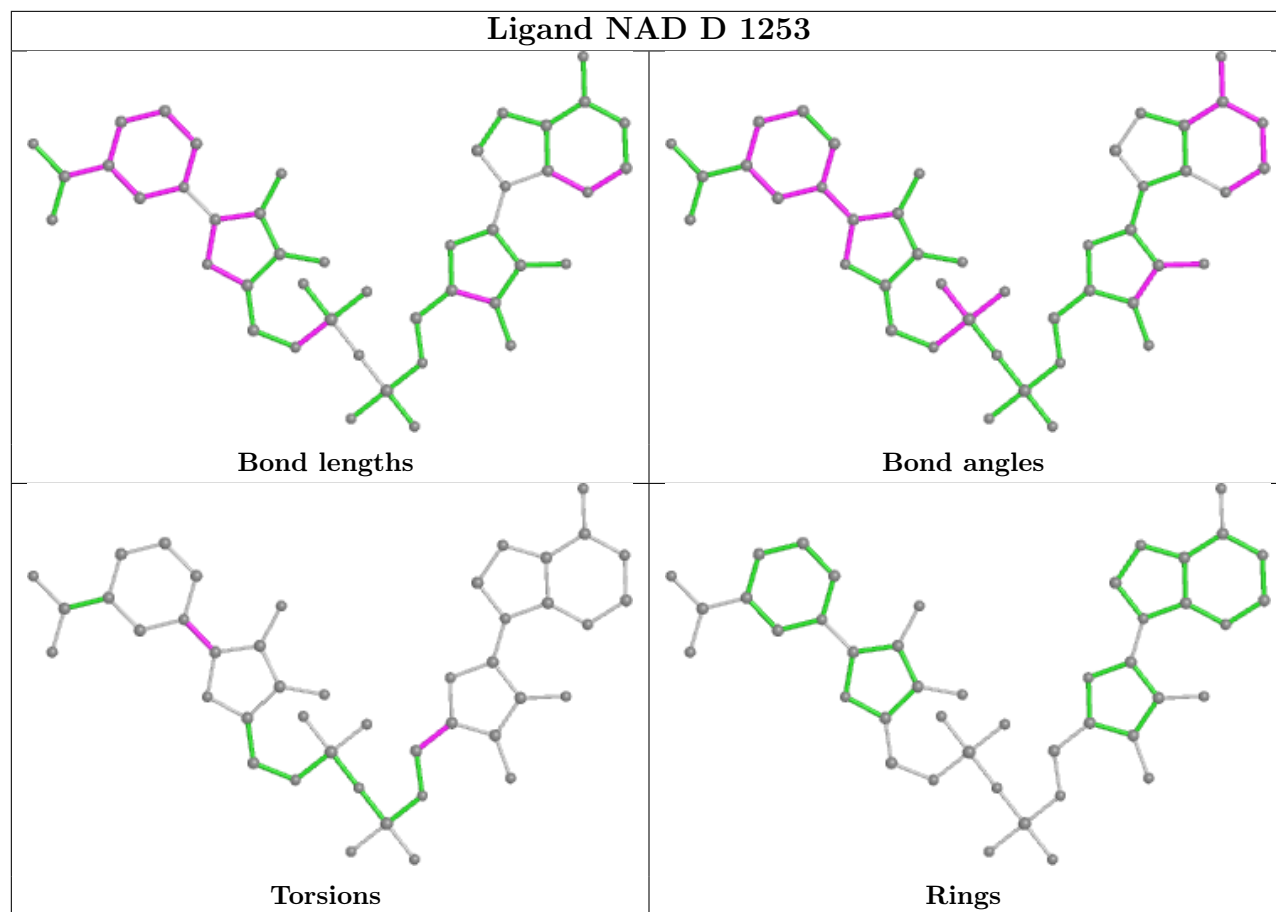


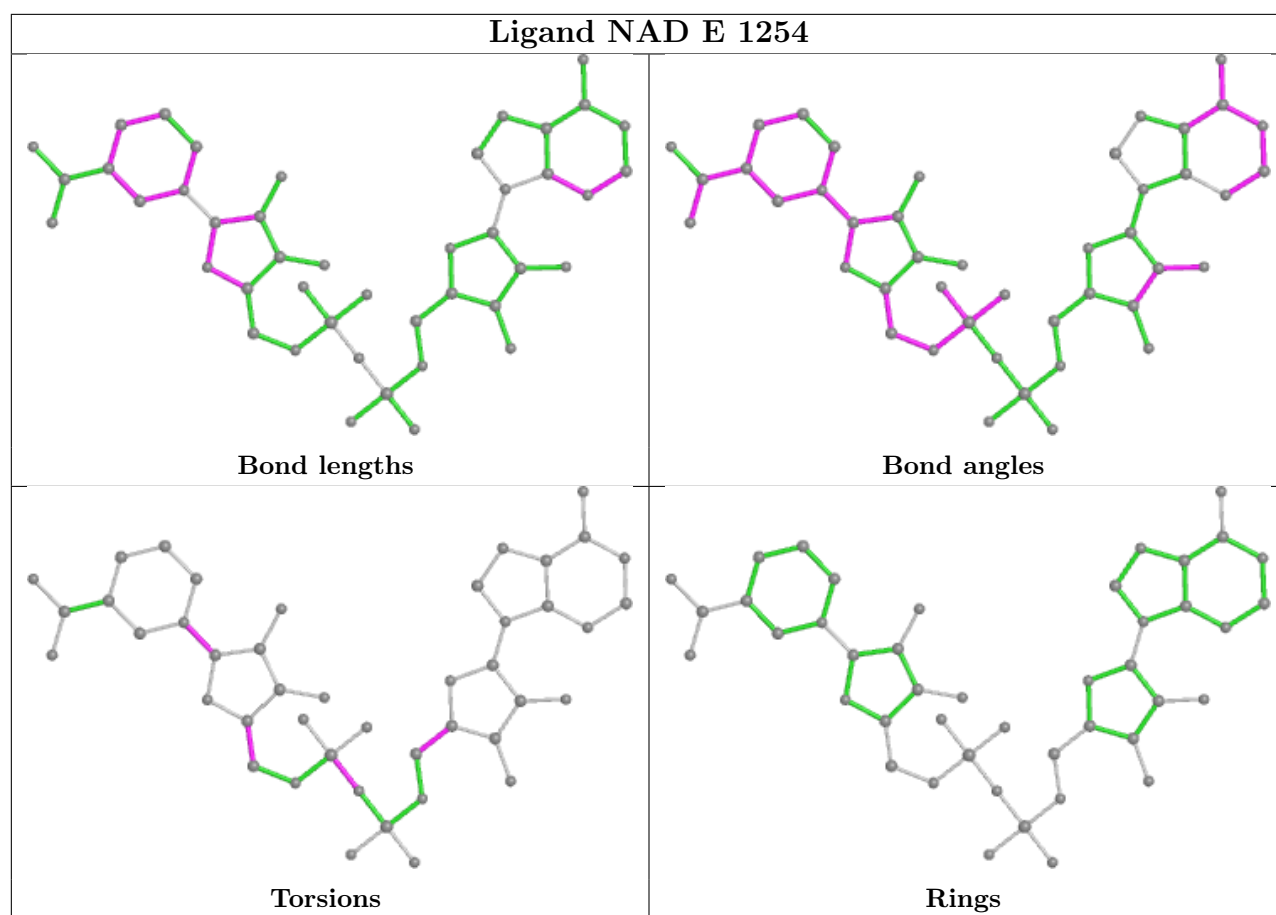












## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/342 (99%)	-0.18	2 (0%) 89 92	10, 21, 35, 62	0
1	B	341/342 (99%)	0.54	31 (9%) 9 12	11, 35, 74, 82	0
1	C	341/342 (99%)	-0.17	6 (1%) 68 74	10, 21, 35, 62	0
1	D	341/342 (99%)	0.97	66 (19%) 1 1	11, 35, 74, 82	0
1	E	341/342 (99%)	0.02	2 (0%) 89 92	10, 21, 35, 62	0
1	F	341/342 (99%)	0.68	35 (10%) 6 9	11, 35, 74, 82	0
1	G	341/342 (99%)	-0.04	5 (1%) 73 79	10, 21, 35, 62	0
1	H	341/342 (99%)	1.34	101 (29%) 0 0	11, 35, 74, 82	0
All	All	2728/2736 (99%)	0.40	248 (9%) 9 12	10, 25, 68, 82	0

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	TYR	9.1
1	D	51	ALA	8.3
1	H	51	ALA	8.3
1	H	75	ALA	8.1
1	D	50	ALA	7.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

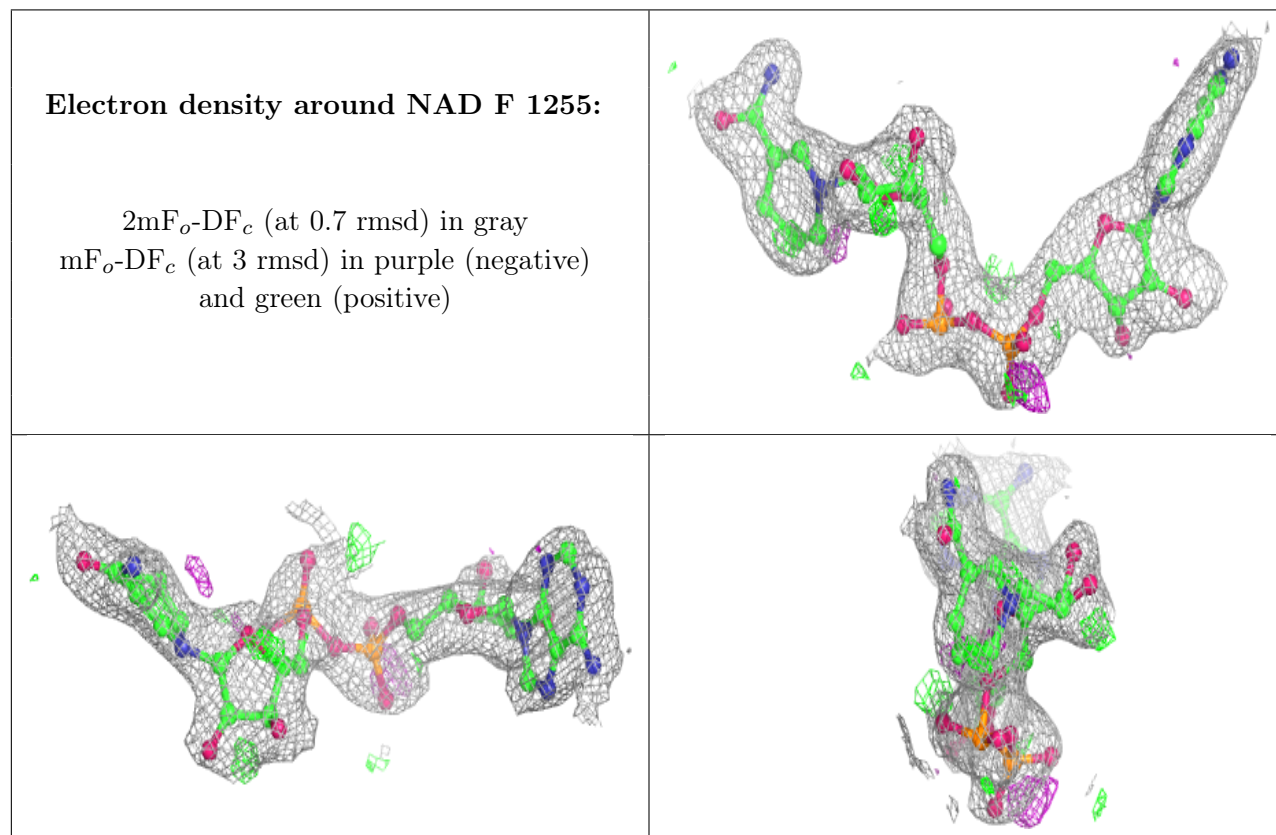
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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.

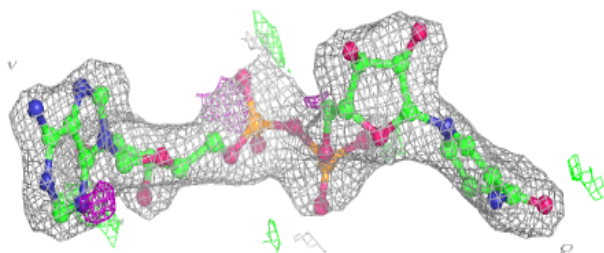
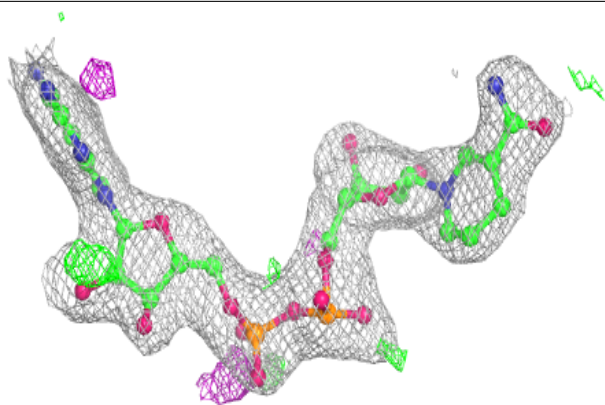
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	F	1255	44/44	0.84	0.20	33,38,46,48	0
3	NAD	B	1251	44/44	0.86	0.17	33,38,46,48	0
3	NAD	H	1258	44/44	0.88	0.19	33,38,46,48	0
4	EDO	C	1264	4/4	0.89	0.18	24,26,27,27	0
4	EDO	D	1265	4/4	0.90	0.20	30,33,35,36	0
4	EDO	H	1271	4/4	0.90	0.22	30,33,35,36	0
3	NAD	D	1253	44/44	0.91	0.16	33,38,46,48	0
4	EDO	G	1270	4/4	0.92	0.15	24,26,27,27	0
3	NAD	E	1254	44/44	0.92	0.16	14,18,20,22	0
3	NAD	A	1250	44/44	0.94	0.14	14,18,20,22	0
3	NAD	G	1256	44/44	0.94	0.13	14,18,20,22	0
3	NAD	C	1252	44/44	0.94	0.15	14,18,20,22	0
4	EDO	B	1262	4/4	0.94	0.29	30,33,35,36	0
4	EDO	E	1267	4/4	0.95	0.16	24,26,27,27	0
4	EDO	F	1268	4/4	0.95	0.23	30,33,35,36	0
2	ZN	F	344	1/1	0.95	0.06	29,29,29,29	0
4	EDO	C	1263	4/4	0.95	0.17	15,19,19,21	0
2	ZN	H	344	1/1	0.96	0.03	29,29,29,29	0
4	EDO	A	1261	4/4	0.96	0.10	24,26,27,27	0
4	EDO	E	1266	4/4	0.97	0.22	15,19,19,21	0
2	ZN	B	343	1/1	0.97	0.13	34,34,34,34	0
2	ZN	G	344	1/1	0.97	0.08	23,23,23,23	0
4	EDO	G	1269	4/4	0.97	0.16	15,19,19,21	0
4	EDO	A	1260	4/4	0.97	0.22	15,19,19,21	0
2	ZN	D	344	1/1	0.97	0.06	29,29,29,29	0
2	ZN	D	343	1/1	0.98	0.04	34,34,34,34	0
2	ZN	G	343	1/1	0.98	0.06	18,18,18,18	0
2	ZN	C	344	1/1	0.98	0.06	23,23,23,23	0
2	ZN	H	343	1/1	0.98	0.05	34,34,34,34	0
2	ZN	F	343	1/1	0.98	0.15	34,34,34,34	0
2	ZN	B	344	1/1	0.99	0.02	29,29,29,29	0
2	ZN	E	343	1/1	0.99	0.07	18,18,18,18	0
2	ZN	A	344	1/1	0.99	0.06	23,23,23,23	0
2	ZN	A	343	1/1	0.99	0.06	18,18,18,18	0
2	ZN	C	343	1/1	1.00	0.06	18,18,18,18	0
2	ZN	E	344	1/1	1.00	0.07	23,23,23,23	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.

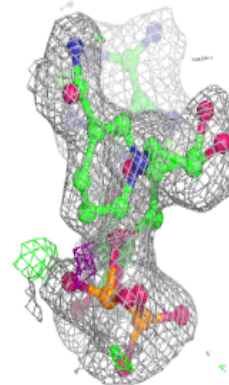
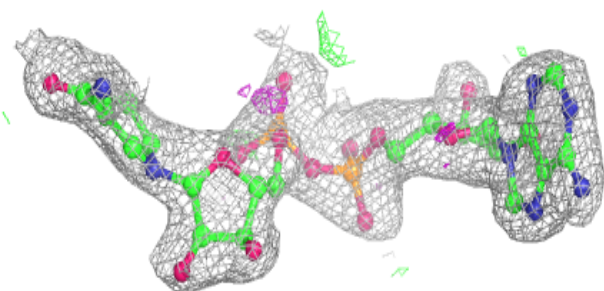
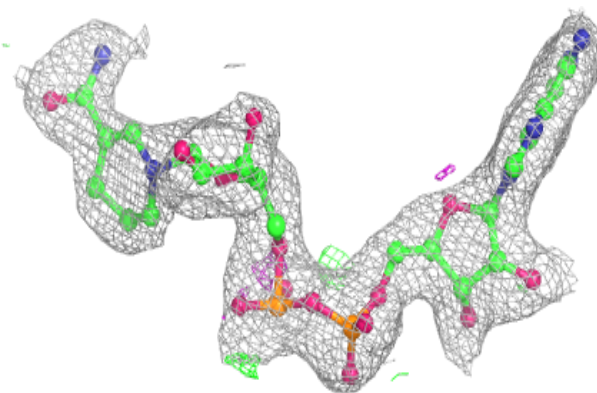


**Electron density around NAD B 1251:**

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

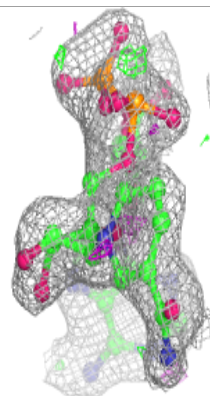
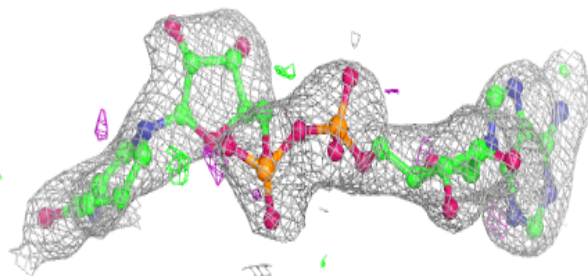
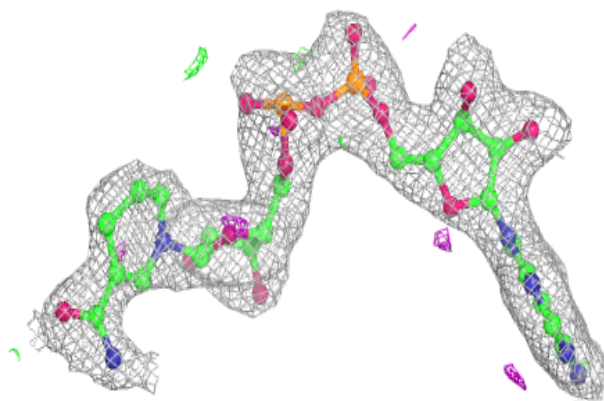
**Electron density around NAD H 1258:**

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

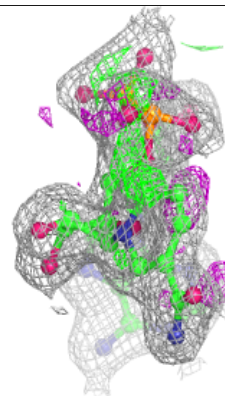
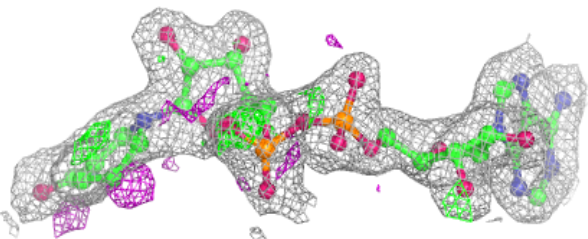
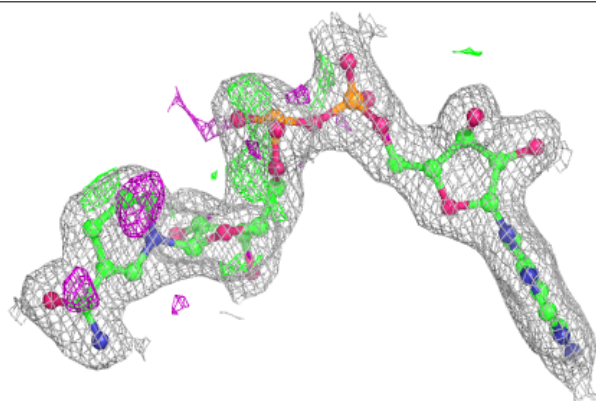


**Electron density around NAD D 1253:**

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

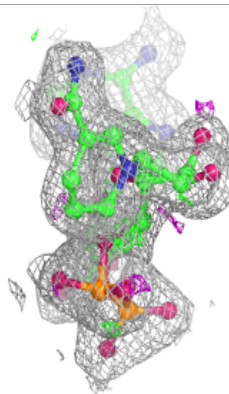
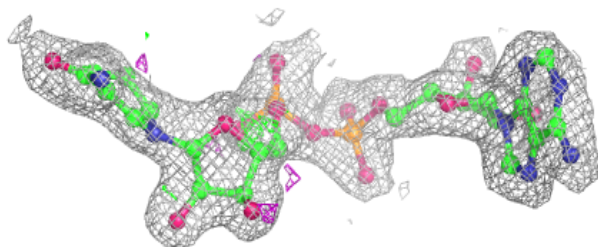
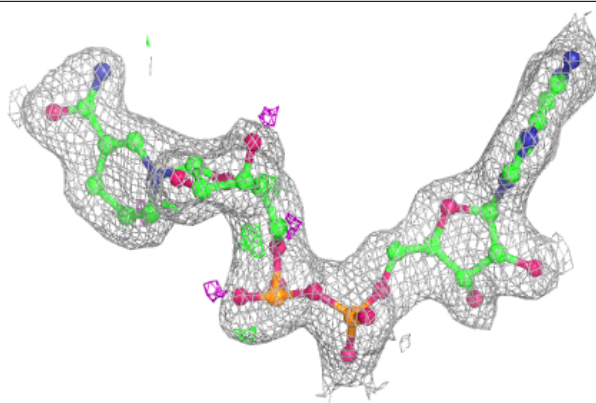
**Electron density around NAD E 1254:**

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

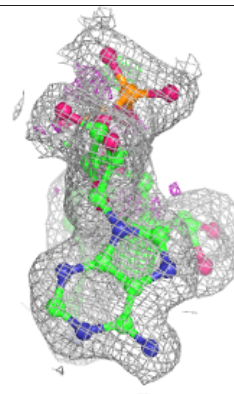
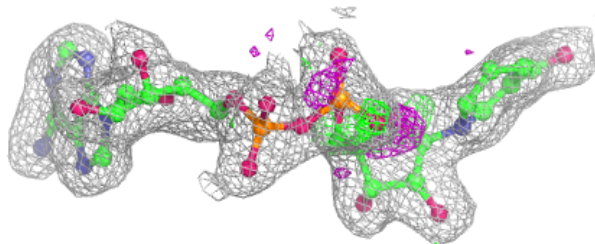
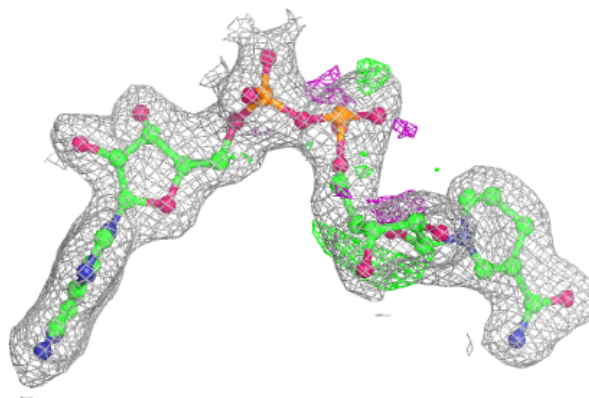


**Electron density around NAD A 1250:**

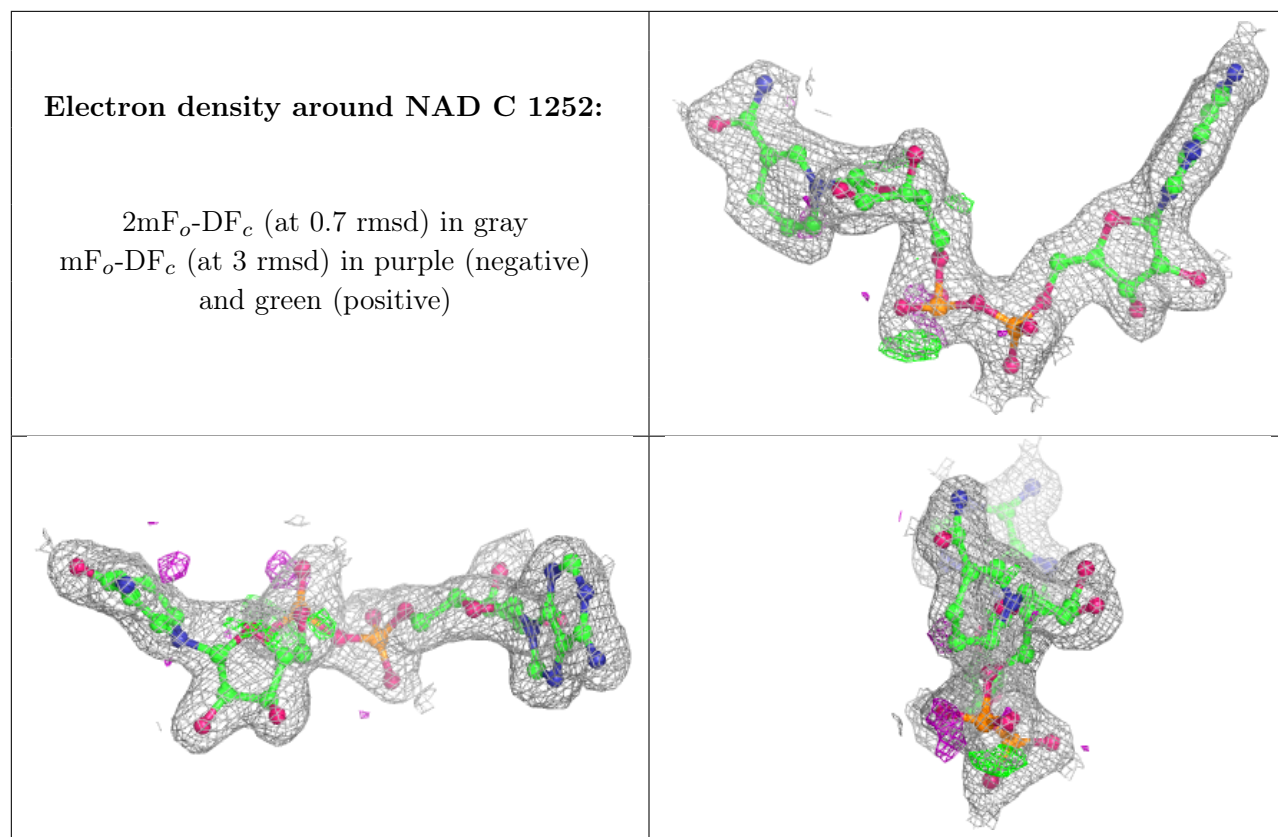
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD G 1256:**

$2mF_o-DF_c$  (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.