wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 10:32 PM JST

PDB ID	:	6AHE
Title	:	Crystal structure of enoyl-ACP reductase from Acinetobacter baumannii in complex with NAD and AFN-1252
Authors	:	Rani, S.T.; Nataraj, V.; Laxminarasimhan, A.; Thomas, A.; Krishnamurthy, N.
Deposited on	:	2018-08-17
Resolution	:	2.29 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

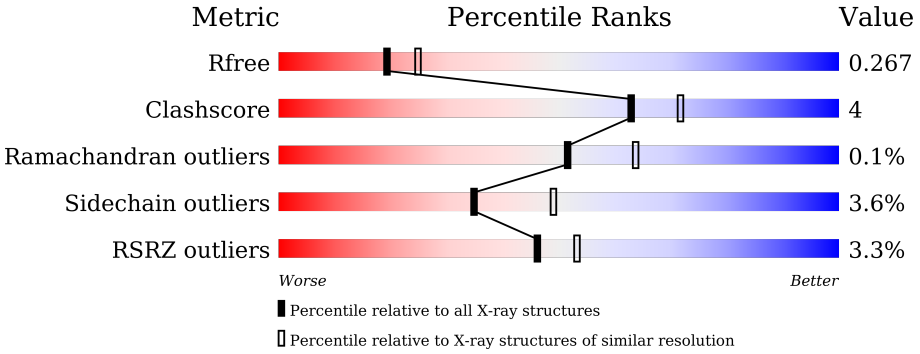
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.29 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	3% 87% 10% •
1	B	267	% 87% 10% •
1	C	267	4% 86% 10% • •
1	D	267	4% 84% 12% • •

2 Entry composition (i)

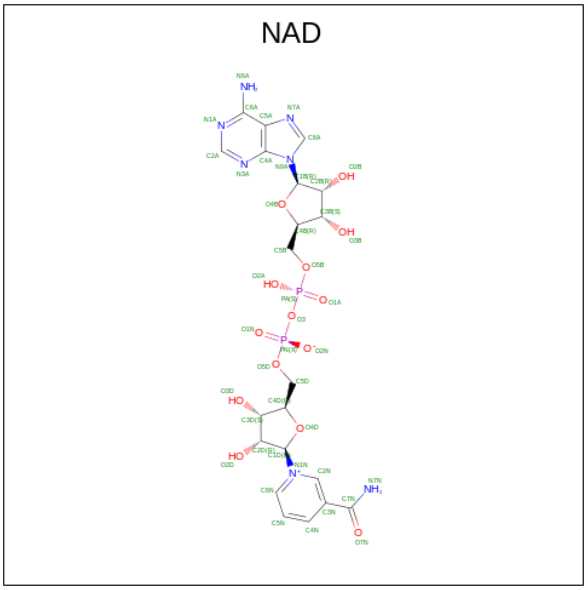
There are 4 unique types of molecules in this entry. The entry contains 8211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1941	1233	335	364	9	0	0	0
			Total	C	N	O	S			
1	D	260	1941	1233	335	364	9	0	0	0
			Total	C	N	O	S			
1	C	260	1945	1236	336	364	9	0	0	0
			Total	C	N	O	S			
1	B	260	1941	1233	335	364	9	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



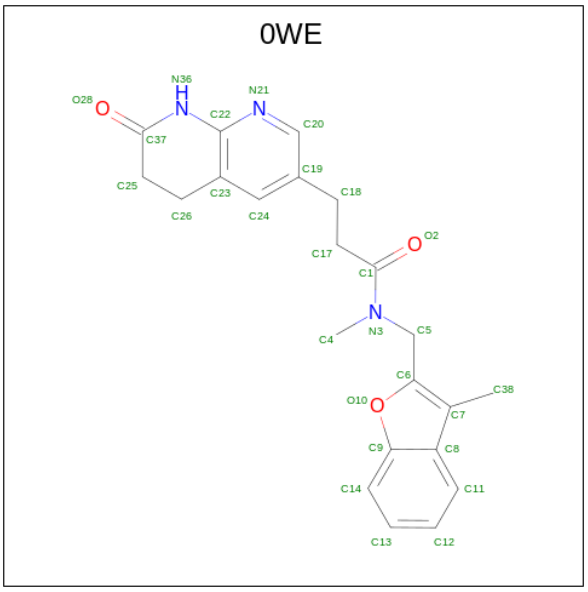
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	D	1	44	21	7	14	2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is N-methyl-N-[(3-methyl-1-benzofuran-2-yl)methyl]-3-(7-oxo-5,6,7,8-tetrahydro-1,8-naphthyridin-3-yl)propanamide (three-letter code: 0WE) (formula: $C_{22}H_{23}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	28	22	3	3	0	0
			Total	C	N	O		
3	D	1	28	22	3	3	0	0
			Total	C	N	O		
3	C	1	28	22	3	3	0	0
			Total	C	N	O		
3	B	1	28	22	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	42	42	42	0	0
			Total	O		
4	D	41	41	41	0	0
			Total	O		
4	C	31	31	31	0	0

Continued on next page...

Continued from previous page...

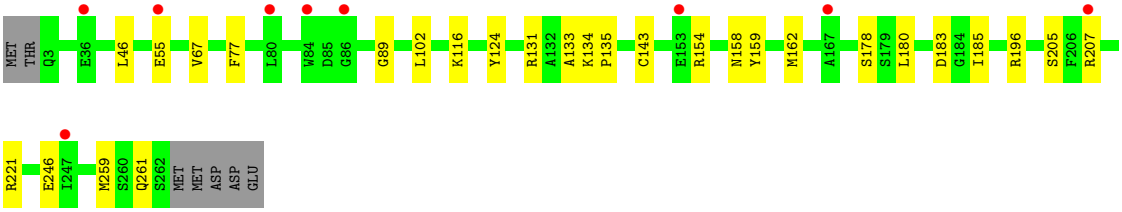
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	41	41	41	0	0

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.

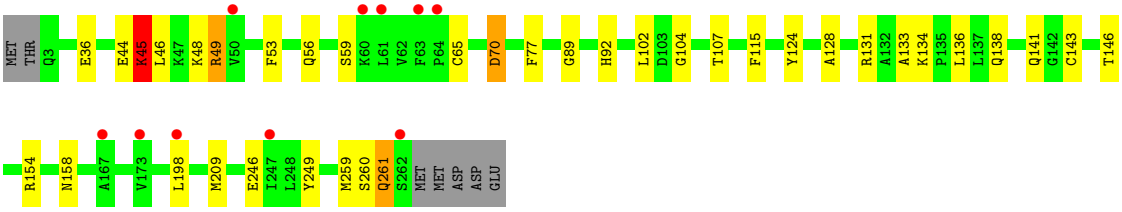
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



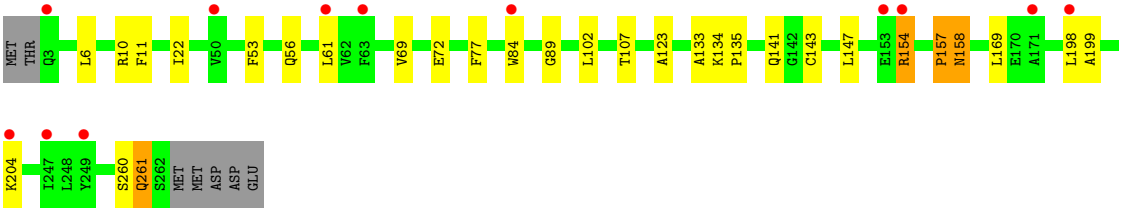
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:



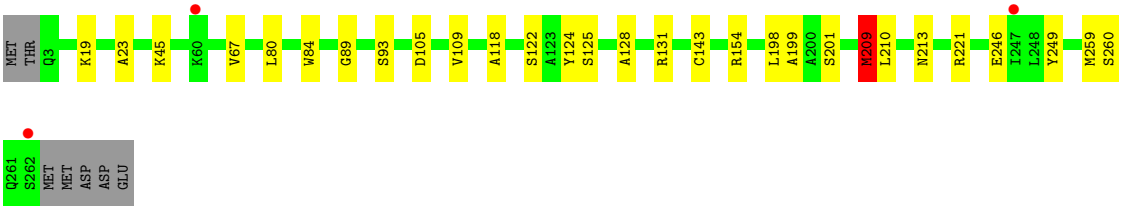
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:


MET
THR
Q3
K19
A23
K45
K60
V67
L80
W84
G89
S93
D105
V109
A118
S122
A123
Y124
S125
A128
R131
C143
R154
L198
A199
A200
S201
M209
L210
N213
R221
E246
I247
L248
Y249
M259
S260
Q261
S262
MET
MET
ASP
ASP
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.53Å 89.57Å 159.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.74 – 2.29 47.67 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (79.74-2.29) 99.4 (47.67-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.204 , 0.268 0.210 , 0.267	Depositor DCC
R_{free} test set	2527 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8211	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 0WE

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	0.72	0/1977	0.85	2/2677 (0.1%)
1	B	0.72	0/1977	0.84	3/2677 (0.1%)
1	C	0.75	0/1981	0.86	3/2681 (0.1%)
1	D	0.76	0/1977	0.88	1/2677 (0.0%)
All	All	0.74	0/7912	0.86	9/10712 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	ASN	N-CA-CB	-9.05	94.30	110.60
1	C	157	PRO	N-CA-C	6.82	129.84	112.10
1	B	221	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	46	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	209	MET	CB-CG-SD	-5.48	95.95	112.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLN	Peptide
1	C	261	GLN	Peptide
1	D	261	GLN	Peptide

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	1941	0	1924	19	0
1	B	1941	0	1924	22	0
1	C	1945	0	1935	18	0
1	D	1941	0	1924	24	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	28	0	23	1	0
3	B	28	0	23	1	0
3	C	28	0	23	2	0
3	D	28	0	23	0	0
4	A	42	0	0	0	0
4	B	41	0	0	0	0
4	C	31	0	0	0	0
4	D	41	0	0	2	0
All	All	8211	0	7903	68	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 4.

The worst 5 of 68 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:D:154:ARG:NH1	1:C:154:ARG:HD3	1.90	0.85
1:C:53:PHE:O	1:C:56:GLN:HB3	1.94	0.68
1:C:260:SER:O	1:C:261:GLN:C	2.32	0.67
1:C:199:ALA:HB1	3:C:301:0WE:H1	1.79	0.64
1:D:104:GLY:H	1:D:158:ASN:HD22	1.45	0.62

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	258/267 (97%)	244 (95%)	14 (5%)	0	100	100
1	B	258/267 (97%)	248 (96%)	10 (4%)	0	100	100
1	C	258/267 (97%)	241 (93%)	17 (7%)	0	100	100
1	D	258/267 (97%)	243 (94%)	14 (5%)	1 (0%)	34	42
All	All	1032/1068 (97%)	976 (95%)	55 (5%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	LYS

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	195/206 (95%)	188 (96%)	7 (4%)	35	49
1	B	195/206 (95%)	186 (95%)	9 (5%)	27	38
1	C	196/206 (95%)	193 (98%)	3 (2%)	65	79
1	D	195/206 (95%)	186 (95%)	9 (5%)	27	38
All	All	781/824 (95%)	753 (96%)	28 (4%)	35	49

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	198	LEU
1	B	260	SER
1	C	141	GLN
1	B	210	LEU
1	C	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	83	HIS
1	C	141	GLN
1	B	141	GLN
1	B	138	GLN
1	D	158	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	0WE	C	301	-	27,31,31	2.03	7 (25%)	30,44,44	2.79	15 (50%)
3	0WE	B	301	-	27,31,31	2.13	5 (18%)	30,44,44	2.67	15 (50%)
3	0WE	A	301	-	27,31,31	2.11	6 (22%)	30,44,44	2.54	14 (46%)
3	0WE	D	301	-	27,31,31	1.99	4 (14%)	30,44,44	2.70	15 (50%)

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	0WE	C	301	-	-	2/11/22/22	0/4/4/4
3	0WE	B	301	-	-	1/11/22/22	0/4/4/4
3	0WE	A	301	-	-	1/11/22/22	0/4/4/4
3	0WE	D	301	-	-	1/11/22/22	0/4/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	0WE	C26-C23	-6.16	1.40	1.51
3	A	301	0WE	C26-C23	-5.93	1.41	1.51
3	D	301	0WE	C26-C23	-5.77	1.41	1.51
3	C	301	0WE	C26-C23	-5.01	1.42	1.51
3	A	301	0WE	C26-C25	-4.74	1.40	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	0WE	C18-C17-C1	6.74	120.39	112.34
3	C	301	0WE	C25-C37-N36	6.72	121.25	116.24
3	D	301	0WE	C38-C7-C6	6.45	137.10	124.94
3	A	301	0WE	C25-C37-N36	6.02	120.72	116.24
3	D	301	0WE	C25-C37-N36	5.70	120.48	116.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	0WE	C17-C18-C19-C20
3	A	301	0WE	C17-C18-C19-C24
3	D	301	0WE	C17-C18-C19-C24
3	C	301	0WE	C17-C18-C19-C24
3	B	301	0WE	C17-C18-C19-C24

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	0WE	2	0
3	B	301	0WE	1	0

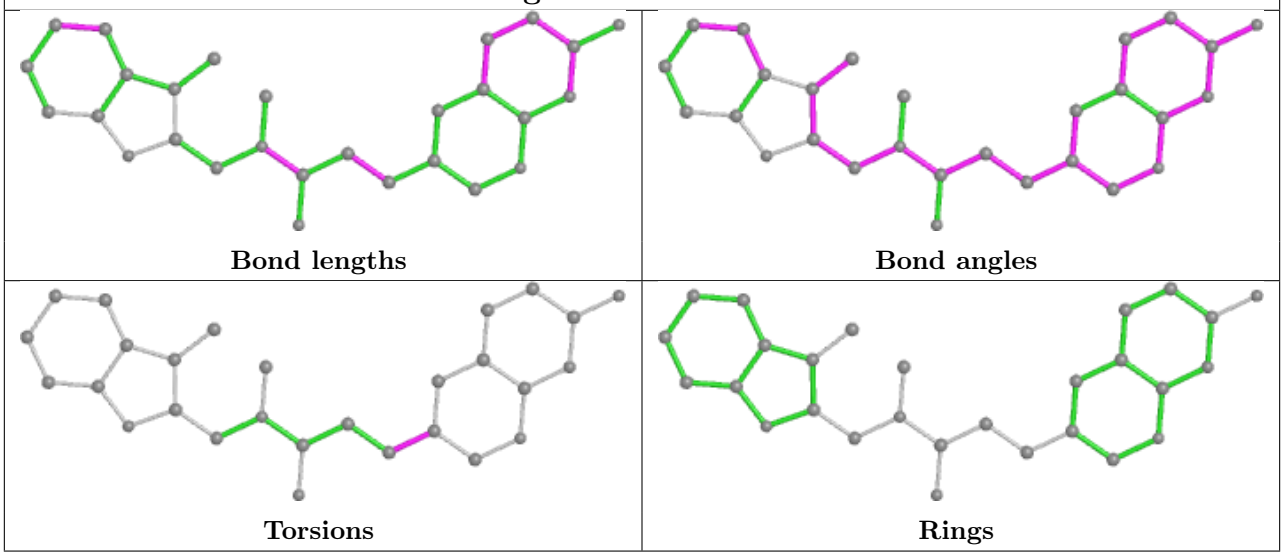
Continued on next page...

Continued from previous page...

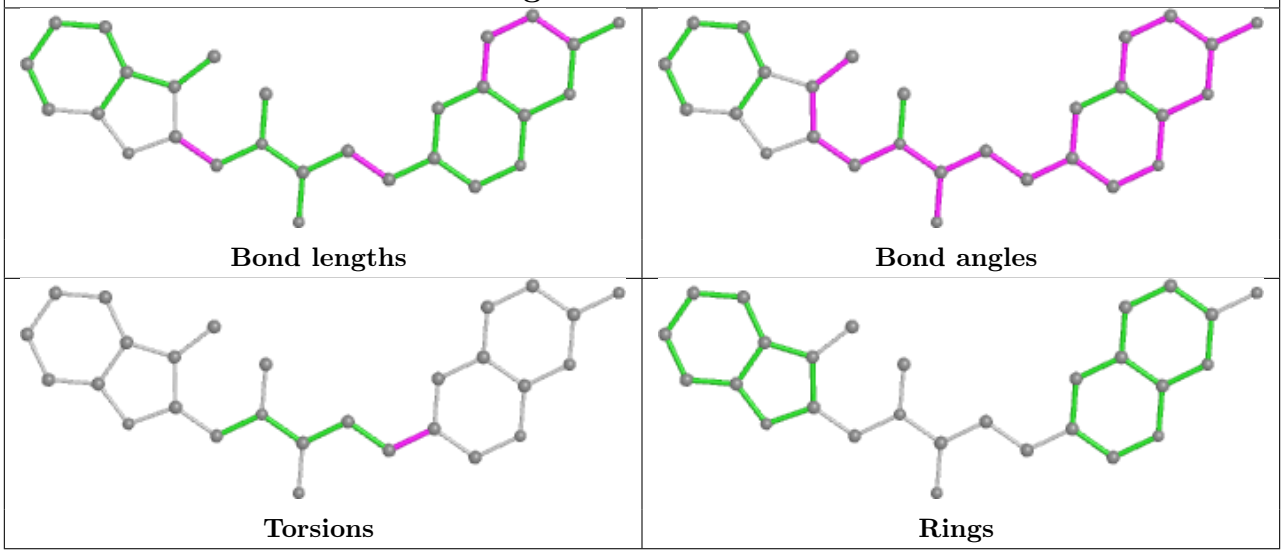
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	0WE	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

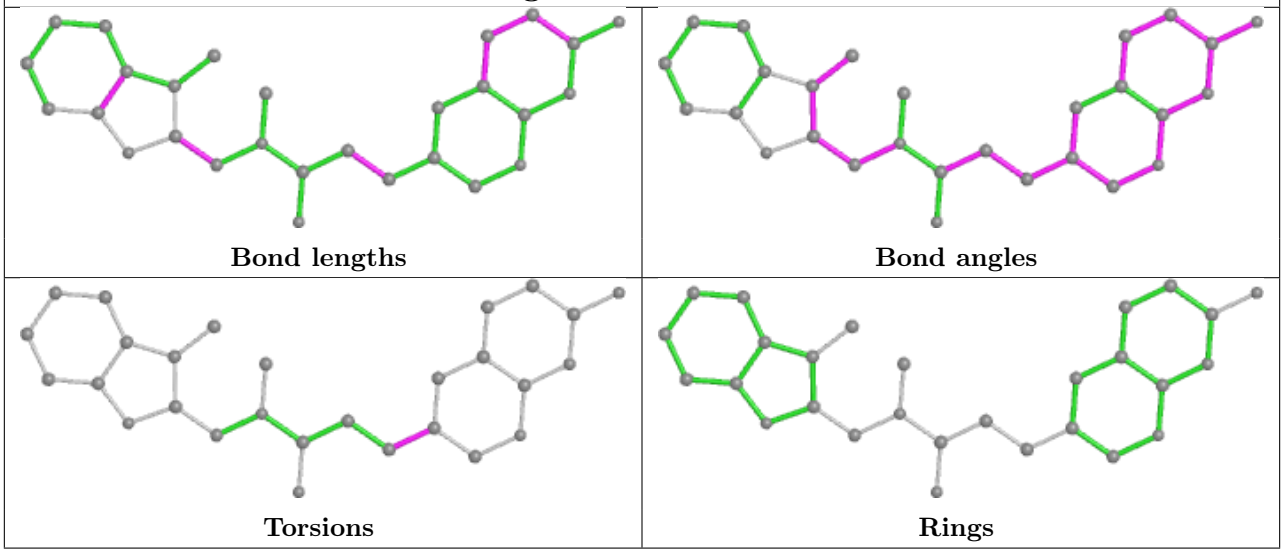
Ligand 0WE C 301



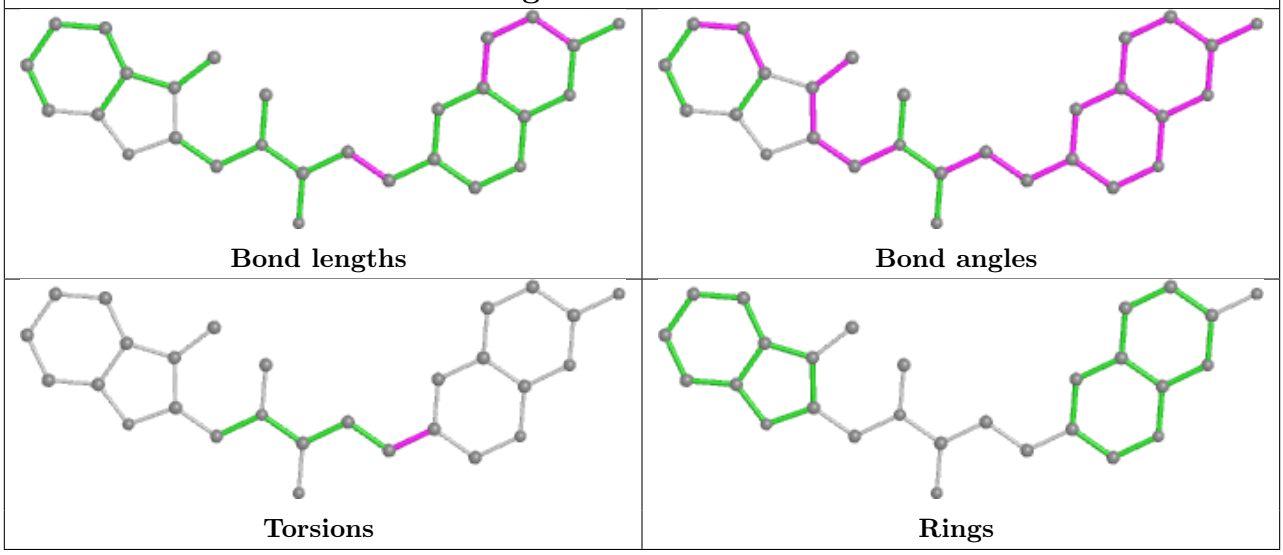
Ligand 0WE B 301



Ligand 0WE A 301



Ligand 0WE D 301



5.5 Carbohydrates (i)

There are no monosaccharides 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	NAD	A	300	-	42,48,48	1.21	3 (7%)	50,73,73	1.35	8 (16%)
2	NAD	C	300	-	42,48,48	1.21	4 (9%)	50,73,73	1.32	7 (14%)
3	0WE	C	301	-	27,31,31	2.03	7 (25%)	30,44,44	2.79	15 (50%)
3	0WE	B	301	-	27,31,31	2.13	5 (18%)	30,44,44	2.67	15 (50%)
2	NAD	D	300	-	42,48,48	1.10	4 (9%)	50,73,73	1.25	8 (16%)
3	0WE	D	301	-	27,31,31	1.99	4 (14%)	30,44,44	2.70	15 (50%)
2	NAD	B	300	-	42,48,48	1.34	6 (14%)	50,73,73	1.55	6 (12%)
3	0WE	A	301	-	27,31,31	2.11	6 (22%)	30,44,44	2.54	14 (46%)

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	A	300	-	-	11/26/62/62	0/5/5/5
2	NAD	C	300	-	-	9/26/62/62	0/5/5/5
3	0WE	C	301	-	-	2/11/22/22	0/4/4/4
3	0WE	B	301	-	-	1/11/22/22	0/4/4/4
2	NAD	D	300	-	-	9/26/62/62	0/5/5/5
3	0WE	D	301	-	-	1/11/22/22	0/4/4/4
2	NAD	B	300	-	-	11/26/62/62	0/5/5/5
3	0WE	A	301	-	-	1/11/22/22	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	0WE	C26-C23	-6.16	1.40	1.51
3	A	301	0WE	C26-C23	-5.93	1.41	1.51
3	D	301	0WE	C26-C23	-5.77	1.41	1.51
3	C	301	0WE	C26-C23	-5.01	1.42	1.51
3	A	301	0WE	C26-C25	-4.74	1.40	1.52

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	0WE	C18-C17-C1	6.74	120.39	112.34
3	C	301	0WE	C25-C37-N36	6.72	121.25	116.24
3	D	301	0WE	C38-C7-C6	6.45	137.10	124.94
3	A	301	0WE	C25-C37-N36	6.02	120.72	116.24
3	D	301	0WE	C25-C37-N36	5.70	120.48	116.24

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	C5B-O5B-PA-O2A
2	A	300	NAD	PN-O3-PA-O5B
2	A	300	NAD	C5D-O5D-PN-O3
2	A	300	NAD	O4D-C1D-N1N-C2N
2	A	300	NAD	O4D-C1D-N1N-C6N

There are no ring outliers.

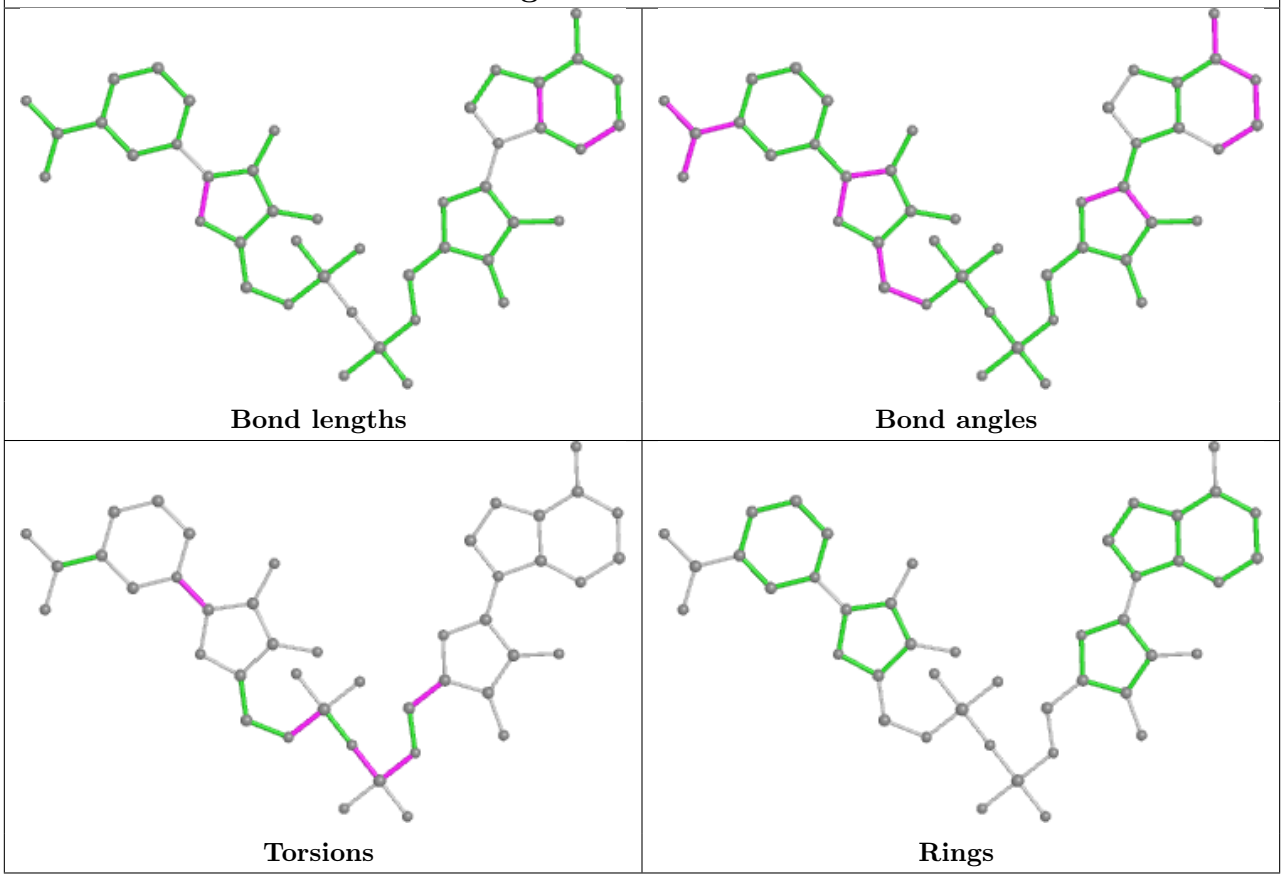
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	NAD	1	0
3	C	301	0WE	2	0
3	B	301	0WE	1	0
2	D	300	NAD	1	0
2	B	300	NAD	2	0
3	A	301	0WE	1	0

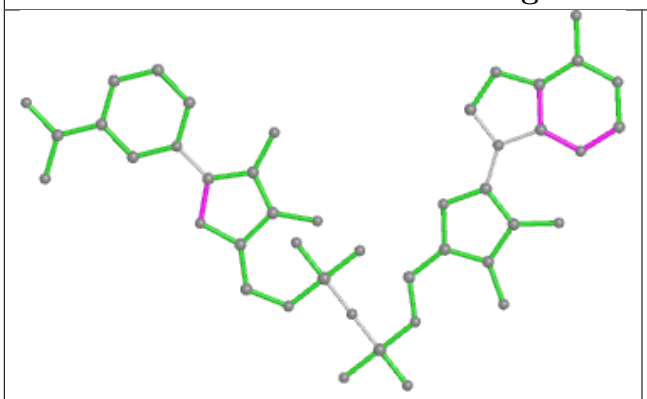
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

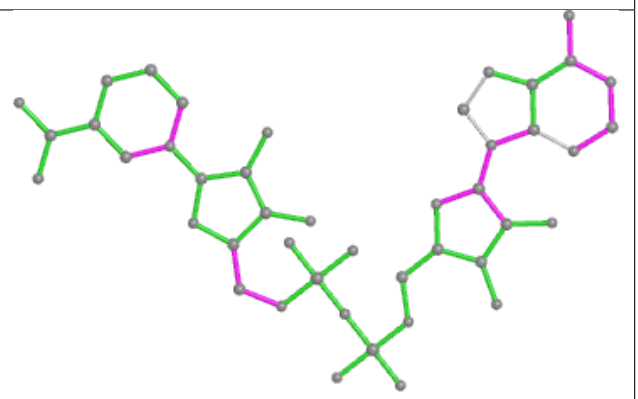
Ligand NAD A 300



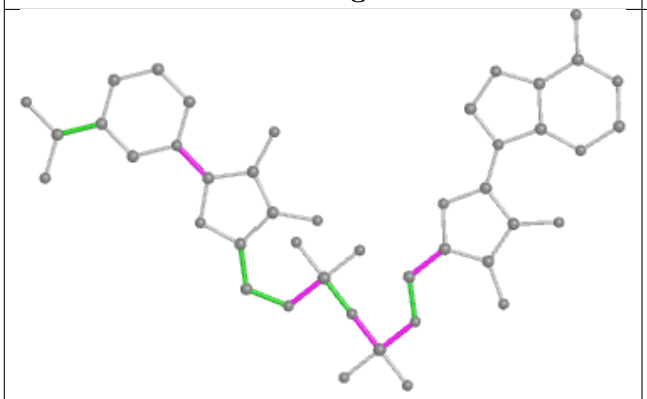
Ligand NAD C 300



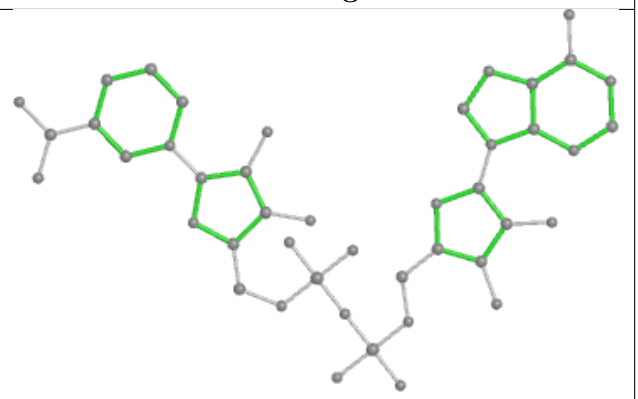
Bond lengths



Bond angles

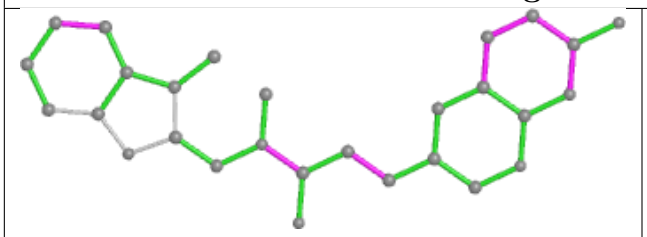


Torsions

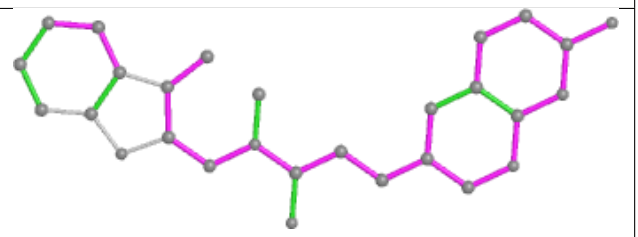


Rings

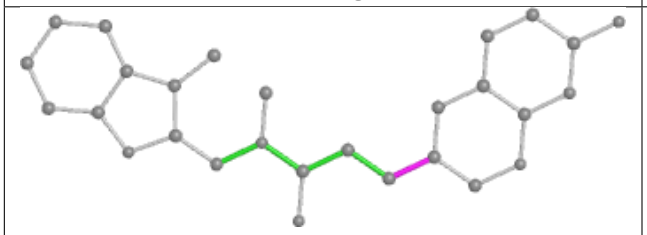
Ligand 0WE C 301



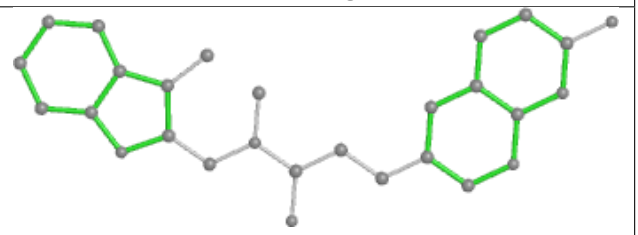
Bond lengths



Bond angles

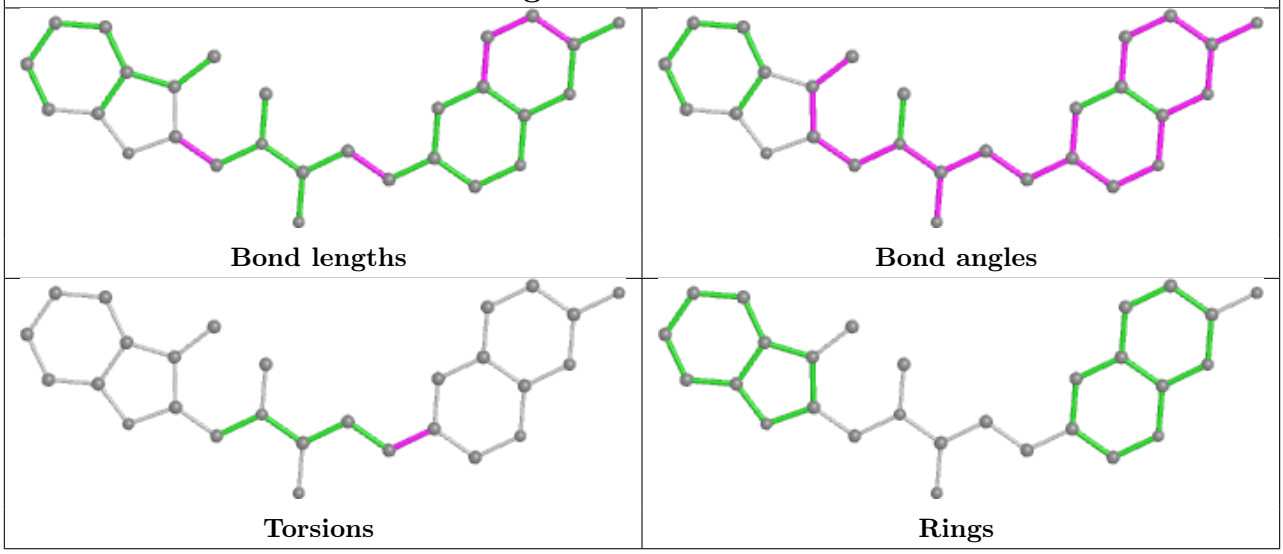


Torsions

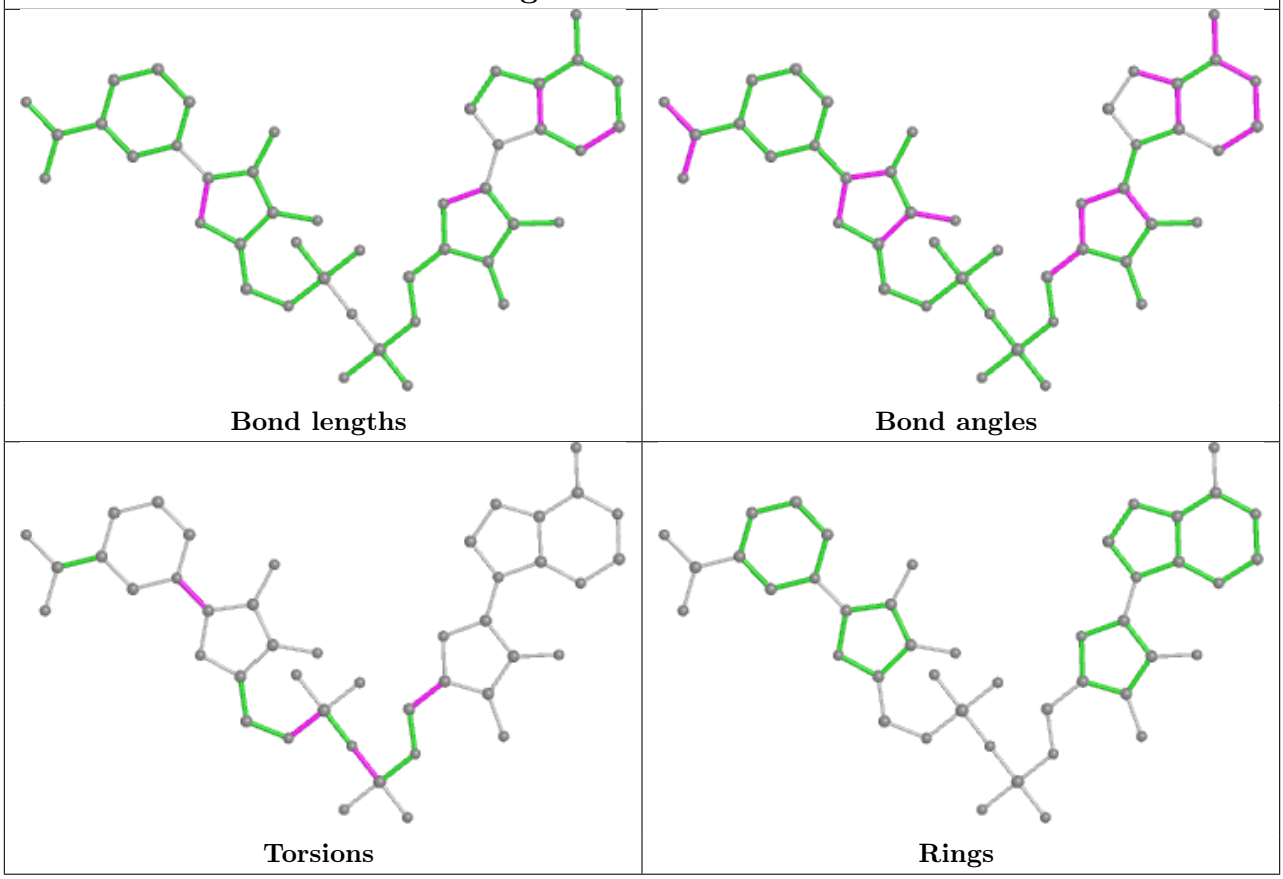


Rings

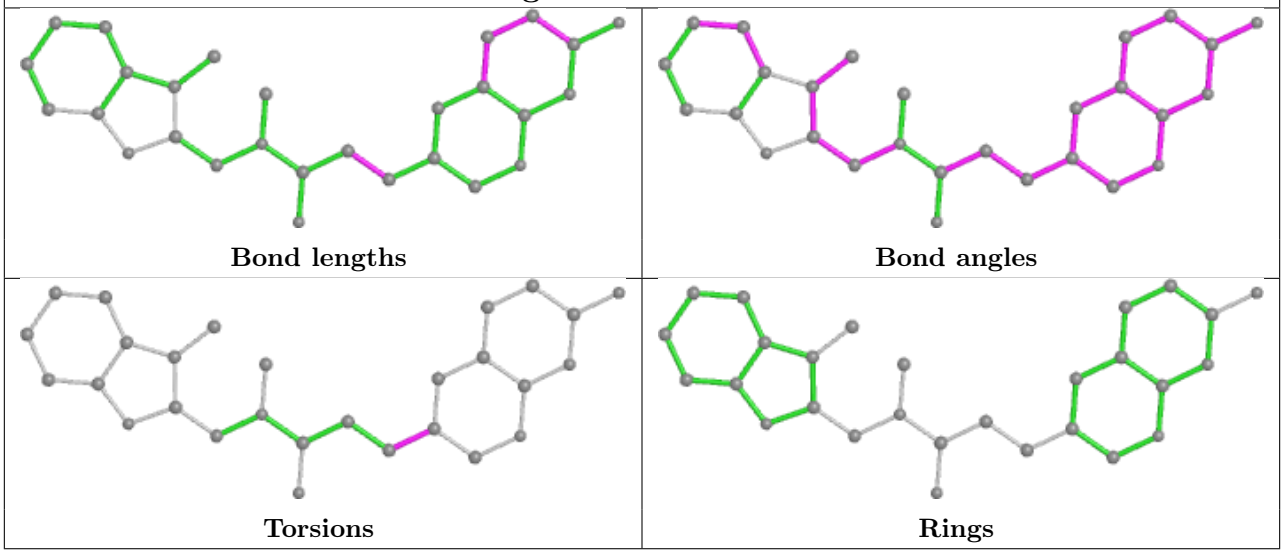
Ligand 0WE B 301



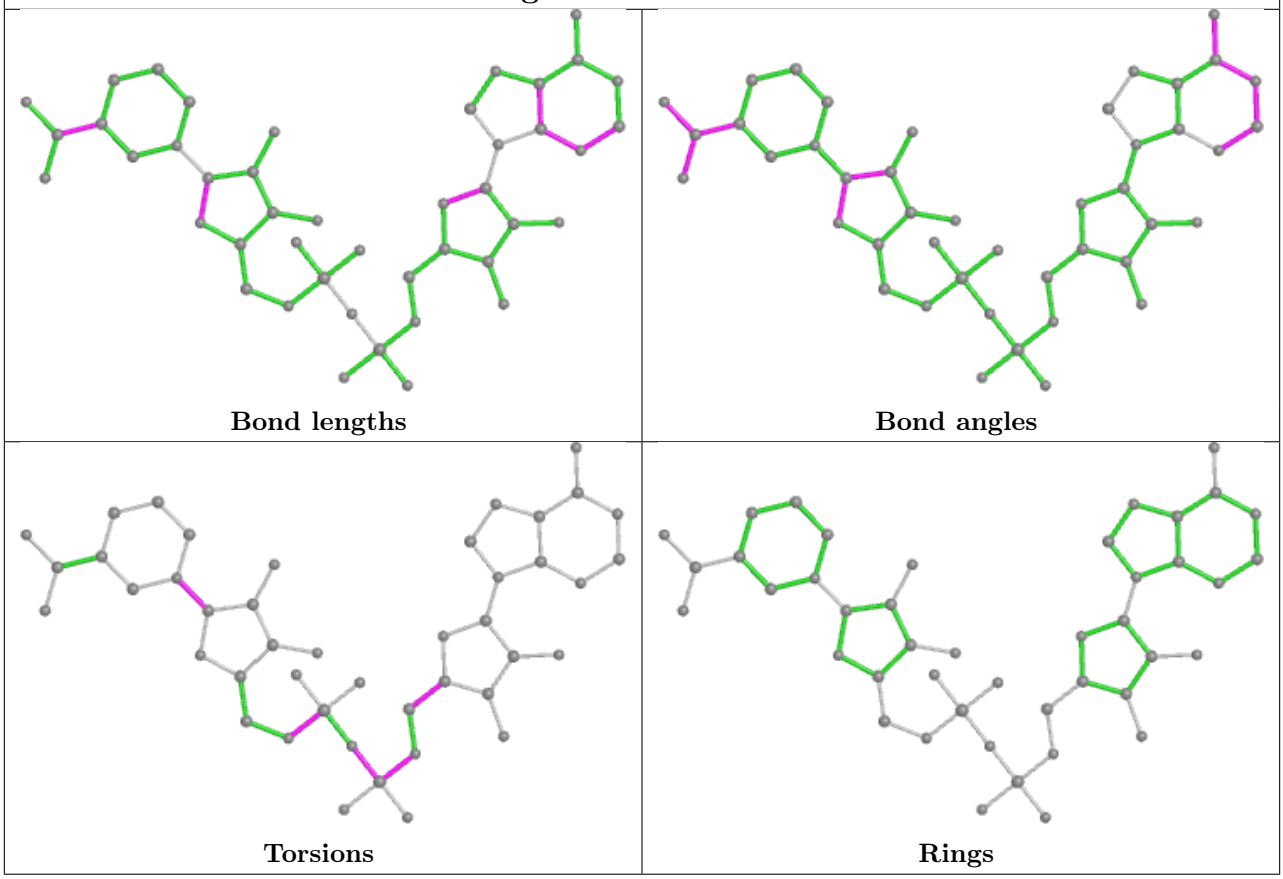
Ligand NAD D 300



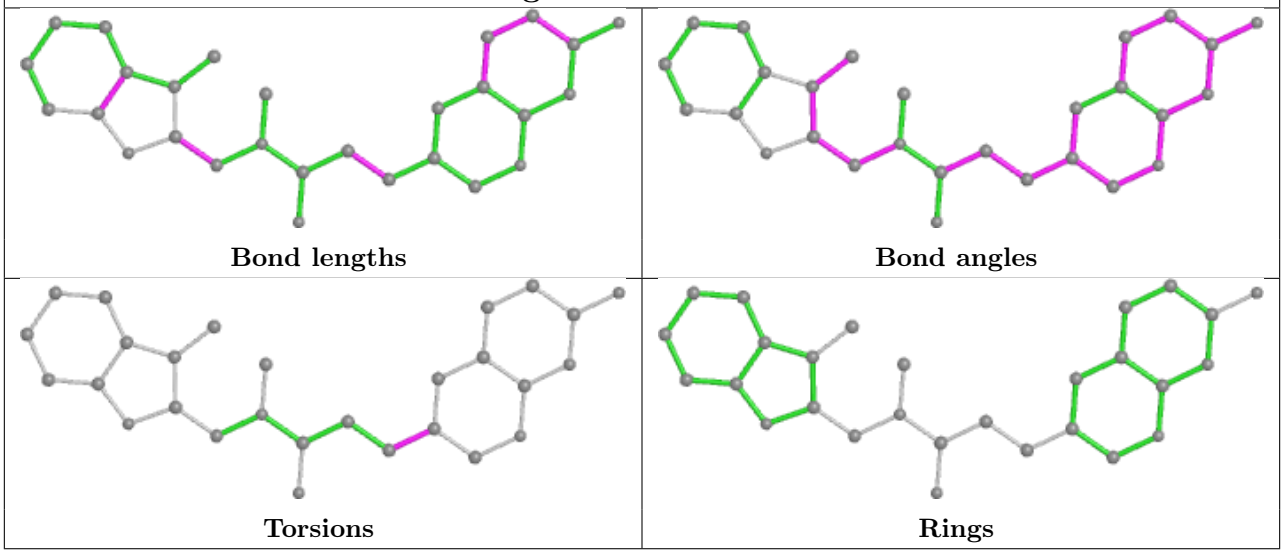
Ligand 0WE D 301



Ligand NAD B 300



Ligand 0WE A 301



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/267 (97%)	-0.03	9 (3%)	44	51	35, 53, 85, 104	0
1	B	260/267 (97%)	-0.07	3 (1%)	79	83	35, 53, 81, 115	0
1	C	260/267 (97%)	0.10	12 (4%)	32	39	36, 54, 80, 105	0
1	D	260/267 (97%)	0.03	10 (3%)	40	47	37, 56, 83, 108	0
All	All	1040/1068 (97%)	0.01	34 (3%)	46	53	35, 54, 83, 115	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	LYS	3.9
1	C	61	LEU	3.7
1	D	60	LYS	3.6
1	B	60	LYS	3.5
1	D	61	LEU	3.4

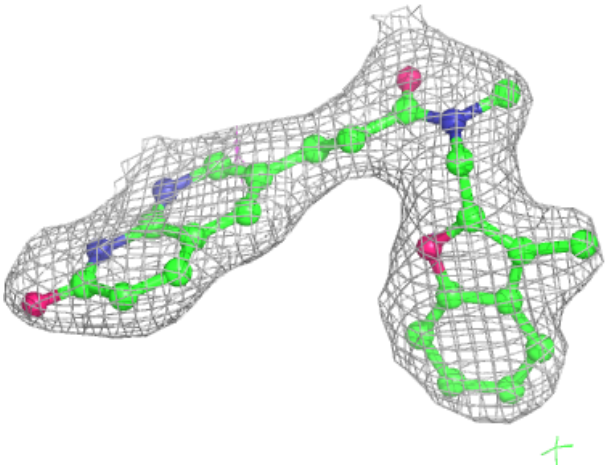
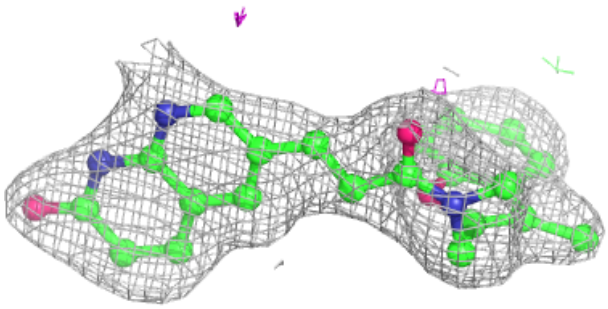
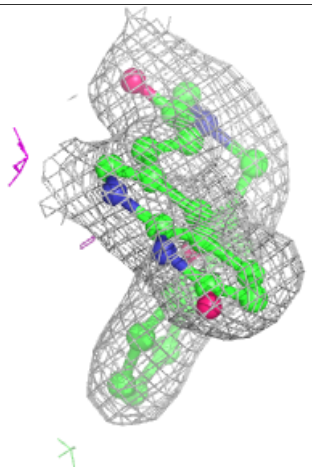
6.2 Non-standard residues in protein, DNA, RNA chains (i)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0WE	C	301	28/28	0.93	0.12	36,45,64,66	0
3	0WE	D	301	28/28	0.95	0.10	42,52,68,75	0
3	0WE	A	301	28/28	0.95	0.13	42,50,63,66	0
3	0WE	B	301	28/28	0.95	0.11	42,49,67,68	0

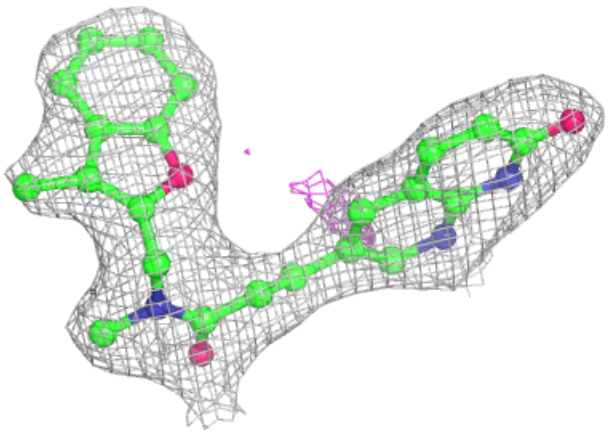
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

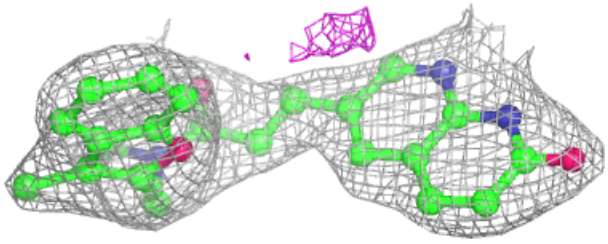
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

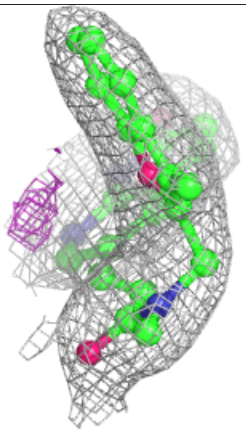
Electron density around 0WE C 301: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around 0WE D 301:

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

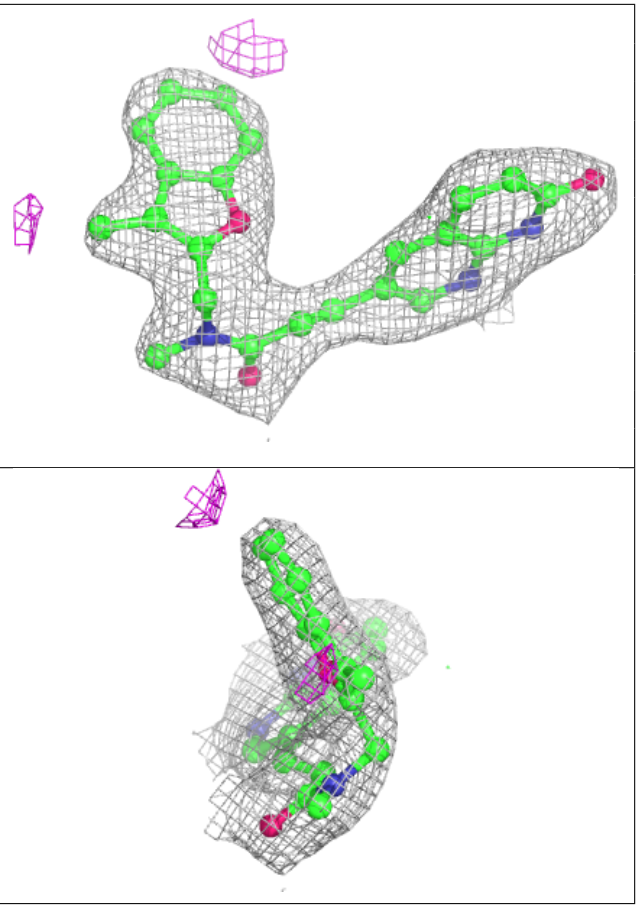






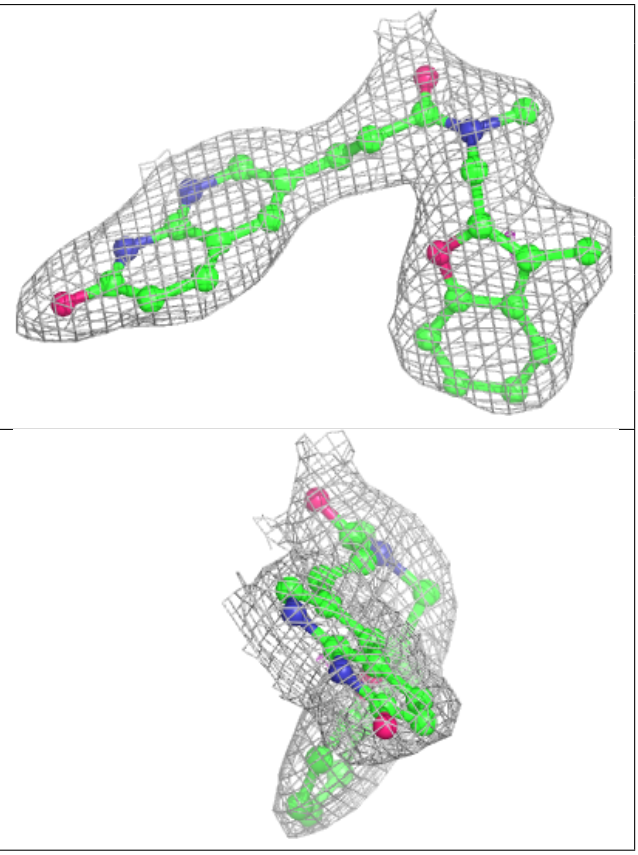
Electron density around 0WE A 301:

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



Electron density around 0WE B 301:

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



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

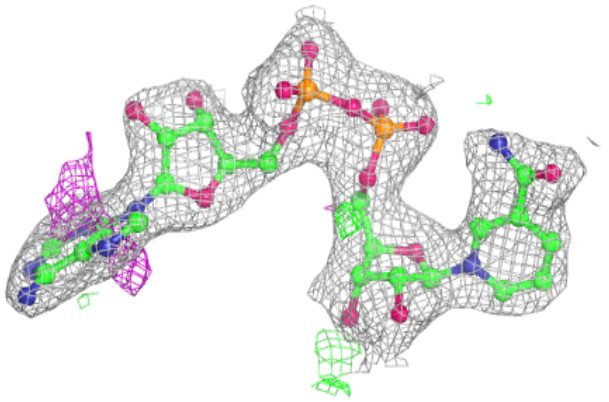
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

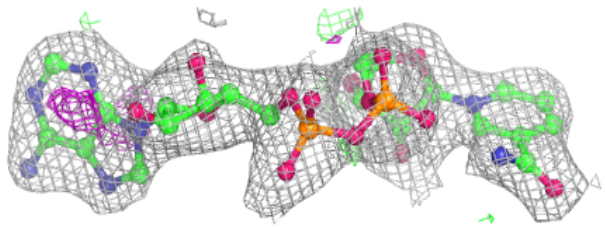
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	300	44/44	0.91	0.14	52,62,73,76	0
3	0WE	C	301	28/28	0.93	0.12	36,45,64,66	0
2	NAD	B	300	44/44	0.94	0.10	40,51,63,72	0
2	NAD	A	300	44/44	0.94	0.11	41,59,70,74	0
3	0WE	D	301	28/28	0.95	0.10	42,52,68,75	0
3	0WE	A	301	28/28	0.95	0.13	42,50,63,66	0
3	0WE	B	301	28/28	0.95	0.11	42,49,67,68	0
2	NAD	D	300	44/44	0.96	0.09	43,56,65,68	0

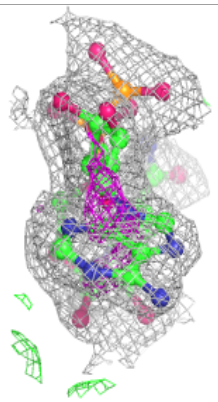
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 300:

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

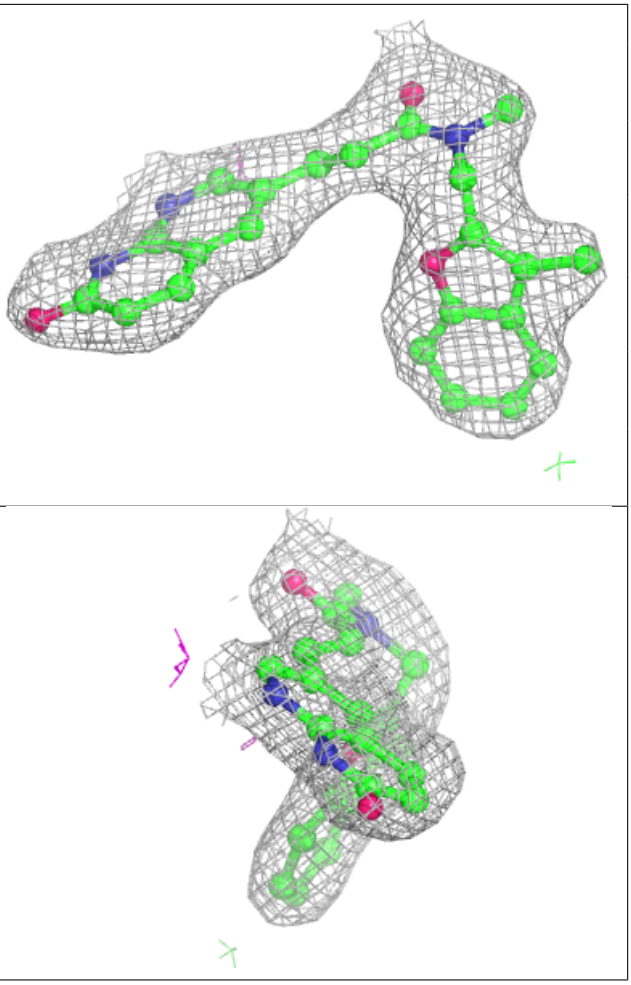


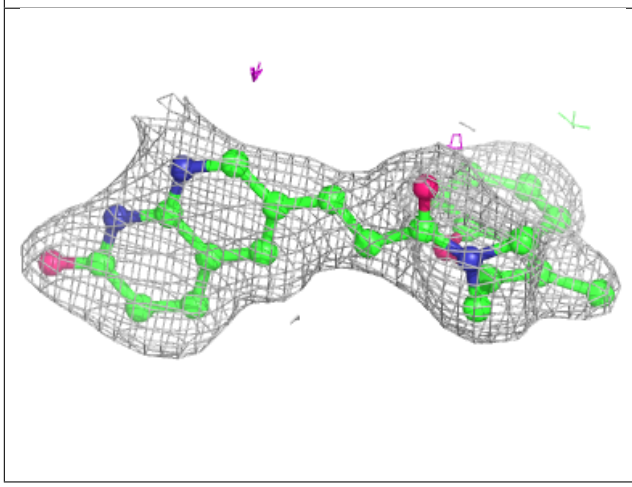




Electron density around 0WE C 301:

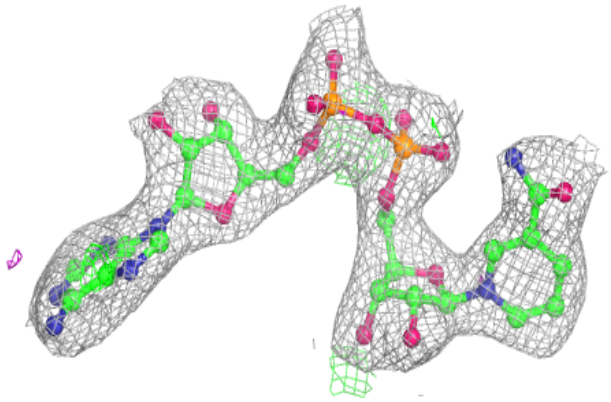
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

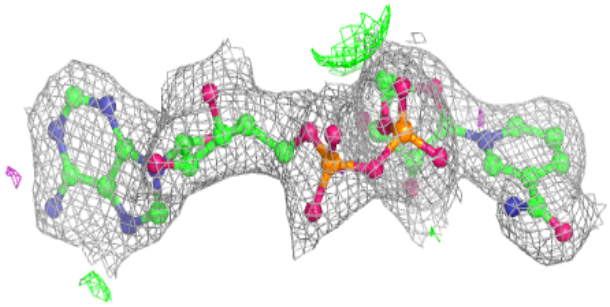


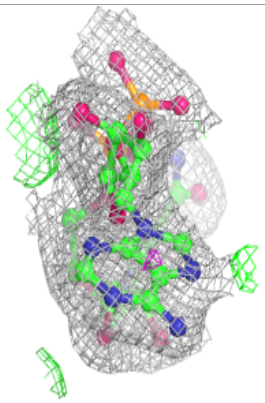


Electron density around NAD B 300:

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

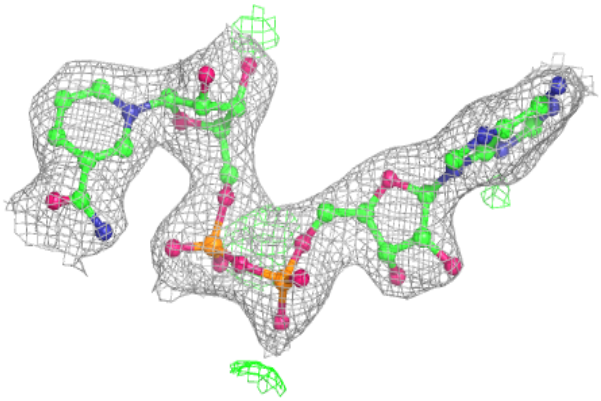


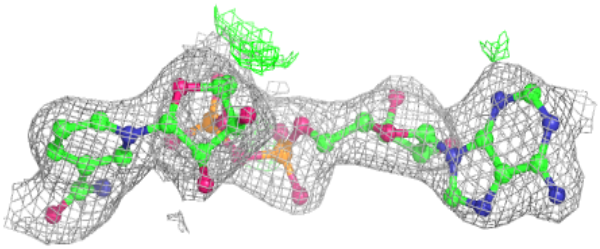


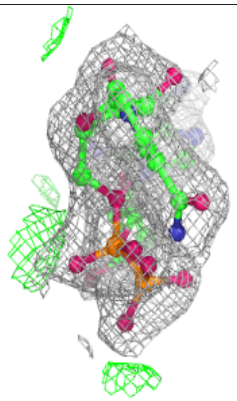


Electron density around NAD A 300:

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

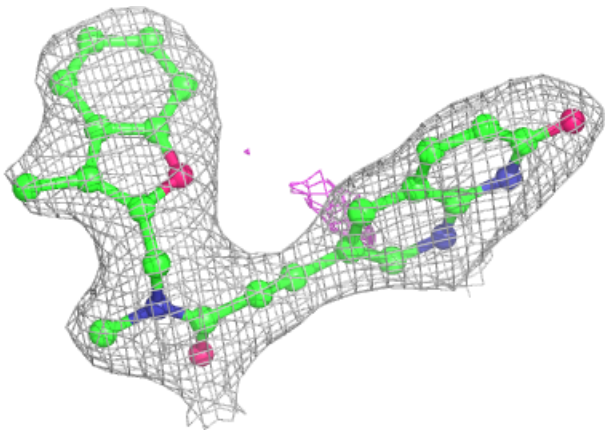


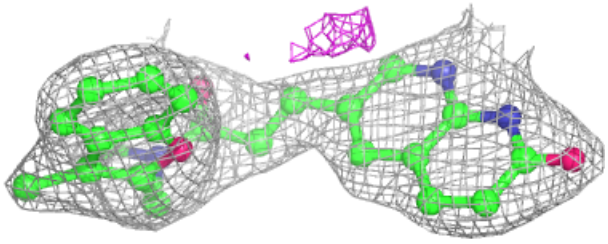


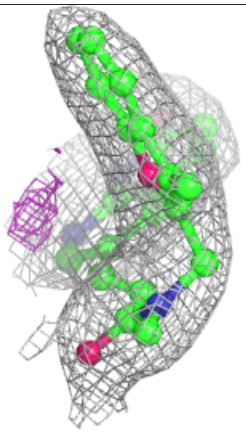


Electron density around 0WE D 301:

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

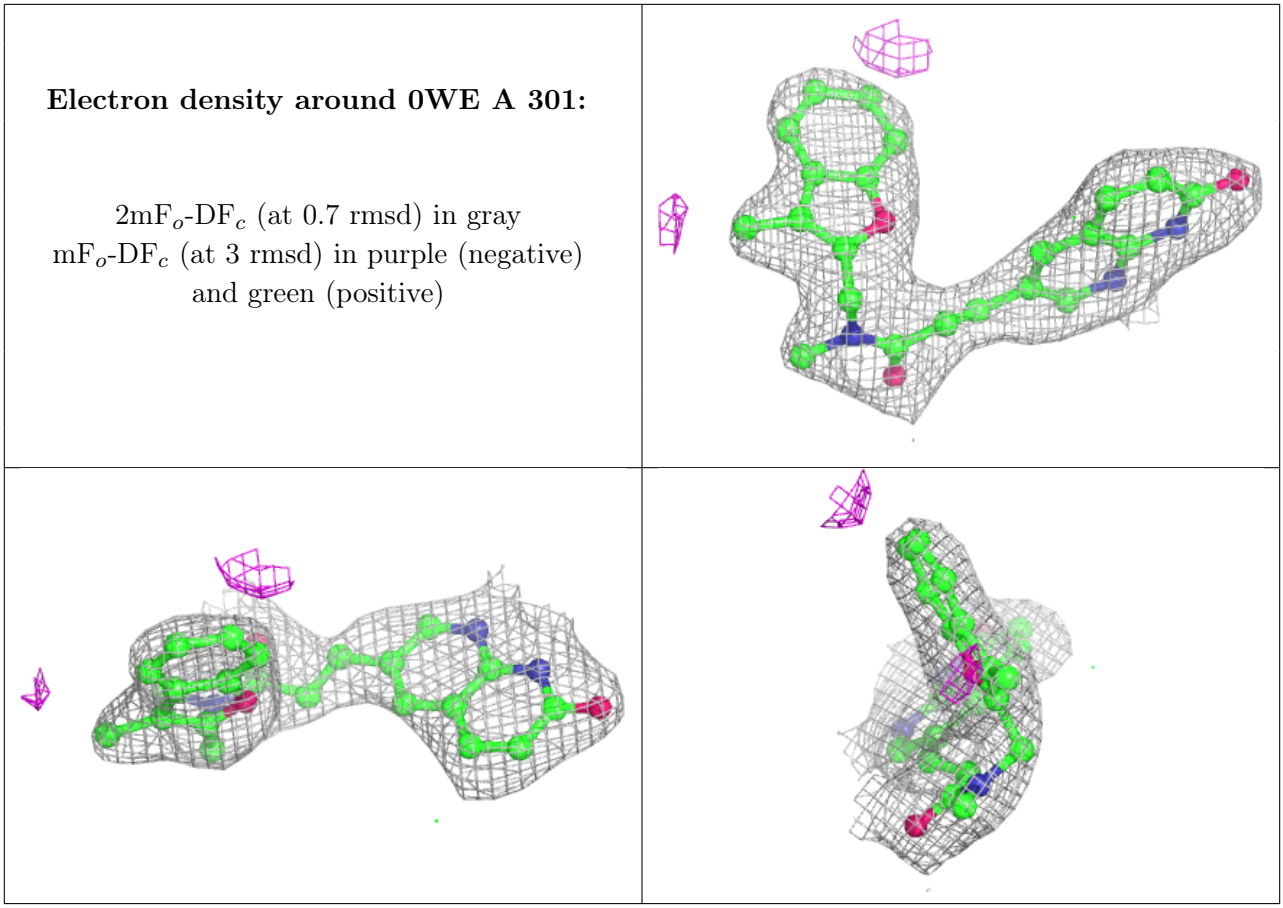






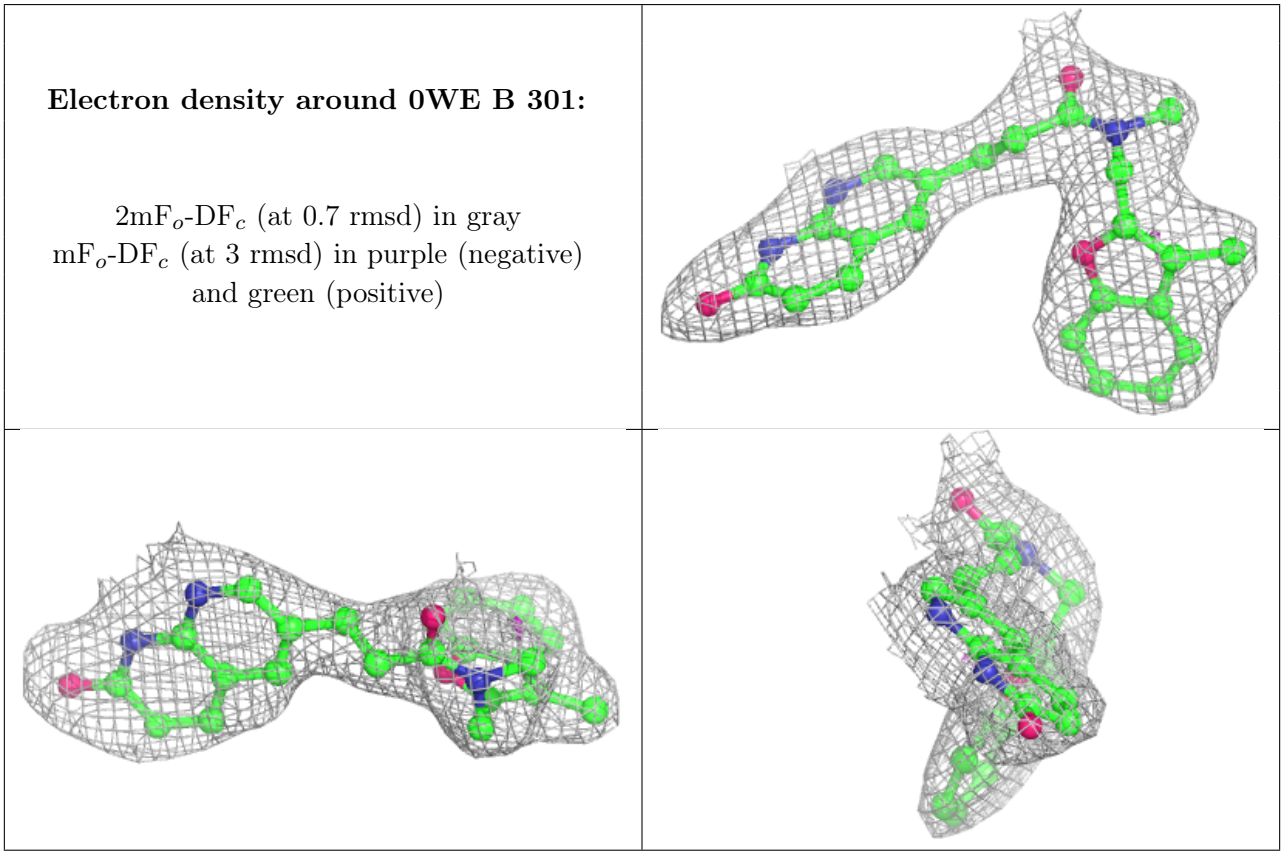
Electron density around 0WE A 301:

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



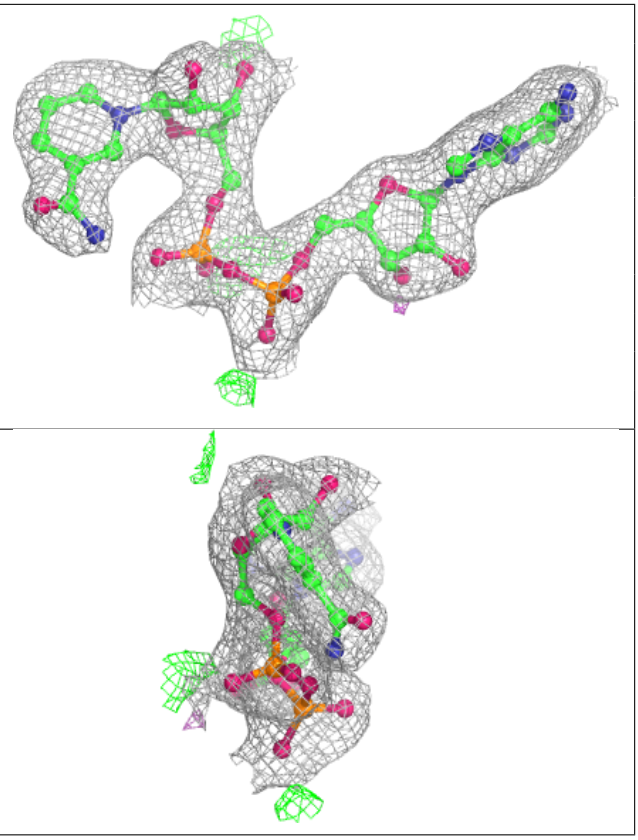
Electron density around 0WE B 301:

$2mF_o$-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 300:

$2mF_o$-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.