



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:51 AM UTC

PDB ID : 6AHE / pdb_00006ahe
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

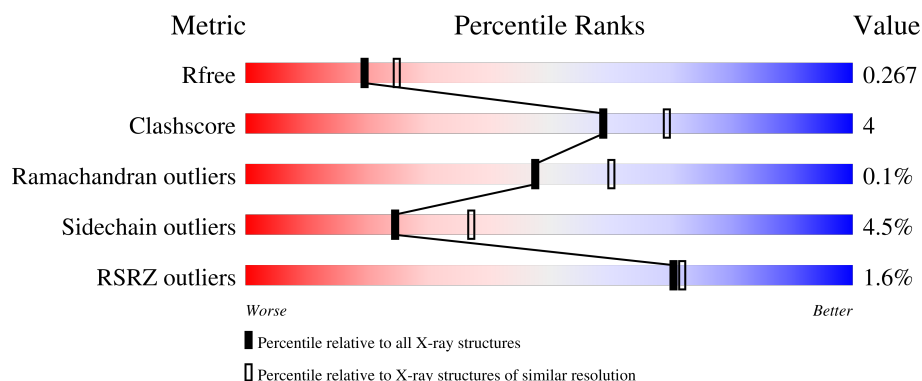
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	267	2% 86% 11% .
1	B	267	% 84% 12% ..
1	C	267	2% 84% 11% ..
1	D	267	% 82% 14% ..

2 Entry composition [i](#)

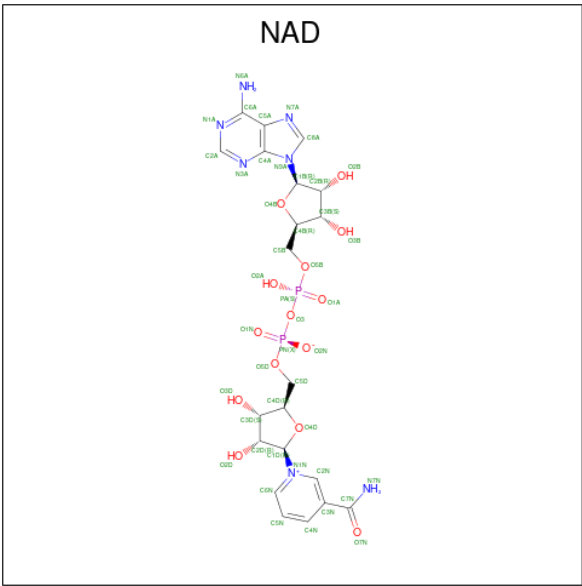
There are 4 unique types of molecules in this entry. The entry contains 8211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	260	Total	C	N	O	S	0	0	0
			1941	1233	335	364	9			
1	D	260	Total	C	N	O	S	0	0	0
			1941	1233	335	364	9			
1	C	260	Total	C	N	O	S	0	0	0
			1945	1236	336	364	9			
1	B	260	Total	C	N	O	S	0	0	0
			1941	1233	335	364	9			

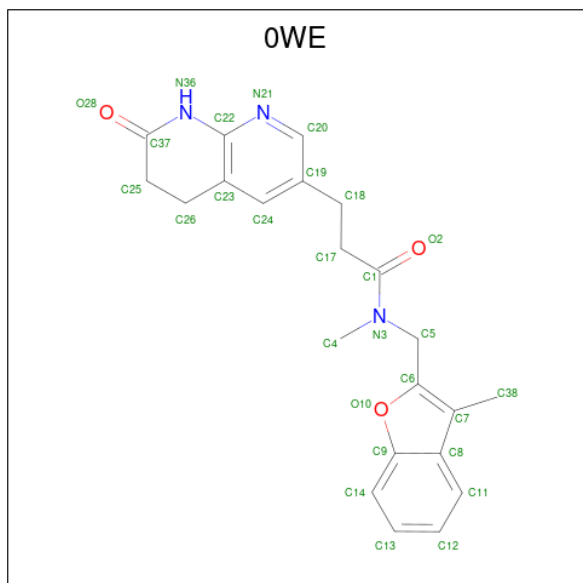
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- 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 (CCD ID: 0WE) (formula: $C_{22}H_{23}N_3O_3$).



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

- Molecule 4 is water.

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

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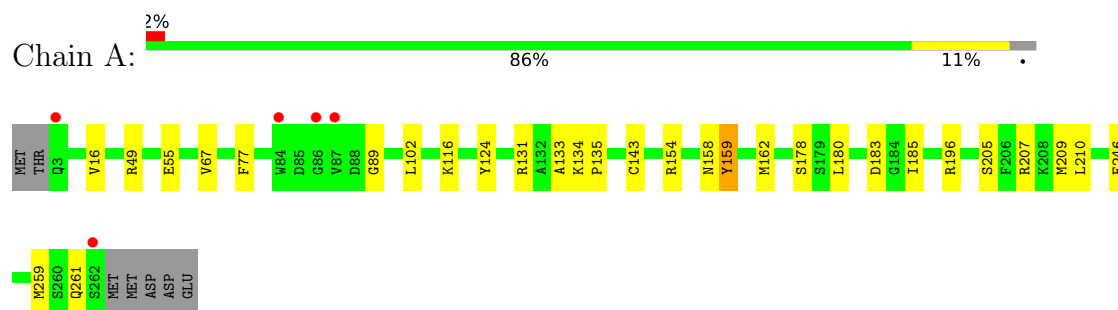
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	41	Total	O	0	0
			41	41		

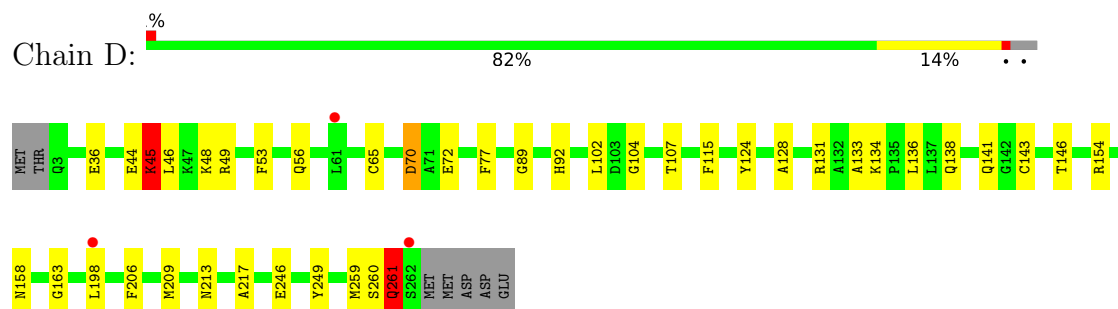
3 Residue-property plots [i](#)

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.

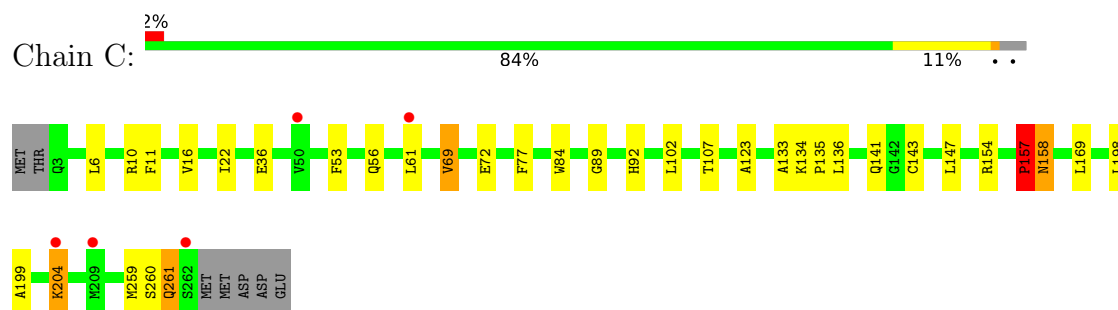
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



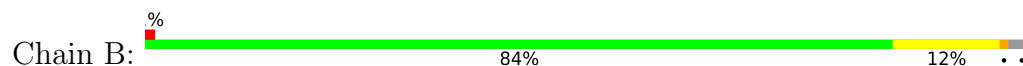
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

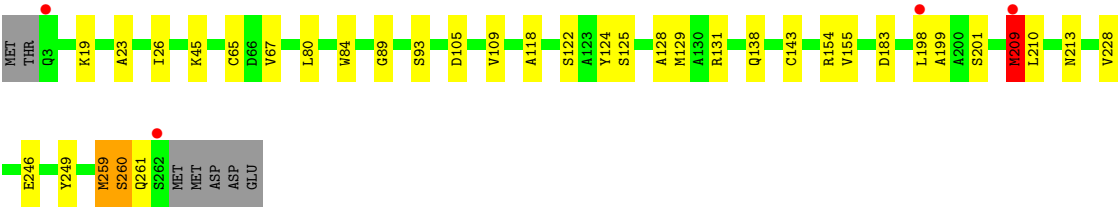


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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





4 Data and refinement statistics

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 79.74 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (79.74-2.29) 99.4 (79.74-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.85%)	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)	0.29 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.96	0/1977	1.18	2/2677 (0.1%)
1	B	0.97	0/1977	1.15	5/2677 (0.2%)
1	C	1.01	1/1981 (0.1%)	1.17	5/2681 (0.2%)
1	D	1.00	0/1977	1.22	7/2677 (0.3%)
All	All	0.99	1/7912 (0.0%)	1.18	19/10712 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	157	PRO	CA-C	5.35	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ASN	N-CA-CB	-10.11	94.30	110.98
1	C	157	PRO	N-CA-C	8.43	129.84	112.47
1	A	159	TYR	N-CA-C	-8.08	102.31	112.90
1	D	261	GLN	CB-CA-C	6.79	118.15	109.80
1	C	136	LEU	N-CA-C	5.91	117.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	VAL	CB-CA-C	5.72	117.58	111.35
1	B	209	MET	CB-CG-SD	-5.58	95.95	112.70
1	B	228	VAL	N-CA-C	-5.43	105.24	110.72
1	D	45	LYS	CB-CA-C	5.37	121.10	110.42
1	D	72	GLU	N-CA-C	5.36	117.82	111.33
1	D	163	GLY	N-CA-C	-5.33	105.95	112.77
1	D	206	PHE	N-CA-C	5.30	117.74	111.33
1	D	217	ALA	CA-C-N	5.27	125.33	119.32
1	D	217	ALA	C-N-CA	5.27	125.33	119.32
1	B	155	VAL	N-CA-C	5.21	115.71	108.84
1	B	26	ILE	N-CA-C	5.10	115.32	110.42
1	B	65	CYS	N-CA-C	5.09	116.19	107.28
1	C	36	GLU	N-CA-C	-5.09	101.42	109.76
1	C	259	MET	N-CA-C	5.08	117.10	109.23

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	16	0
1	B	1941	0	1924	23	0
1	C	1945	0	1935	18	0
1	D	1941	0	1924	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	70	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.

All (70) 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:259:MET:HE3	1:B:209:MET:HE2	1.23	1.19
1:A:259:MET:CE	1:B:209:MET:HE2	1.91	0.99
1:A:259:MET:HE3	1:B:209:MET:CE	2.01	0.90
1:D:154:ARG:NH1	1:C:154:ARG:HD3	1.90	0.85
1:C:260:SER:O	1:C:261:GLN:C	2.32	0.72
1:C:53:PHE:O	1:C:56:GLN:HB3	1.94	0.68
1:C:199:ALA:HB1	3:C:301:OWE:H1	1.79	0.64
1:D:104:GLY:H	1:D:158:ASN:HD22	1.45	0.62
1:D:102:LEU:O	1:D:158:ASN:HB3	2.00	0.61
1:D:104:GLY:H	1:D:158:ASN:ND2	1.98	0.61
1:D:260:SER:O	1:D:261:GLN:C	2.43	0.61
1:D:44:GLU:O	1:D:45:LYS:C	2.43	0.61
1:C:199:ALA:O	3:C:301:OWE:H5	2.02	0.60
1:C:89:GLY:HA2	1:C:143:CYS:O	2.03	0.59
1:A:67:VAL:HG22	2:A:300:NAD:N1A	2.18	0.58
1:D:89:GLY:HA2	1:D:143:CYS:O	2.04	0.57
1:D:154:ARG:CZ	1:C:154:ARG:HD3	2.35	0.57
1:D:44:GLU:HA	1:D:44:GLU:OE1	2.05	0.56
1:B:105:ASP:O	1:B:109:VAL:HG22	2.08	0.54
1:C:6:LEU:HD13	1:C:11:PHE:CE1	2.44	0.53
1:C:134:LYS:HB3	1:C:135:PRO:HD3	1.91	0.52
1:D:44:GLU:O	1:D:46:LEU:N	2.43	0.52
1:A:180:LEU:HB3	1:A:185:ILE:HB	1.91	0.52
1:A:154:ARG:CZ	1:B:154:ARG:CZ	2.88	0.51
1:A:89:GLY:HA2	1:A:143:CYS:O	2.11	0.51
1:C:69:VAL:HG12	1:C:72:GLU:H	1.77	0.50
1:B:80:LEU:HD11	1:B:84:TRP:CE3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:O	1:D:56:GLN:HB2	2.14	0.48
1:C:10:ARG:HB3	1:C:84:TRP:CH2	2.48	0.48
1:B:199:ALA:O	3:B:301:OWE:H5	2.14	0.48
1:D:134:LYS:O	1:D:138:GLN:HB2	2.13	0.48
1:B:93:SER:OG	2:B:300:NAD:H52N	2.14	0.48
1:A:134:LYS:HB3	1:A:135:PRO:HD3	1.96	0.48
1:A:246:GLU:HA	1:A:246:GLU:OE1	2.14	0.47
1:D:48:LYS:HB3	4:D:426:HOH:O	2.15	0.47
1:B:118:ALA:O	1:B:122:SER:HB2	2.15	0.47
1:B:124:TYR:CE2	1:B:128:ALA:HB2	2.50	0.47
1:B:154:ARG:HH21	1:B:154:ARG:HG3	1.79	0.47
1:A:77:PHE:CE2	1:A:133:ALA:HB2	2.50	0.46
1:D:49:ARG:HD2	1:D:49:ARG:H	1.80	0.46
1:A:159:TYR:O	1:A:162:MET:HB2	2.15	0.46
1:C:107:THR:O	1:B:131:ARG:HD3	2.16	0.45
1:B:67:VAL:HB	1:B:125:SER:HB2	1.99	0.45
1:B:260:SER:O	1:B:261:GLN:C	2.60	0.45
1:A:102:LEU:HD21	1:A:162:MET:HG2	1.98	0.44
1:D:124:TYR:CE2	1:D:128:ALA:HB2	2.52	0.44
1:B:89:GLY:HA2	1:B:143:CYS:O	2.17	0.44
1:D:77:PHE:CE2	1:D:133:ALA:HB2	2.52	0.44
1:D:70:ASP:OD1	1:D:70:ASP:N	2.52	0.43
1:B:129:MET:HE2	1:B:129:MET:HB3	1.94	0.43
1:A:158:ASN:O	3:A:301:OWE:H21	2.18	0.43
1:D:92:HIS:O	1:D:146:THR:HA	2.18	0.43
1:D:44:GLU:C	1:D:46:LEU:N	2.76	0.43
1:D:246:GLU:OE1	1:B:249:TYR:HB2	2.18	0.43
1:C:204:LYS:H	1:C:204:LYS:HG2	1.35	0.43
1:D:249:TYR:HB2	1:B:246:GLU:OE1	2.19	0.43
1:C:22:ILE:HG21	1:C:147:LEU:HG	2.00	0.43
1:A:259:MET:HE1	1:B:209:MET:HE2	1.93	0.42
1:A:131:ARG:HD3	1:D:107:THR:O	2.19	0.42
1:B:67:VAL:HG22	2:B:300:NAD:N1A	2.34	0.42
1:A:124:TYR:HB2	1:D:115:PHE:CD1	2.54	0.41
1:D:259:MET:O	1:C:157:PRO:HD3	2.20	0.41
1:C:123:ALA:HA	1:C:169:LEU:HD13	2.02	0.41
1:C:77:PHE:CE2	1:C:133:ALA:HB2	2.56	0.41
1:B:138:GLN:HE21	1:B:183:ASP:CG	2.29	0.41
1:D:124:TYR:OH	1:D:131:ARG:NH2	2.52	0.40
2:D:300:NAD:H8A	4:D:413:HOH:O	2.20	0.40
1:B:23:ALA:HB2	1:B:93:SER:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:MET:HE2	1:B:259:MET:HB2	1.83	0.40
1:C:102:LEU:O	1:C:158:ASN:HB3	2.21	0.40

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%)	30	38
All	All	1032/1068 (97%)	976 (95%)	55 (5%)	1 (0%)	48	60

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%)	185 (95%)	10 (5%)	21	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	195/206 (95%)	186 (95%)	9 (5%)	24	36
1	C	196/206 (95%)	188 (96%)	8 (4%)	27	41
1	D	195/206 (95%)	187 (96%)	8 (4%)	27	41
All	All	781/824 (95%)	746 (96%)	35 (4%)	24	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	55	GLU
1	A	116	LYS
1	A	178	SER
1	A	183	ASP
1	A	196	ARG
1	A	205	SER
1	A	207	ARG
1	A	209	MET
1	A	210	LEU
1	D	36	GLU
1	D	65	CYS
1	D	70	ASP
1	D	136	LEU
1	D	141	GLN
1	D	198	LEU
1	D	209	MET
1	D	213	ASN
1	C	16	VAL
1	C	61	LEU
1	C	69	VAL
1	C	92	HIS
1	C	141	GLN
1	C	157	PRO
1	C	198	LEU
1	C	204	LYS
1	B	19	LYS
1	B	45	LYS
1	B	198	LEU
1	B	201	SER
1	B	209	MET
1	B	210	LEU
1	B	213	ASN

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Mol	Chain	Res	Type
1	B	259	MET
1	B	260	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	138	GLN
1	A	141	GLN
1	A	213	ASN
1	D	141	GLN
1	D	150	GLN
1	D	158	ASN
1	D	222	ASN
1	C	28	GLN
1	C	83	HIS
1	C	141	GLN
1	C	213	ASN
1	B	56	GLN
1	B	138	GLN
1	B	141	GLN
1	B	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	301	-	29,31,31	2.13	5 (17%)	40,44,44	2.54	18 (45%)
3	0WE	D	301	-	29,31,31	2.11	6 (20%)	40,44,44	2.82	18 (45%)
3	0WE	C	301	-	29,31,31	2.18	6 (20%)	40,44,44	2.76	18 (45%)
3	0WE	B	301	-	29,31,31	2.22	6 (20%)	40,44,44	2.73	20 (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	A	301	-	-	2/13/22/22	0/4/4/4
3	0WE	D	301	-	-	2/13/22/22	0/4/4/4
3	0WE	C	301	-	-	2/13/22/22	0/4/4/4
3	0WE	B	301	-	-	1/13/22/22	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	0WE	C26-C23	-6.32	1.40	1.51
3	A	301	0WE	C26-C23	-6.08	1.41	1.51
3	D	301	0WE	C26-C23	-5.91	1.41	1.51
3	C	301	0WE	C26-C23	-5.13	1.42	1.51
3	D	301	0WE	C25-C37	-4.78	1.39	1.50
3	A	301	0WE	C26-C25	-4.76	1.40	1.52
3	C	301	0WE	C26-C25	-4.75	1.40	1.52
3	C	301	0WE	O10-C9	-4.71	1.30	1.38
3	B	301	0WE	O10-C9	-4.64	1.31	1.38
3	A	301	0WE	C25-C37	-4.58	1.40	1.50
3	B	301	0WE	C26-C25	-4.57	1.40	1.52
3	D	301	0WE	C26-C25	-4.41	1.41	1.52
3	B	301	0WE	C25-C37	-4.23	1.41	1.50
3	C	301	0WE	C25-C37	-4.23	1.41	1.50
3	A	301	0WE	O10-C9	-4.18	1.31	1.38
3	B	301	0WE	C18-C17	-4.08	1.33	1.52
3	C	301	0WE	C18-C17	-3.91	1.34	1.52
3	D	301	0WE	C18-C17	-3.83	1.34	1.52
3	D	301	0WE	O10-C9	-3.79	1.32	1.38
3	A	301	0WE	C18-C17	-3.79	1.34	1.52
3	C	301	0WE	C1-N3	-2.55	1.31	1.34
3	D	301	0WE	C8-C7	-2.25	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	0WE	C8-C7	-2.11	1.40	1.44

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	0WE	C38-C7-C6	8.77	137.10	127.10
3	B	301	0WE	C18-C17-C1	7.09	120.39	112.33
3	C	301	0WE	C38-C7-C6	6.44	134.44	127.10
3	C	301	0WE	C6-C5-N3	-6.40	103.03	113.11
3	A	301	0WE	C6-C5-N3	-6.33	103.14	113.11
3	B	301	0WE	C6-C5-N3	-6.31	103.16	113.11
3	D	301	0WE	C38-C7-C8	-6.26	113.69	124.76
3	D	301	0WE	C18-C17-C1	5.98	119.13	112.33
3	A	301	0WE	O10-C6-C5	5.55	124.83	116.06
3	B	301	0WE	O10-C6-C5	5.39	124.57	116.06
3	B	301	0WE	C38-C7-C6	5.37	133.22	127.10
3	C	301	0WE	O10-C6-C5	4.40	123.01	116.06
3	C	301	0WE	C25-C37-N36	4.40	121.25	116.31
3	C	301	0WE	C9-O10-C6	4.38	110.37	106.04
3	C	301	0WE	C38-C7-C8	-4.26	117.22	124.76
3	A	301	0WE	C9-O10-C6	4.24	110.23	106.04
3	A	301	0WE	C25-C26-C23	4.13	120.19	111.97
3	D	301	0WE	C9-O10-C6	4.09	110.08	106.04
3	A	301	0WE	C25-C37-N36	3.93	120.72	116.31
3	C	301	0WE	C24-C19-C20	3.86	120.48	116.90
3	B	301	0WE	C25-C26-C23	3.83	119.60	111.97
3	C	301	0WE	C18-C17-C1	3.83	116.69	112.33
3	C	301	0WE	O28-C37-N36	-3.83	117.33	121.39
3	C	301	0WE	C25-C26-C23	3.78	119.50	111.97
3	D	301	0WE	O10-C6-C5	3.76	122.00	116.06
3	D	301	0WE	C25-C37-N36	3.71	120.48	116.31
3	D	301	0WE	C25-C26-C23	3.69	119.31	111.97
3	D	301	0WE	C17-C18-C19	3.64	125.48	112.70
3	D	301	0WE	C6-C5-N3	-3.63	107.39	113.11
3	B	301	0WE	C38-C7-C8	-3.63	118.34	124.76
3	A	301	0WE	C17-C18-C19	3.61	125.40	112.70
3	B	301	0WE	C9-O10-C6	3.58	109.58	106.04
3	A	301	0WE	C38-C7-C6	3.56	131.17	127.10
3	A	301	0WE	C18-C17-C1	3.47	116.27	112.33
3	B	301	0WE	C25-C37-N36	3.36	120.08	116.31
3	C	301	0WE	C17-C18-C19	3.30	124.31	112.70
3	A	301	0WE	O28-C37-N36	-3.26	117.93	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	0WE	C17-C18-C19	3.21	124.00	112.70
3	B	301	0WE	N36-C22-N21	2.97	120.82	116.38
3	A	301	0WE	C24-C19-C20	2.97	119.65	116.90
3	C	301	0WE	C19-C20-N21	-2.94	119.62	123.99
3	D	301	0WE	C8-C7-C6	2.86	109.21	105.85
3	B	301	0WE	C4-N3-C5	-2.81	112.74	116.89
3	A	301	0WE	C20-N21-C22	2.79	121.66	116.19
3	C	301	0WE	N36-C22-N21	2.64	120.32	116.38
3	A	301	0WE	C19-C20-N21	-2.63	120.08	123.99
3	A	301	0WE	C38-C7-C8	-2.61	120.14	124.76
3	B	301	0WE	C24-C19-C20	2.61	119.32	116.90
3	A	301	0WE	C18-C19-C20	-2.59	117.13	121.73
3	C	301	0WE	C5-N3-C1	2.57	128.13	120.58
3	A	301	0WE	C4-N3-C5	-2.53	113.16	116.89
3	B	301	0WE	C20-N21-C22	2.53	121.14	116.19
3	C	301	0WE	C20-N21-C22	2.50	121.08	116.19
3	A	301	0WE	C8-C7-C6	2.40	108.67	105.85
3	D	301	0WE	C26-C25-C37	2.39	119.08	113.77
3	D	301	0WE	C13-C12-C11	2.38	123.18	120.24
3	B	301	0WE	C19-C20-N21	-2.38	120.46	123.99
3	B	301	0WE	C26-C25-C37	2.35	118.99	113.77
3	B	301	0WE	C5-N3-C1	2.34	127.47	120.58
3	C	301	0WE	C12-C13-C14	2.33	123.11	120.24
3	D	301	0WE	C24-C19-C20	2.30	119.03	116.90
3	D	301	0WE	C20-N21-C22	2.30	120.69	116.19
3	D	301	0WE	O28-C37-N36	-2.27	118.98	121.39
3	C	301	0WE	C13-C14-C9	-2.24	115.53	119.60
3	D	301	0WE	C11-C8-C9	2.23	121.39	118.88
3	B	301	0WE	C17-C1-N3	2.22	121.87	118.08
3	B	301	0WE	C8-C7-C6	2.20	108.44	105.85
3	A	301	0WE	N36-C22-N21	2.17	119.62	116.38
3	D	301	0WE	C18-C19-C20	-2.15	117.92	121.73
3	C	301	0WE	C8-C7-C6	2.11	108.33	105.85
3	B	301	0WE	O2-C1-C17	-2.10	115.58	121.26
3	B	301	0WE	C13-C14-C9	-2.08	115.81	119.60
3	D	301	0WE	C12-C11-C8	-2.04	116.11	119.80
3	A	301	0WE	C26-C25-C37	2.01	118.22	113.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

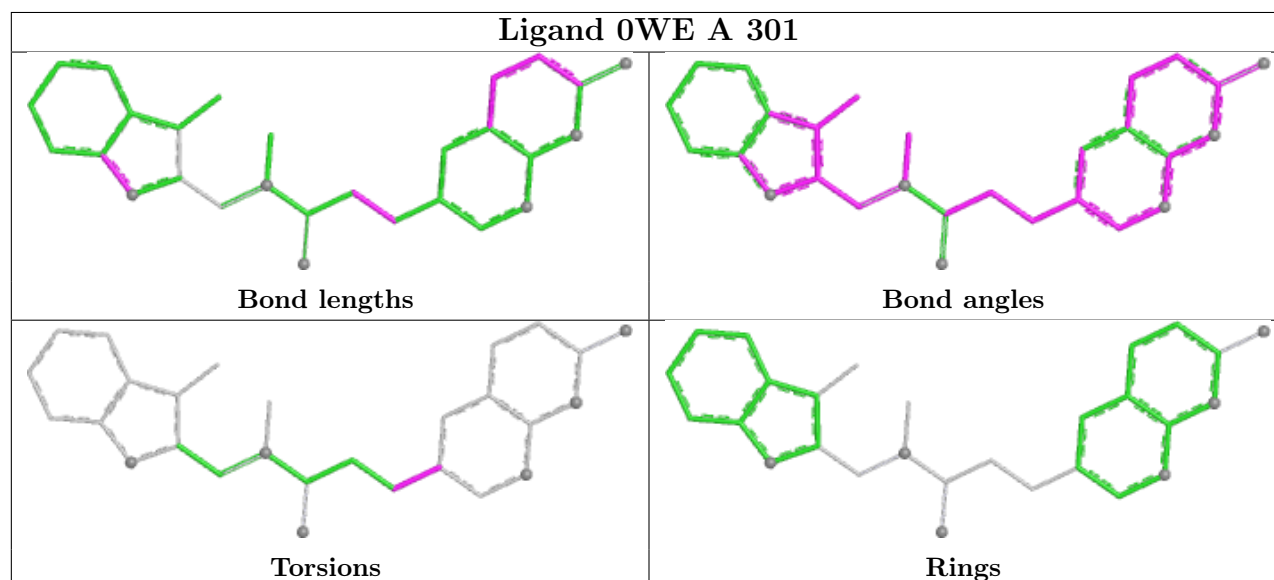
Mol	Chain	Res	Type	Atoms
3	C	301	0WE	C17-C18-C19-C20
3	D	301	0WE	C17-C18-C19-C24
3	A	301	0WE	C17-C18-C19-C24
3	C	301	0WE	C17-C18-C19-C24
3	B	301	0WE	C17-C18-C19-C24
3	A	301	0WE	C17-C18-C19-C20
3	D	301	0WE	C17-C18-C19-C20

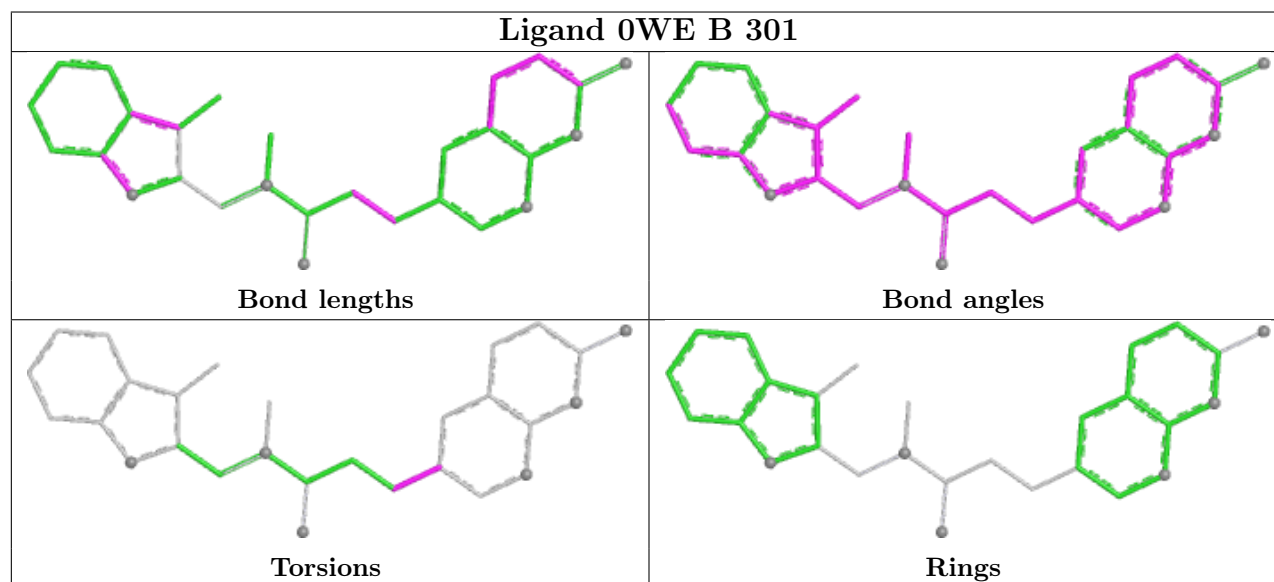
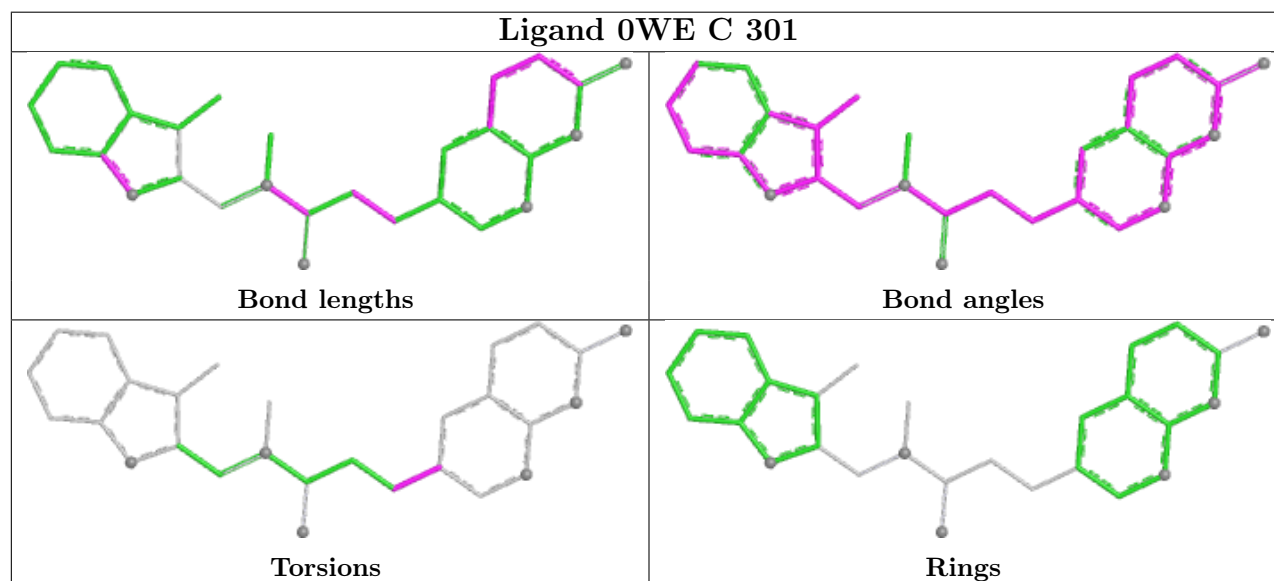
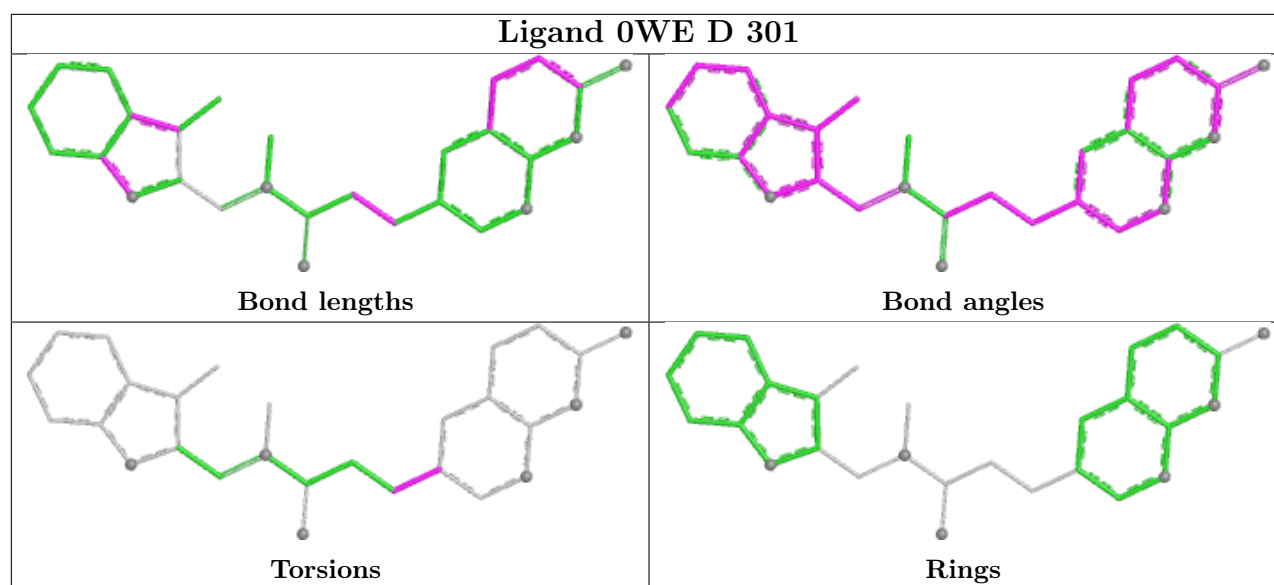
There are no ring outliers.

3 monomers are involved in 4 short contacts:

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





5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	300	-	46,48,48	1.66	8 (17%)	64,73,73	1.95	14 (21%)
3	0WE	A	301	-	29,31,31	2.13	5 (17%)	40,44,44	2.54	18 (45%)
2	NAD	C	300	-	46,48,48	1.77	7 (15%)	64,73,73	1.77	16 (25%)
3	0WE	C	301	-	29,31,31	2.18	6 (20%)	40,44,44	2.76	18 (45%)
2	NAD	A	300	-	46,48,48	1.65	8 (17%)	64,73,73	1.70	16 (25%)
3	0WE	B	301	-	29,31,31	2.22	6 (20%)	40,44,44	2.73	20 (50%)
3	0WE	D	301	-	29,31,31	2.11	6 (20%)	40,44,44	2.82	18 (45%)
2	NAD	D	300	-	46,48,48	1.57	7 (15%)	64,73,73	1.93	14 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	300	-	-	12/30/62/62	0/5/5/5
3	0WE	A	301	-	-	2/13/22/22	0/4/4/4
2	NAD	C	300	-	-	7/30/62/62	0/5/5/5
3	0WE	C	301	-	-	2/13/22/22	0/4/4/4
2	NAD	A	300	-	-	10/30/62/62	0/5/5/5
3	0WE	B	301	-	-	1/13/22/22	0/4/4/4
3	0WE	D	301	-	-	2/13/22/22	0/4/4/4
2	NAD	D	300	-	-	10/30/62/62	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	0WE	C26-C23	-6.32	1.40	1.51
2	A	300	NAD	C5A-C4A	6.09	1.49	1.39
3	A	301	0WE	C26-C23	-6.08	1.41	1.51
3	D	301	0WE	C26-C23	-5.91	1.41	1.51
2	B	300	NAD	C5A-C4A	5.85	1.49	1.39
2	C	300	NAD	C5A-C4A	5.54	1.49	1.39
3	C	301	0WE	C26-C23	-5.13	1.42	1.51
2	C	300	NAD	PA-O3	5.13	1.65	1.59
2	D	300	NAD	C5A-C4A	4.83	1.47	1.39
3	D	301	0WE	C25-C37	-4.78	1.39	1.50
3	A	301	0WE	C26-C25	-4.76	1.40	1.52
3	C	301	0WE	C26-C25	-4.75	1.40	1.52
3	C	301	0WE	O10-C9	-4.71	1.30	1.38
3	B	301	0WE	O10-C9	-4.64	1.31	1.38
3	A	301	0WE	C25-C37	-4.58	1.40	1.50
3	B	301	0WE	C26-C25	-4.57	1.40	1.52
2	C	300	NAD	PN-O3	4.48	1.64	1.59
3	D	301	0WE	C26-C25	-4.41	1.41	1.52
2	D	300	NAD	PA-O3	4.30	1.64	1.59
3	B	301	0WE	C25-C37	-4.23	1.41	1.50
3	C	301	0WE	C25-C37	-4.23	1.41	1.50
3	A	301	0WE	O10-C9	-4.18	1.31	1.38
2	D	300	NAD	PN-O3	4.13	1.64	1.59
3	B	301	0WE	C18-C17	-4.08	1.33	1.52
3	C	301	0WE	C18-C17	-3.91	1.34	1.52
2	A	300	NAD	O4D-C1D	3.88	1.46	1.40
2	B	300	NAD	PA-O3	3.88	1.63	1.59
3	D	301	0WE	C18-C17	-3.83	1.34	1.52
3	D	301	0WE	O10-C9	-3.79	1.32	1.38
3	A	301	0WE	C18-C17	-3.79	1.34	1.52
2	C	300	NAD	O4D-C1D	3.70	1.45	1.40
2	D	300	NAD	O4D-C1D	3.29	1.45	1.40
2	A	300	NAD	PA-O3	3.24	1.63	1.59
2	A	300	NAD	PN-O3	3.08	1.62	1.59
2	B	300	NAD	O4D-C1D	2.90	1.44	1.40
2	B	300	NAD	C5A-C6A	2.85	1.48	1.41
2	B	300	NAD	C4A-N3A	2.83	1.39	1.34
2	C	300	NAD	C5A-C6A	2.79	1.48	1.41
2	B	300	NAD	C8A-N7A	2.72	1.36	1.31
2	A	300	NAD	C5A-C6A	2.69	1.48	1.41
2	D	300	NAD	C5A-C6A	2.63	1.48	1.41
2	B	300	NAD	PN-O3	2.61	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NAD	C5A-N7A	-2.58	1.34	1.39
2	B	300	NAD	C3N-C7N	2.57	1.54	1.50
3	C	301	0WE	C1-N3	-2.55	1.31	1.34
2	C	300	NAD	C8A-N7A	2.50	1.36	1.31
2	A	300	NAD	C8A-N7A	2.45	1.36	1.31
2	D	300	NAD	C5A-N7A	-2.31	1.34	1.39
3	D	301	0WE	C8-C7	-2.25	1.40	1.44
2	C	300	NAD	C4A-N3A	2.22	1.38	1.34
3	B	301	0WE	C8-C7	-2.11	1.40	1.44
2	A	300	NAD	C4A-N3A	2.11	1.38	1.34
2	D	300	NAD	C8A-N7A	2.03	1.35	1.31

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	0WE	C38-C7-C6	8.77	137.10	127.10
3	B	301	0WE	C18-C17-C1	7.09	120.39	112.33
3	C	301	0WE	C38-C7-C6	6.44	134.44	127.10
3	C	301	0WE	C6-C5-N3	-6.40	103.03	113.11
3	A	301	0WE	C6-C5-N3	-6.33	103.14	113.11
3	B	301	0WE	C6-C5-N3	-6.31	103.16	113.11
3	D	301	0WE	C38-C7-C8	-6.26	113.69	124.76
2	D	300	NAD	C5A-C4A-N3A	-6.11	118.30	126.72
3	D	301	0WE	C18-C17-C1	5.98	119.13	112.33
3	A	301	0WE	O10-C6-C5	5.55	124.83	116.06
2	B	300	NAD	C5A-C4A-N3A	-5.41	119.27	126.72
2	D	300	NAD	N3A-C4A-N9A	5.39	136.34	127.17
3	B	301	0WE	O10-C6-C5	5.39	124.57	116.06
3	B	301	0WE	C38-C7-C6	5.37	133.22	127.10
2	D	300	NAD	O4B-C1B-N9A	5.36	118.38	108.09
2	B	300	NAD	N3A-C4A-N9A	5.20	136.00	127.17
2	A	300	NAD	C5A-C4A-N3A	-5.02	119.80	126.72
2	C	300	NAD	N3A-C4A-N9A	4.86	135.44	127.17
2	B	300	NAD	C3N-C7N-N7N	4.81	123.67	117.74
2	C	300	NAD	C4A-N9A-C8A	4.77	110.75	105.74
2	A	300	NAD	N3A-C4A-N9A	4.62	135.02	127.17
2	B	300	NAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	B	300	NAD	O4B-C1B-N9A	4.52	116.77	108.09
3	C	301	0WE	O10-C6-C5	4.40	123.01	116.06
3	C	301	0WE	C25-C37-N36	4.40	121.25	116.31
3	C	301	0WE	C9-O10-C6	4.38	110.37	106.04
2	C	300	NAD	N3A-C2A-N1A	-4.28	122.10	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	NAD	C5A-C4A-N3A	-4.28	120.83	126.72
2	B	300	NAD	O7N-C7N-N7N	-4.27	116.45	122.62
3	C	301	0WE	C38-C7-C8	-4.26	117.22	124.76
3	A	301	0WE	C9-O10-C6	4.24	110.23	106.04
3	A	301	0WE	C25-C26-C23	4.13	120.19	111.97
3	D	301	0WE	C9-O10-C6	4.09	110.08	106.04
3	A	301	0WE	C25-C37-N36	3.93	120.72	116.31
2	B	300	NAD	C2A-N3A-C4A	3.89	121.34	111.83
2	D	300	NAD	C2A-N3A-C4A	3.88	121.31	111.83
3	C	301	0WE	C24-C19-C20	3.86	120.48	116.90
3	B	301	0WE	C25-C26-C23	3.83	119.60	111.97
3	C	301	0WE	C18-C17-C1	3.83	116.69	112.33
3	C	301	0WE	O28-C37-N36	-3.83	117.33	121.39
3	C	301	0WE	C25-C26-C23	3.78	119.50	111.97
3	D	301	0WE	O10-C6-C5	3.76	122.00	116.06
3	D	301	0WE	C25-C37-N36	3.71	120.48	116.31
3	D	301	0WE	C25-C26-C23	3.69	119.31	111.97
3	D	301	0WE	C17-C18-C19	3.64	125.48	112.70
2	D	300	NAD	O2N-PN-O3	3.63	117.09	107.27
3	D	301	0WE	C6-C5-N3	-3.63	107.39	113.11
3	B	301	0WE	C38-C7-C8	-3.63	118.34	124.76
3	A	301	0WE	C17-C18-C19	3.61	125.40	112.70
3	B	301	0WE	C9-O10-C6	3.58	109.58	106.04
3	A	301	0WE	C38-C7-C6	3.56	131.17	127.10
2	A	300	NAD	O4B-C1B-N9A	3.52	114.86	108.09
3	A	301	0WE	C18-C17-C1	3.47	116.27	112.33
2	D	300	NAD	N3A-C2A-N1A	-3.46	123.35	128.58
2	C	300	NAD	C2A-N3A-C4A	3.41	120.16	111.83
2	D	300	NAD	C4A-N9A-C8A	3.37	109.27	105.74
3	B	301	0WE	C25-C37-N36	3.36	120.08	116.31
3	C	301	0WE	C17-C18-C19	3.30	124.31	112.70
3	A	301	0WE	O28-C37-N36	-3.26	117.93	121.39
2	D	300	NAD	C4A-C5A-N7A	-3.22	106.91	110.58
2	B	300	NAD	C4A-N9A-C8A	3.22	109.11	105.74
3	B	301	0WE	C17-C18-C19	3.21	124.00	112.70
2	A	300	NAD	C3N-C7N-N7N	3.03	121.47	117.74
2	C	300	NAD	C4B-O4B-C1B	-3.03	102.78	109.47
3	B	301	0WE	N36-C22-N21	2.97	120.82	116.38
3	A	301	0WE	C24-C19-C20	2.97	119.65	116.90
3	C	301	0WE	C19-C20-N21	-2.94	119.62	123.99
3	D	301	0WE	C8-C7-C6	2.86	109.21	105.85
2	A	300	NAD	C2A-N3A-C4A	2.84	118.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	C4A-C5A-N7A	-2.84	107.33	110.58
3	B	301	0WE	C4-N3-C5	-2.81	112.74	116.89
3	A	301	0WE	C20-N21-C22	2.79	121.66	116.19
2	D	300	NAD	C5A-N7A-C8A	2.77	107.81	103.45
2	B	300	NAD	O3-PN-O1N	-2.76	102.39	110.70
2	C	300	NAD	C2A-N1A-C6A	2.75	123.25	118.73
2	A	300	NAD	N3A-C2A-N1A	-2.73	124.45	128.58
2	C	300	NAD	N6A-C6A-N1A	2.72	124.43	118.38
2	A	300	NAD	O7N-C7N-N7N	-2.70	118.71	122.62
3	C	301	0WE	N36-C22-N21	2.64	120.32	116.38
3	A	301	0WE	C19-C20-N21	-2.63	120.08	123.99
2	B	300	NAD	C2A-N1A-C6A	2.63	123.05	118.73
2	A	300	NAD	C4A-N9A-C8A	2.62	108.49	105.74
3	A	301	0WE	C38-C7-C8	-2.61	120.14	124.76
3	B	301	0WE	C24-C19-C20	2.61	119.32	116.90
2	A	300	NAD	N6A-C6A-N1A	2.61	124.18	118.38
3	A	301	0WE	C18-C19-C20	-2.59	117.13	121.73
3	C	301	0WE	C5-N3-C1	2.57	128.13	120.58
3	A	301	0WE	C4-N3-C5	-2.53	113.16	116.89
2	A	300	NAD	O5D-C5D-C4D	2.53	117.60	108.99
3	B	301	0WE	C20-N21-C22	2.53	121.14	116.19
3	C	301	0WE	C20-N21-C22	2.50	121.08	116.19
2	C	300	NAD	O5D-C5D-C4D	2.44	117.29	108.99
2	C	300	NAD	N9A-C8A-N7A	-2.41	110.51	113.94
2	C	300	NAD	C6N-N1N-C2N	-2.41	119.83	121.88
3	A	301	0WE	C8-C7-C6	2.40	108.67	105.85
3	D	301	0WE	C26-C25-C37	2.39	119.08	113.77
2	B	300	NAD	N6A-C6A-N1A	2.39	123.70	118.38
3	D	301	0WE	C13-C12-C11	2.38	123.18	120.24
3	B	301	0WE	C19-C20-N21	-2.38	120.46	123.99
2	D	300	NAD	O4B-C4B-C5B	2.36	116.90	109.33
2	A	300	NAD	O3-PN-O1N	-2.35	103.62	110.70
3	B	301	0WE	C26-C25-C37	2.35	118.99	113.77
3	B	301	0WE	C5-N3-C1	2.34	127.47	120.58
3	C	301	0WE	C12-C13-C14	2.33	123.11	120.24
2	D	300	NAD	N9A-C8A-N7A	-2.33	110.64	113.94
2	A	300	NAD	C5A-N7A-C8A	2.31	107.08	103.45
3	D	301	0WE	C24-C19-C20	2.30	119.03	116.90
3	D	301	0WE	C20-N21-C22	2.30	120.69	116.19
3	D	301	0WE	O28-C37-N36	-2.27	118.98	121.39
3	C	301	0WE	C13-C14-C9	-2.24	115.53	119.60
2	C	300	NAD	O4B-C1B-N9A	2.24	112.39	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	0WE	C11-C8-C9	2.23	121.39	118.88
3	B	301	0WE	C17-C1-N3	2.22	121.87	118.08
2	D	300	NAD	O3D-C3D-C4D	-2.21	104.74	111.08
3	B	301	0WE	C8-C7-C6	2.20	108.44	105.85
2	B	300	NAD	C4A-C5A-N7A	-2.20	108.07	110.58
2	A	300	NAD	C2A-N1A-C6A	2.19	122.33	118.73
2	C	300	NAD	O2N-PN-O3	2.18	113.16	107.27
2	D	300	NAD	N6A-C6A-N1A	2.17	123.22	118.38
3	A	301	0WE	N36-C22-N21	2.17	119.62	116.38
3	D	301	0WE	C18-C19-C20	-2.15	117.92	121.73
2	C	300	NAD	C5A-C6A-N6A	-2.11	118.05	123.29
3	C	301	0WE	C8-C7-C6	2.11	108.33	105.85
3	B	301	0WE	O2-C1-C17	-2.10	115.58	121.26
2	C	300	NAD	C5N-C4N-C3N	-2.10	118.30	120.36
3	B	301	0WE	C13-C14-C9	-2.08	115.81	119.60
2	B	300	NAD	C5A-C6A-N6A	-2.08	118.14	123.29
2	A	300	NAD	O2N-PN-O3	2.05	112.83	107.27
3	D	301	0WE	C12-C11-C8	-2.04	116.11	119.80
2	D	300	NAD	O7N-C7N-N7N	-2.04	119.67	122.62
2	C	300	NAD	O2A-PA-O1A	2.04	121.92	112.44
2	B	300	NAD	O2A-PA-O1A	2.01	121.79	112.44
3	A	301	0WE	C26-C25-C37	2.01	118.22	113.77
2	A	300	NAD	C4D-O4D-C1D	2.00	111.76	109.92

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	C5B-O5B-PA-O2A
2	A	300	NAD	C5B-O5B-PA-O3
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
2	A	300	NAD	C2D-C1D-N1N-C2N
2	A	300	NAD	C2D-C1D-N1N-C6N
2	D	300	NAD	PN-O3-PA-O5B
2	D	300	NAD	C5D-O5D-PN-O3
2	D	300	NAD	C5D-O5D-PN-O1N
2	D	300	NAD	C5D-O5D-PN-O2N
2	D	300	NAD	O4D-C1D-N1N-C2N
2	D	300	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	D	300	NAD	C2D-C1D-N1N-C2N
2	D	300	NAD	C2D-C1D-N1N-C6N
2	C	300	NAD	C5D-O5D-PN-O3
2	C	300	NAD	C5D-O5D-PN-O1N
2	C	300	NAD	C5D-O5D-PN-O2N
2	C	300	NAD	O4D-C1D-N1N-C2N
2	C	300	NAD	O4D-C1D-N1N-C6N
2	C	300	NAD	C2D-C1D-N1N-C6N
2	B	300	NAD	C5B-O5B-PA-O2A
2	B	300	NAD	C5D-O5D-PN-O3
2	B	300	NAD	O4D-C1D-N1N-C2N
2	B	300	NAD	O4D-C1D-N1N-C6N
2	B	300	NAD	C2D-C1D-N1N-C2N
2	B	300	NAD	C2D-C1D-N1N-C6N
2	C	300	NAD	PN-O3-PA-O5B
2	B	300	NAD	PN-O3-PA-O5B
3	C	301	0WE	C17-C18-C19-C20
2	A	300	NAD	C5B-O5B-PA-O1A
2	A	300	NAD	C5D-O5D-PN-O1N
2	B	300	NAD	C5B-O5B-PA-O1A
2	B	300	NAD	C5B-O5B-PA-O3
2	B	300	NAD	C5D-O5D-PN-O1N
3	D	301	0WE	C17-C18-C19-C24
3	A	301	0WE	C17-C18-C19-C24
3	C	301	0WE	C17-C18-C19-C24
3	B	301	0WE	C17-C18-C19-C24
2	B	300	NAD	C3D-C4D-C5D-O5D
3	A	301	0WE	C17-C18-C19-C20
3	D	301	0WE	C17-C18-C19-C20
2	D	300	NAD	PA-O3-PN-O1N
2	D	300	NAD	PA-O3-PN-O2N
2	B	300	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 8 short contacts:

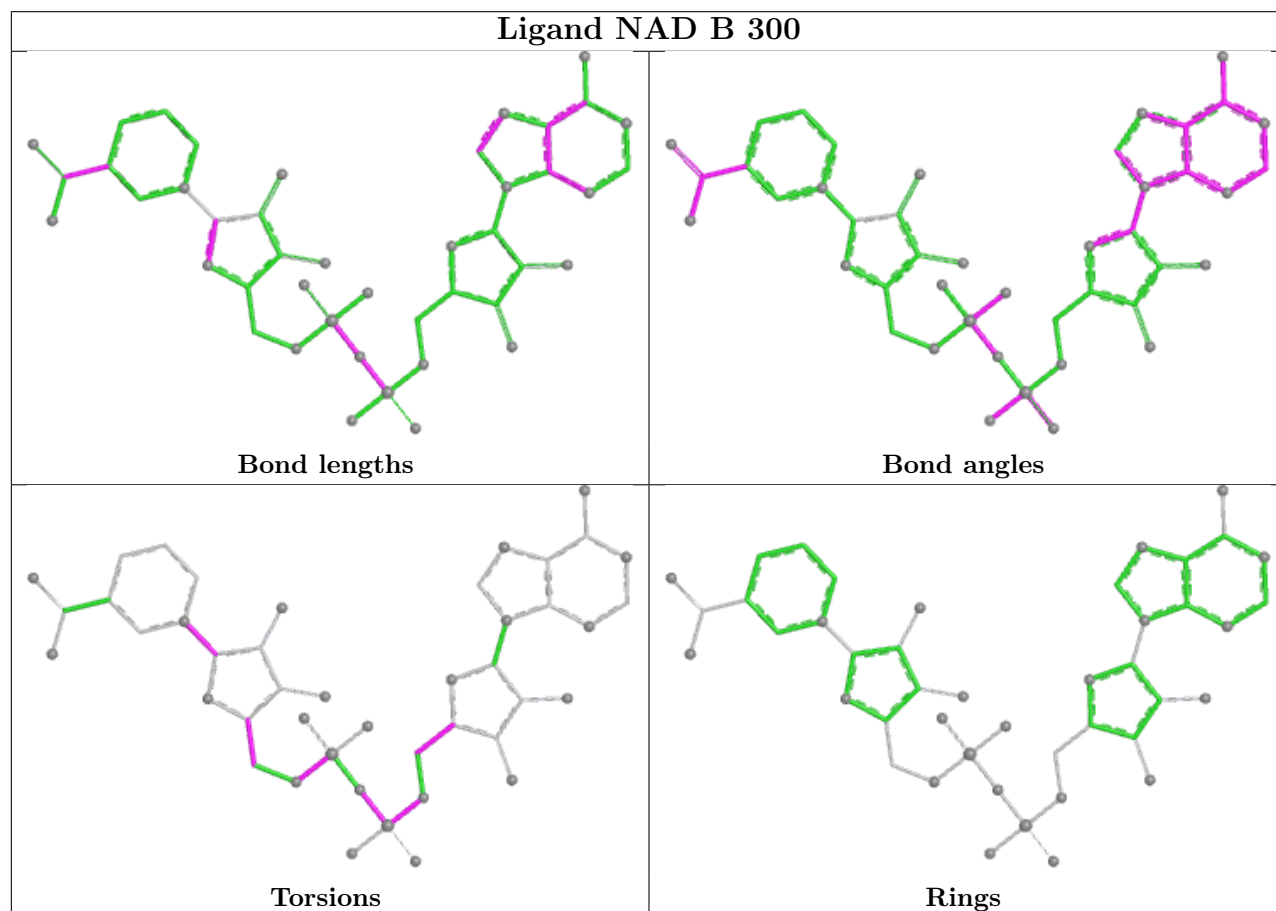
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	NAD	2	0
3	A	301	0WE	1	0
3	C	301	0WE	2	0
2	A	300	NAD	1	0
3	B	301	0WE	1	0

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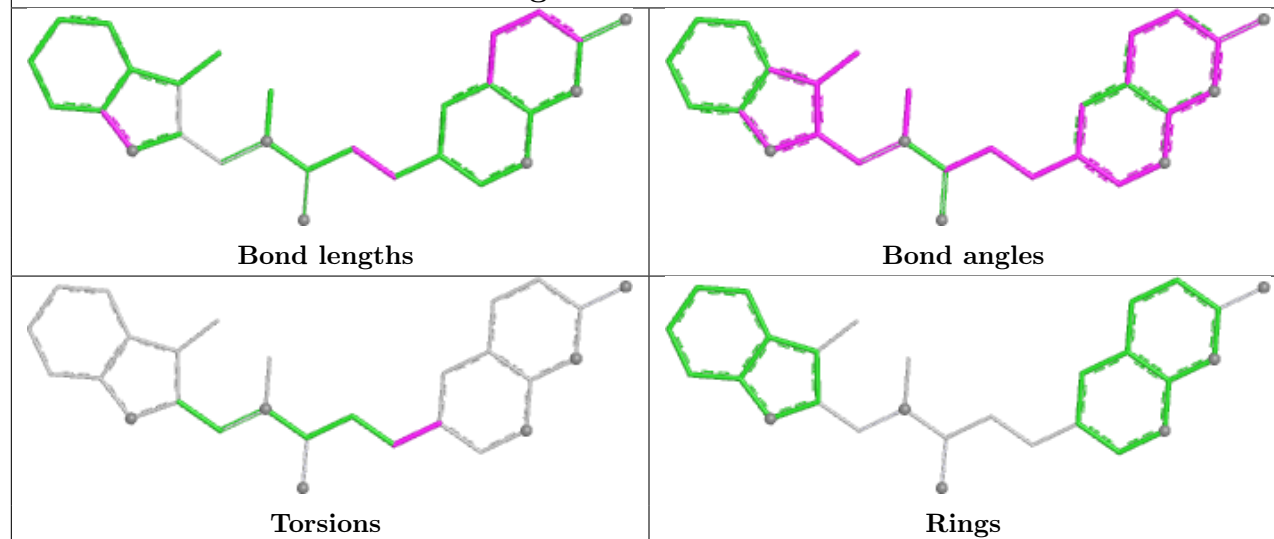
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	NAD	1	0

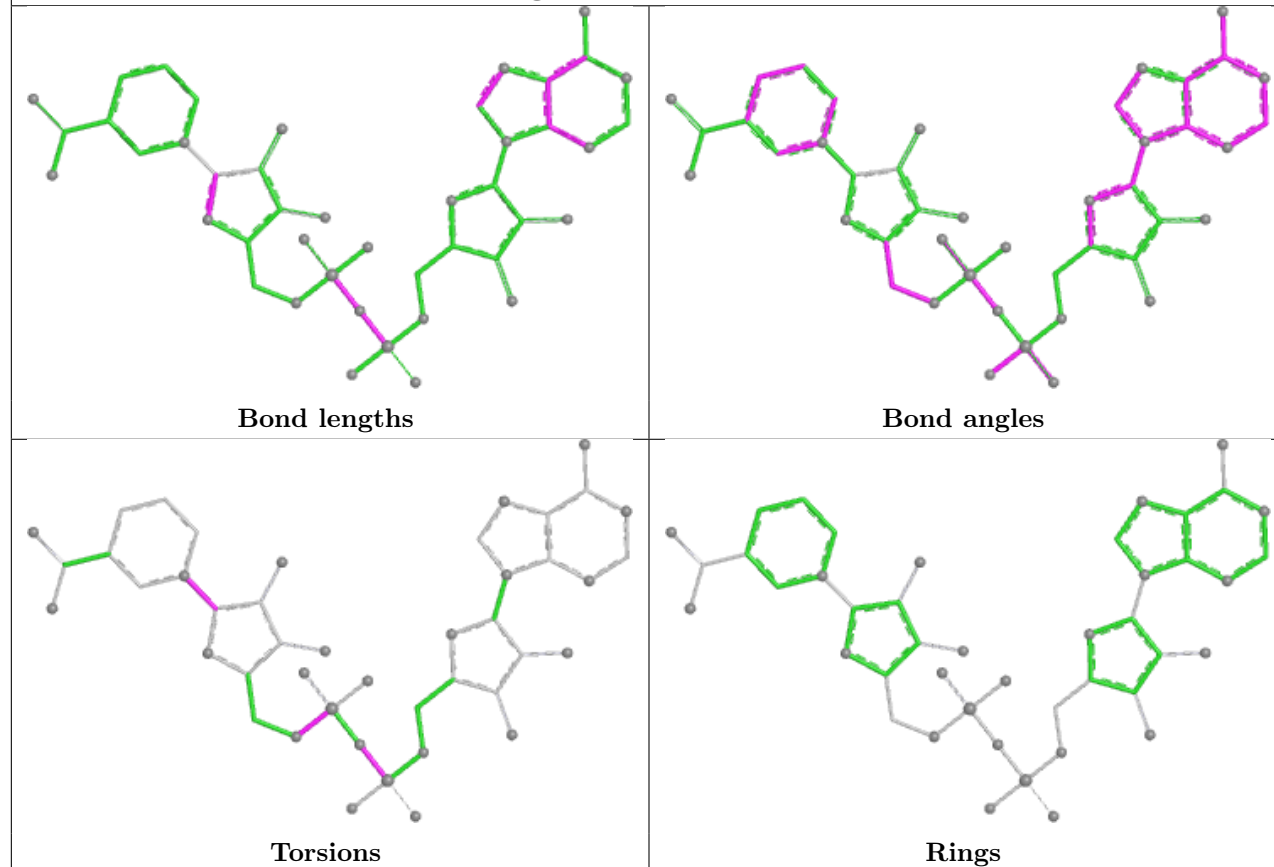
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



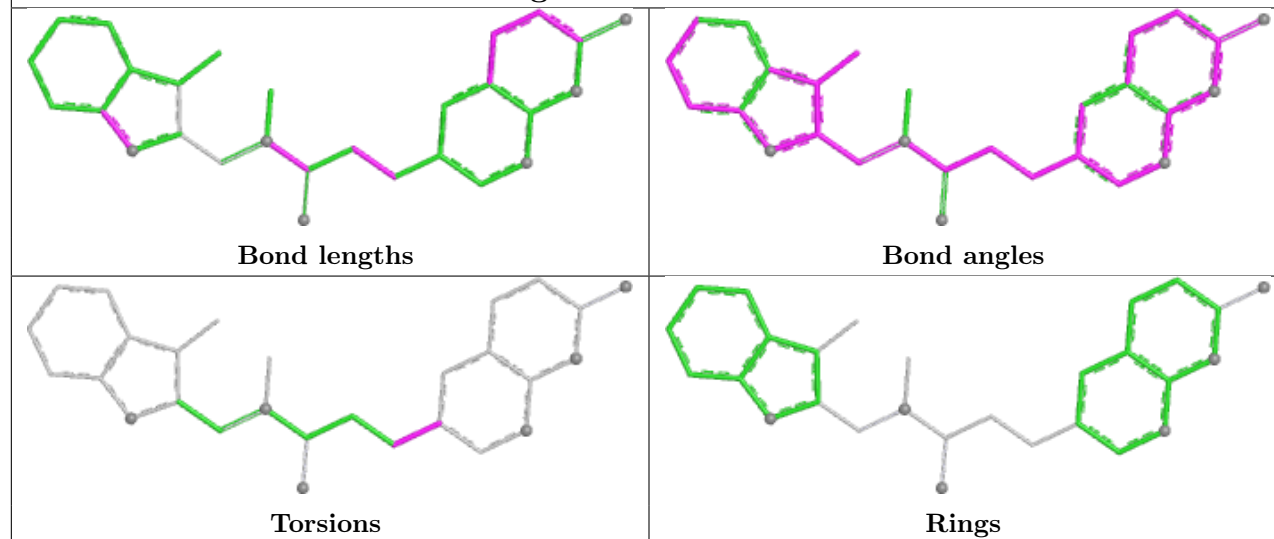
Ligand OWE A 301



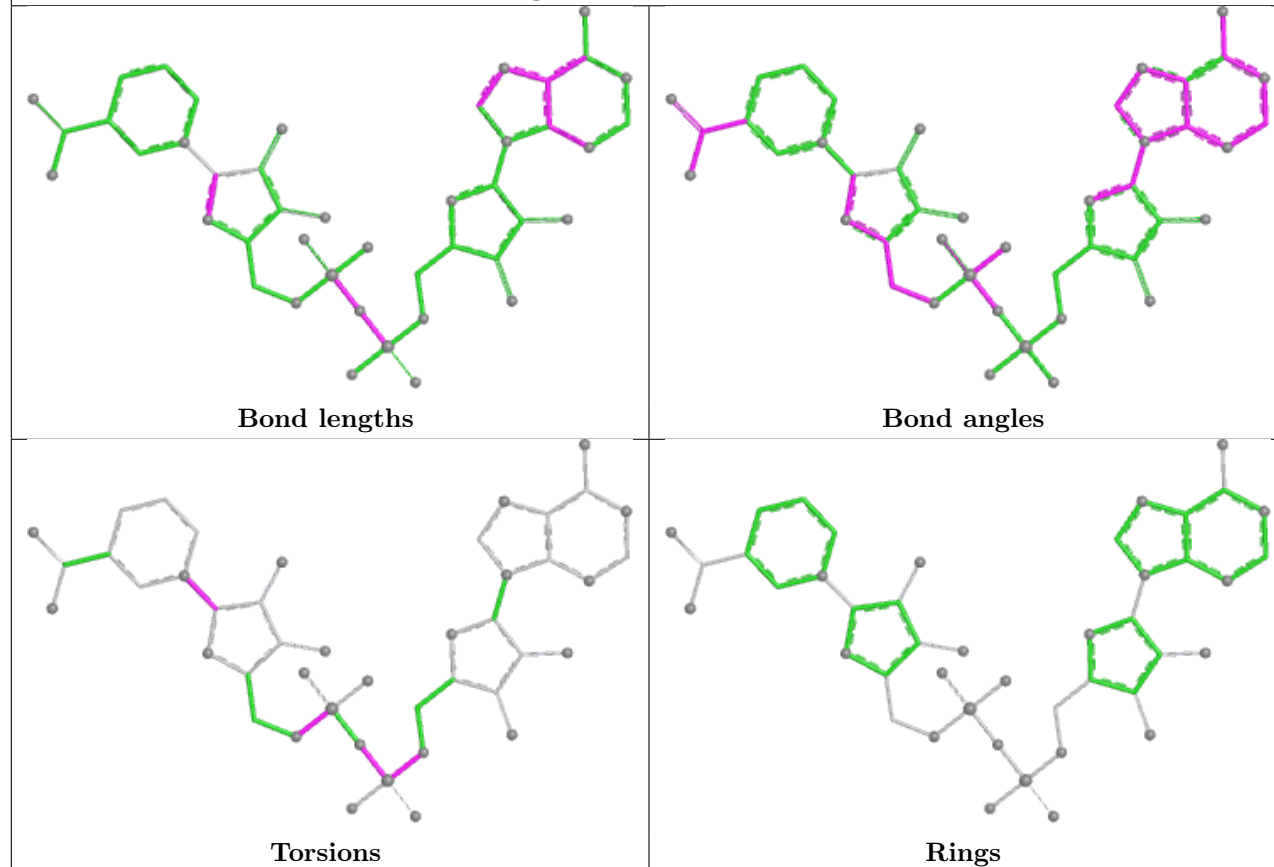
Ligand NAD C 300



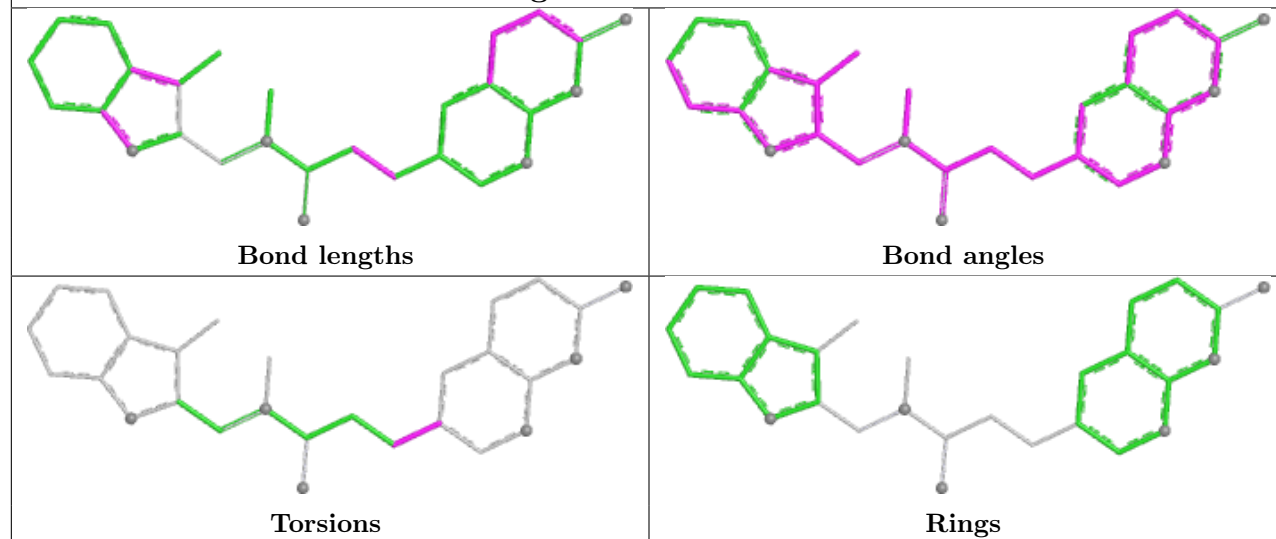
Ligand OWE C 301



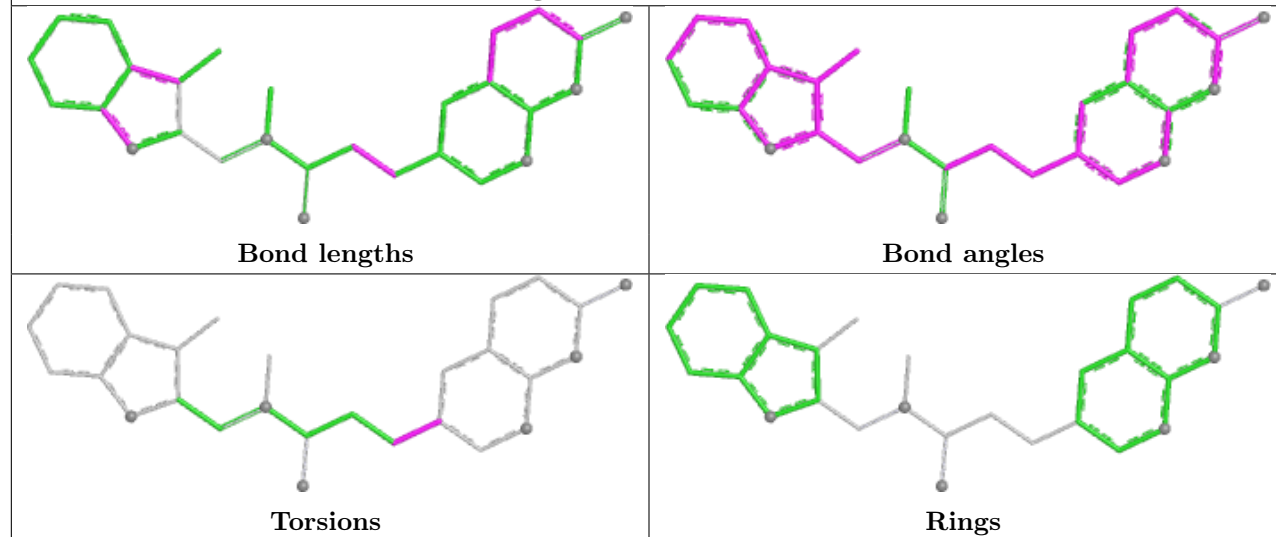
Ligand NAD A 300

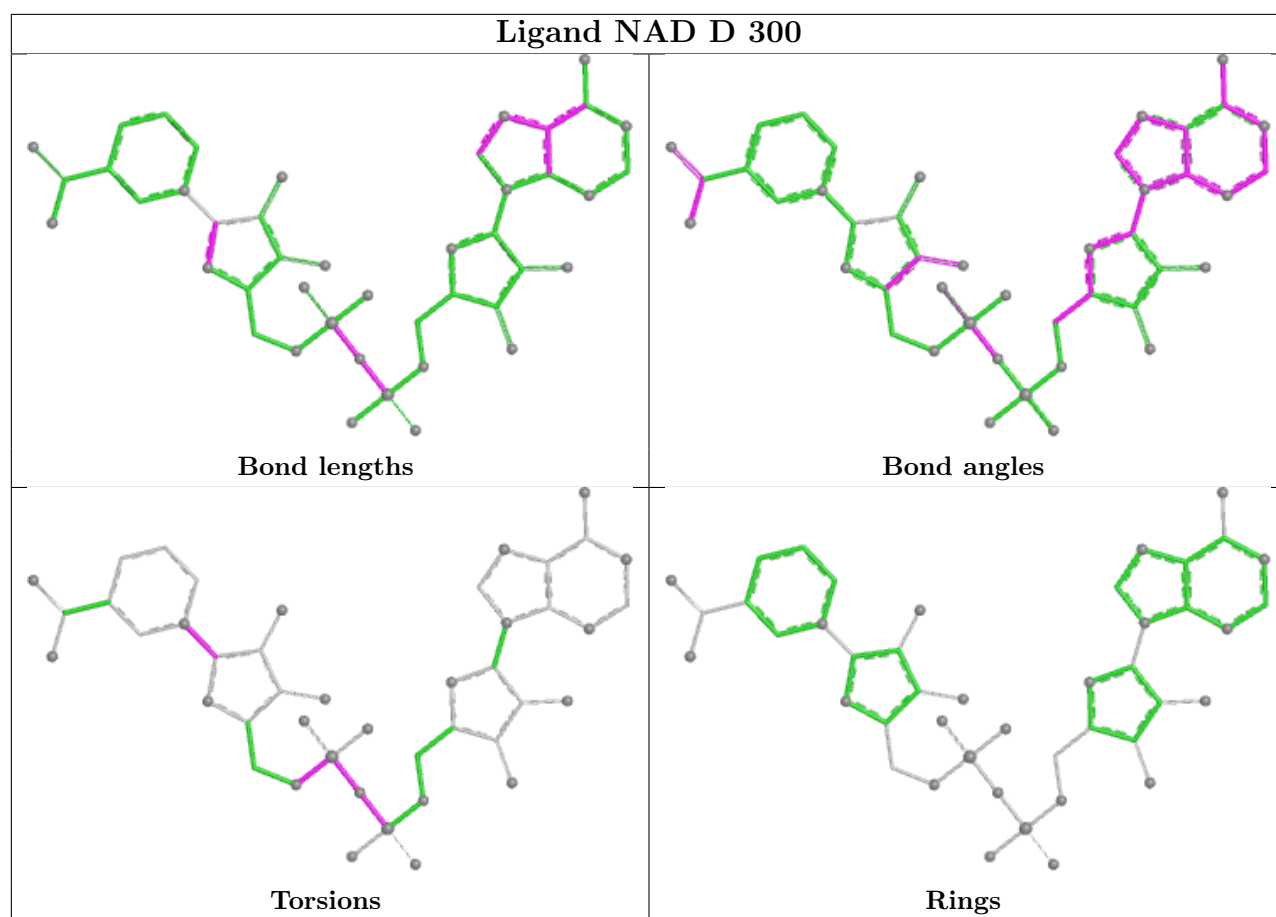


Ligand 0WE B 301



Ligand 0WE D 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

6.1 Protein, DNA and RNA chains

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%)	0.07	5 (1%) 66 68	35, 53, 85, 104	0
1	B	260/267 (97%)	0.04	4 (1%) 72 73	35, 53, 81, 115	0
1	C	260/267 (97%)	0.18	5 (1%) 66 68	36, 54, 80, 105	0
1	D	260/267 (97%)	0.17	3 (1%) 76 77	37, 56, 83, 108	0
All	All	1040/1068 (97%)	0.11	17 (1%) 70 72	35, 54, 83, 115	0

All (17) RSRZ outliers are listed below:

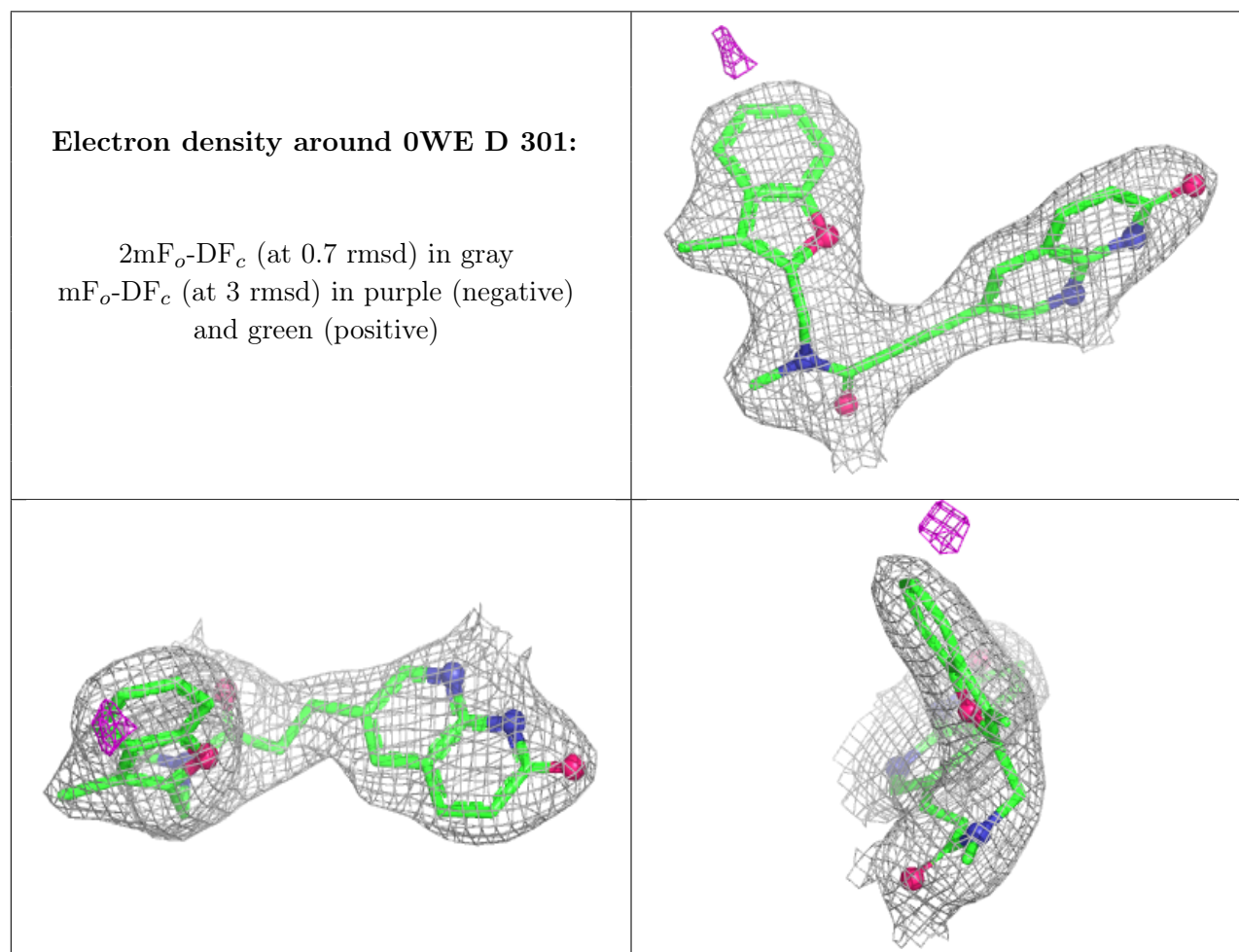
Mol	Chain	Res	Type	RSRZ
1	B	262	SER	6.6
1	A	262	SER	6.6
1	D	262	SER	6.2
1	C	262	SER	5.7
1	A	84	TRP	3.6
1	C	204	LYS	3.3
1	B	3	GLN	3.1
1	B	198	LEU	3.1
1	A	3	GLN	2.8
1	B	209	MET	2.6
1	C	50	VAL	2.6
1	A	87	VAL	2.4
1	D	198	LEU	2.4
1	D	61	LEU	2.4
1	C	61	LEU	2.2
1	C	209	MET	2.2
1	A	86	GLY	2.1

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.

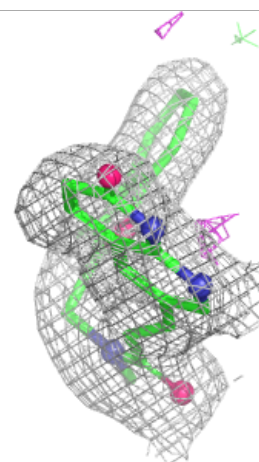
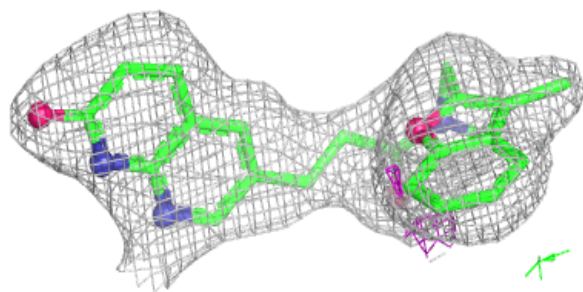
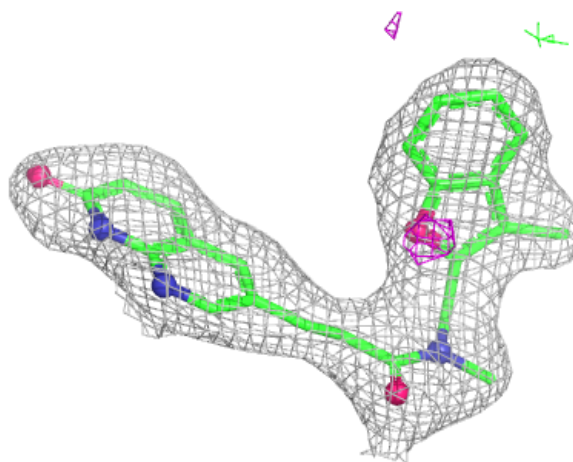
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	0WE	D	301	28/28	0.93	0.08	42,52,68,75	0
3	0WE	C	301	28/28	0.93	0.09	36,45,64,66	0
3	0WE	A	301	28/28	0.94	0.08	42,50,63,66	0
3	0WE	B	301	28/28	0.94	0.08	42,49,67,68	0

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.



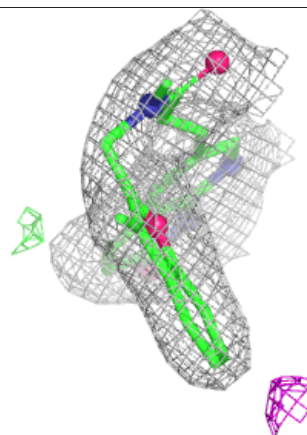
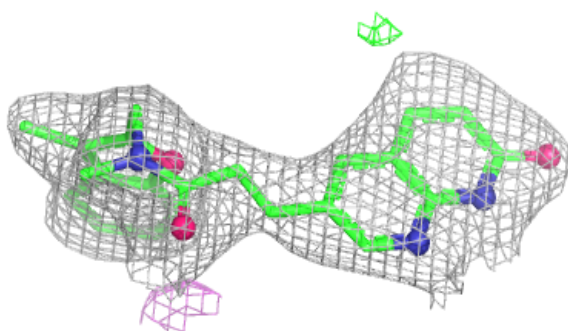
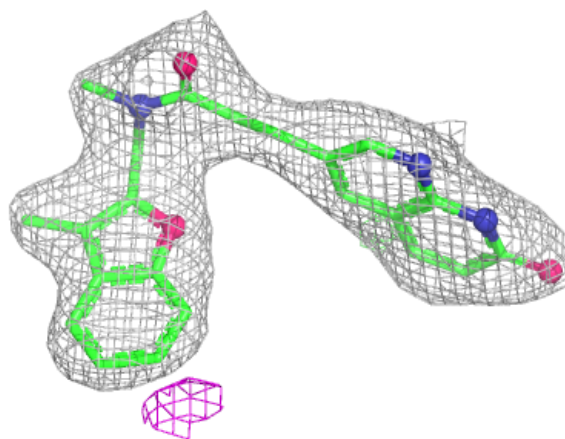
Electron density around 0WE C 301:

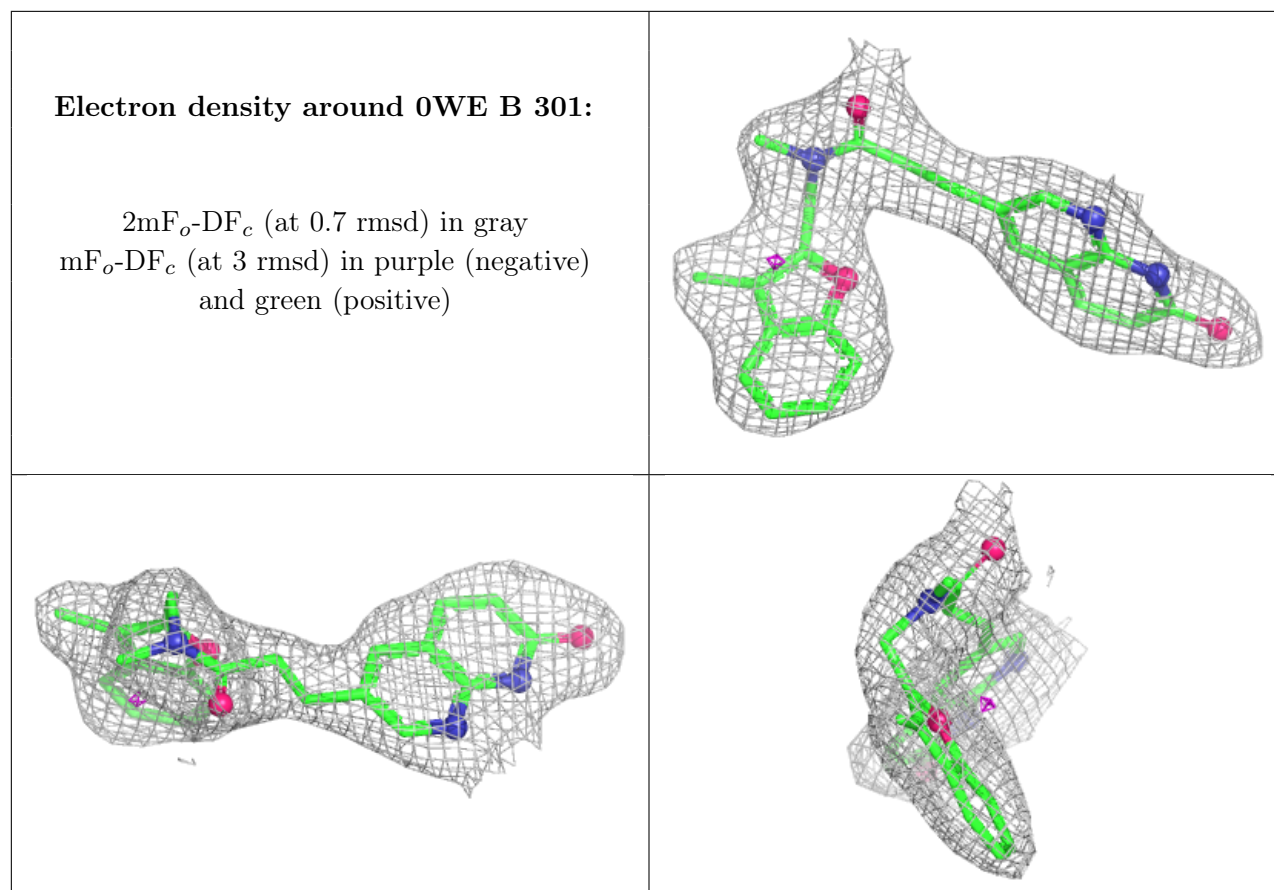
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OWE 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)





6.3 Carbohydrates [i](#)

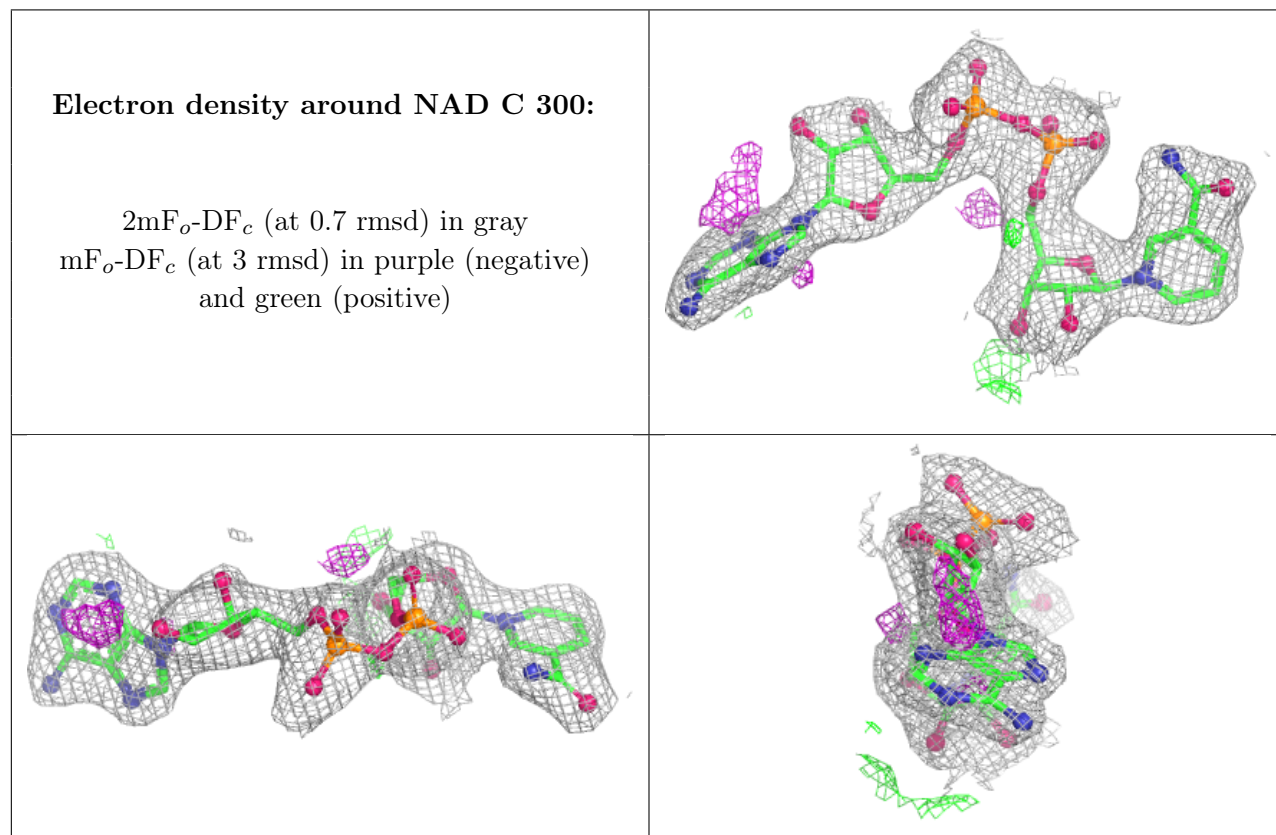
There are no oligosaccharides in this entry.

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.

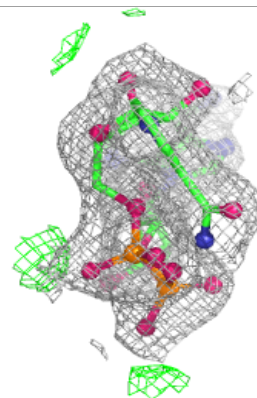
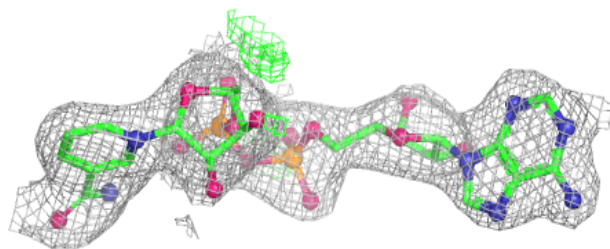
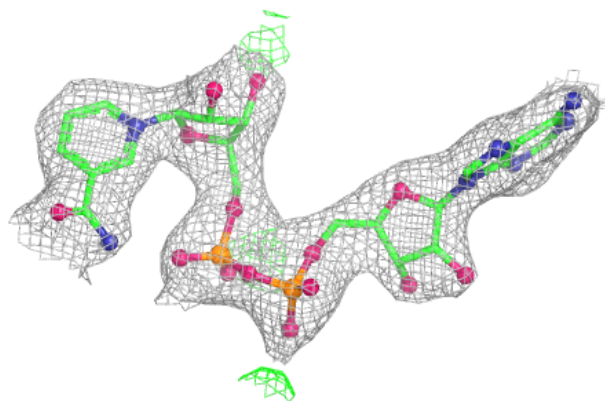
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	C	300	44/44	0.90	0.10	52,62,73,76	0
2	NAD	A	300	44/44	0.93	0.08	41,59,70,74	0
3	0WE	D	301	28/28	0.93	0.08	42,52,68,75	0
3	0WE	C	301	28/28	0.93	0.09	36,45,64,66	0
3	0WE	A	301	28/28	0.94	0.08	42,50,63,66	0
2	NAD	D	300	44/44	0.94	0.08	43,56,65,68	0
2	NAD	B	300	44/44	0.94	0.08	40,51,63,72	0
3	0WE	B	301	28/28	0.94	0.08	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.



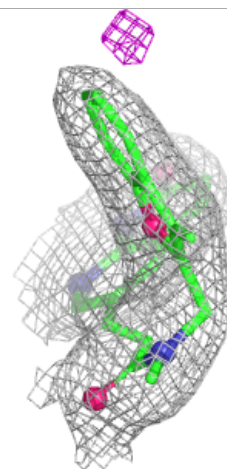
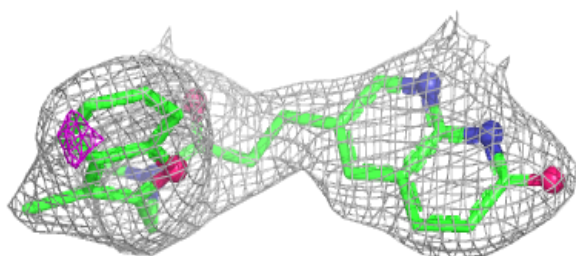
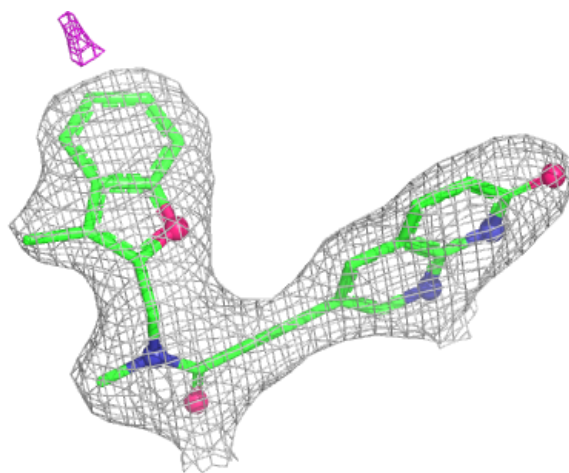
Electron density around NAD A 300:

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



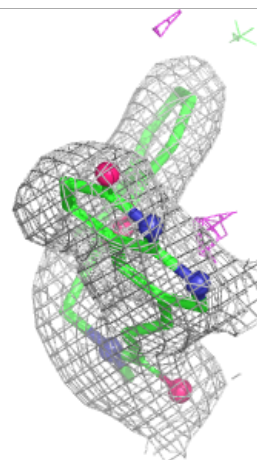
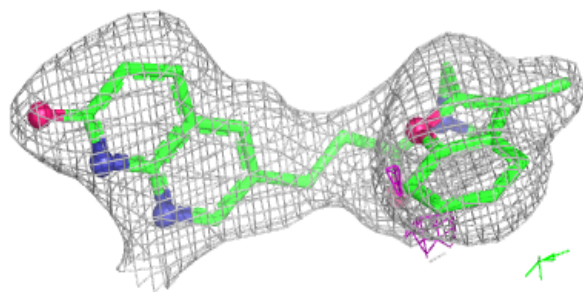
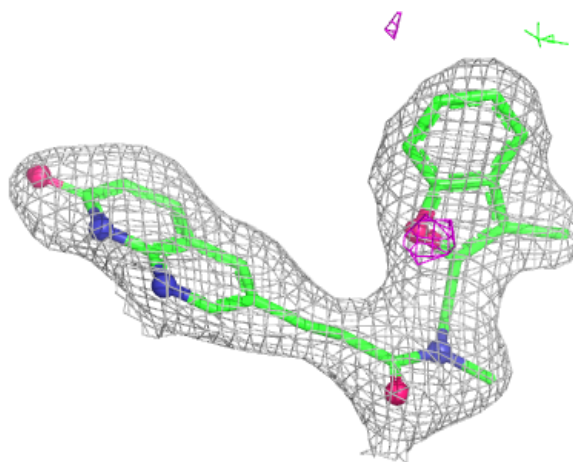
Electron density around 0WE D 301:

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



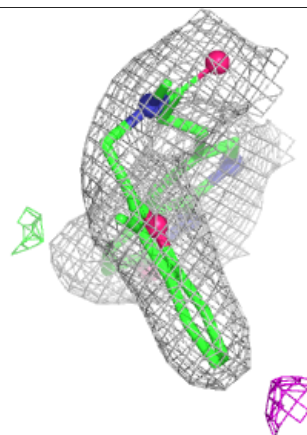
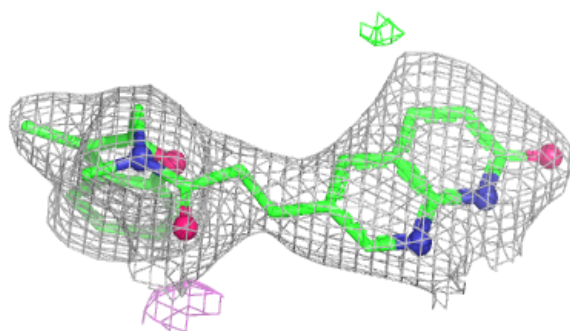
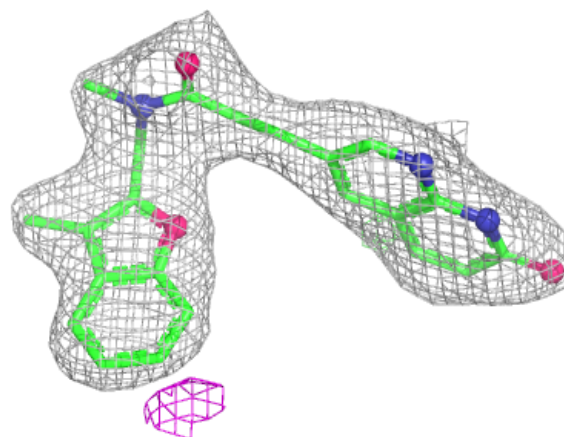
Electron density around 0WE C 301:

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

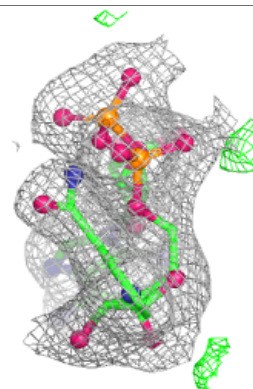
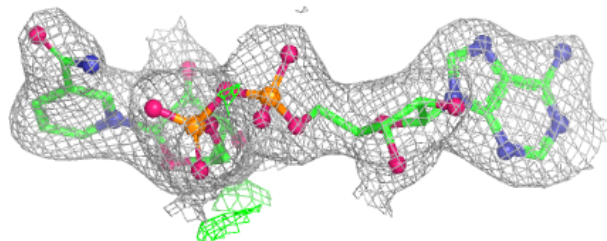
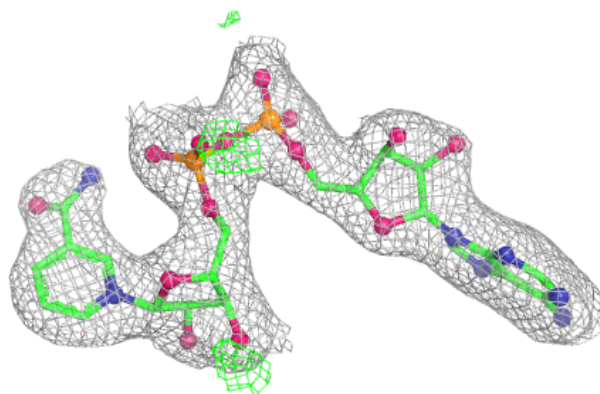


Electron density around OWE A 301:

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

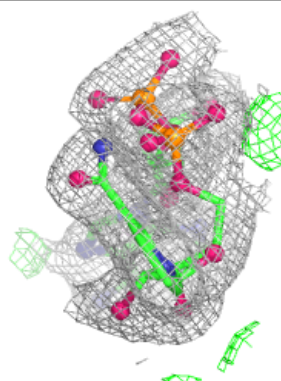
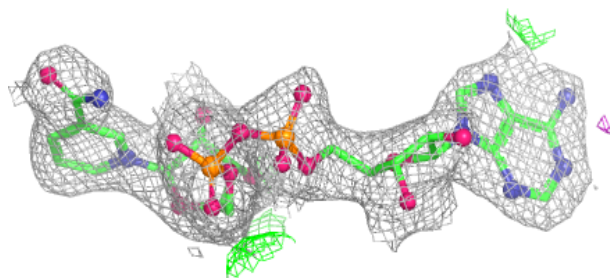
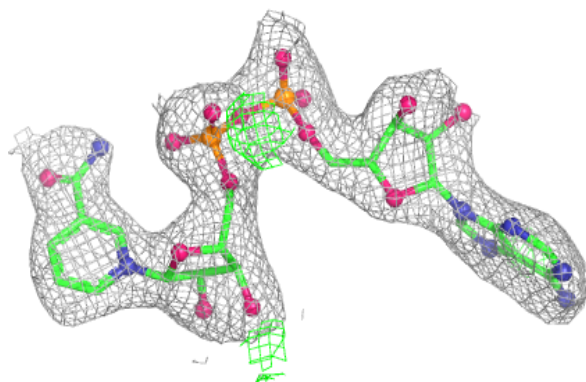
**Electron density around NAD D 300:**

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

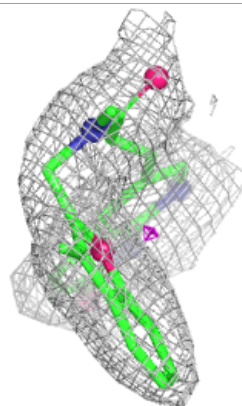
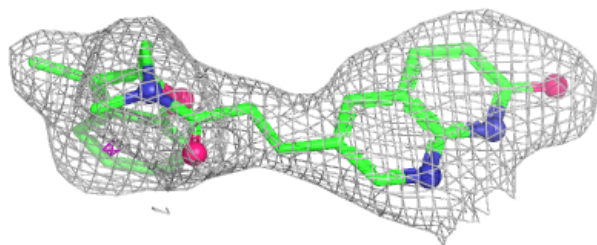
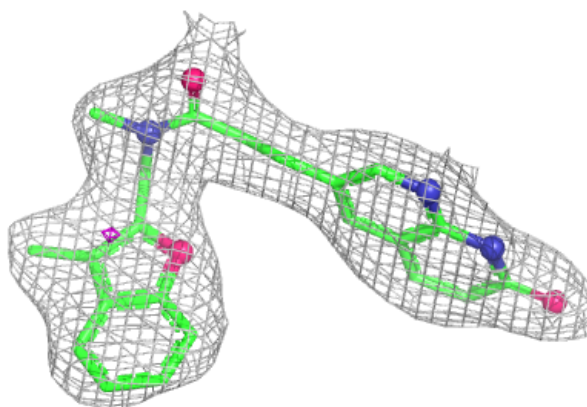


Electron density around NAD B 300:

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

**Electron density around OWE 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.