



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:08 AM UTC

PDB ID : 4UVI / pdb_00004uvi
Title : Discovery of pyrimidine isoxazoles InhA in complex with compound 23
Authors : Read, J.A.; Gingell, H.; Madhavapeddi, P.; Ghorpade, S.; Cowan, S.
Deposited on : 2014-08-05
Resolution : 1.73 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

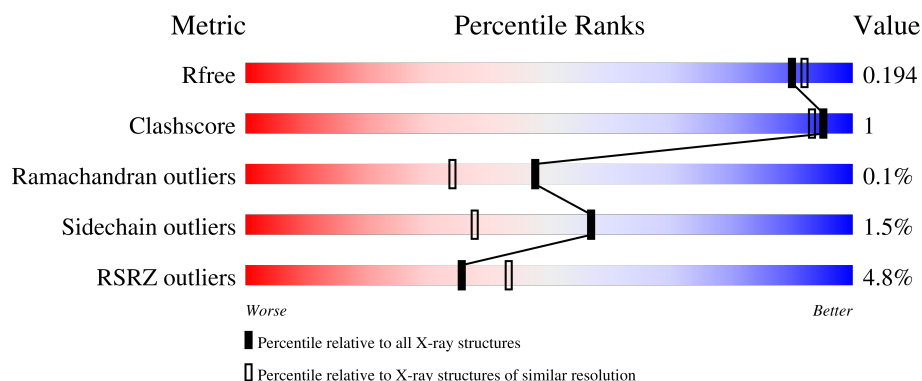
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	269	2% 92% 5%
1	B	269	6% 94% 5%
1	C	269	3% 88% 7%
1	D	269	8% 95%

2 Entry composition [i](#)

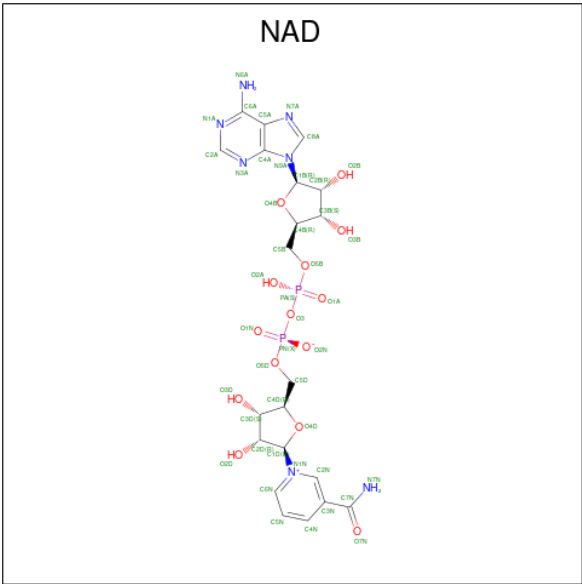
There are 4 unique types of molecules in this entry. The entry contains 8794 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	261	Total	C	N	O	S	0	1	0
			1910	1211	330	360	9			
1	B	267	Total	C	N	O	S	0	1	0
			1967	1246	340	371	10			
1	C	249	Total	C	N	O	S	0	0	0
			1839	1169	318	343	9			
1	D	264	Total	C	N	O	S	0	1	0
			1920	1220	330	360	10			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



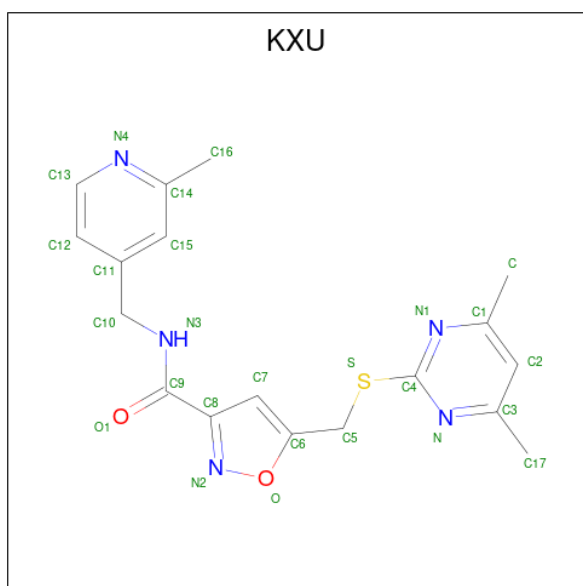
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 5-[[[(4,6-dimethylpyrimidin-2-yl)sulfanyl]methyl]-N-[(2-methylpyridin-4-yl)methyl]-1,2-oxazole-3-carboxamide (CCD ID: KXU) (formula: C₁₈H₁₉N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	18	5	2	1		
3	B	1	Total	C	N	O	S	0	0
			26	18	5	2	1		
3	C	1	Total	C	N	O	S	0	0
			26	18	5	2	1		
3	D	1	Total	C	N	O	S	0	0
			26	18	5	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	226	Total	O	0	0
			226	226		
4	B	240	Total	O	0	0
			240	240		

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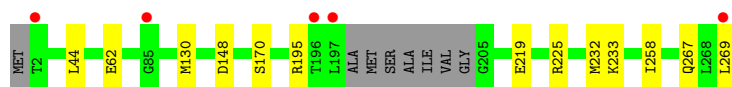
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	212	Total 212	O 212	0	0
4	D	200	Total 200	O 200	0	0

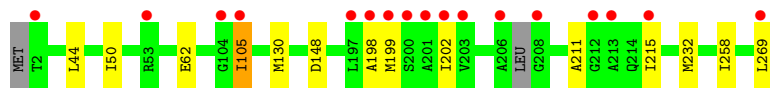
3 Residue-property plots [i](#)

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.

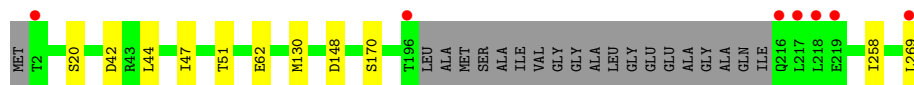
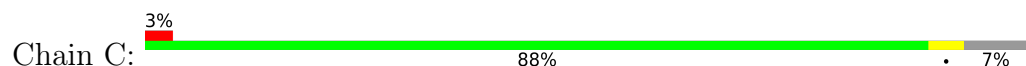
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



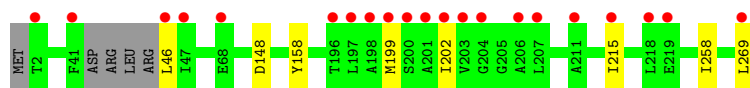
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• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.14Å 111.66Å 67.72Å 90.00° 98.62° 90.00°	Depositor
Resolution (Å)	66.96 – 1.73 66.96 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.6 (66.96-1.73) 96.2 (66.96-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.73Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.169 , 0.194 (Not available) , 0.194	Depositor DCC
R_{free} test set	4764 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8794	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: KXU, NAD

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	0.83	0/1947	1.08	1/2648 (0.0%)
1	B	0.82	0/2004	1.11	1/2722 (0.0%)
1	C	0.84	0/1876	1.05	1/2552 (0.0%)
1	D	0.84	0/1957	1.11	1/2662 (0.0%)
All	All	0.83	0/7784	1.08	4/10584 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASP	CA-CB-CG	7.56	120.16	112.60
1	D	148	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	148	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	148	ASP	CA-CB-CG	6.36	118.96	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1910	0	1878	6	0
1	B	1967	0	1949	8	0
1	C	1839	0	1821	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1920	0	1900	3	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	26	0	19	0	0
3	B	26	0	19	1	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
4	A	226	0	0	0	0
4	B	240	0	0	0	0
4	C	212	0	0	0	0
4	D	200	0	0	0	0
All	All	8794	0	7728	19	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 1.

All (19) 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:B:105:ILE:H	1:B:105:ILE:HD13	1.46	0.79
1:A:44:LEU:HD21	1:A:62:GLU:HB2	1.73	0.71
1:B:44:LEU:HD21	1:B:62:GLU:HB2	1.74	0.68
1:A:258:ILE:HD12	1:D:258:ILE:HD12	1.80	0.63
1:B:258:ILE:HD12	1:C:258:ILE:HD12	1.85	0.57
1:C:44:LEU:HD21	1:C:62:GLU:HG3	1.85	0.57
1:D:158:TYR:OH	1:D:199:MET:HE1	2.08	0.54
1:B:211:ALA:O	1:B:215:ILE:HG12	2.08	0.52
1:D:199:MET:HA	1:D:202:ILE:HD12	1.94	0.50
1:C:47:ILE:O	1:C:51:THR:HG23	2.15	0.47
1:A:219:GLU:HB3	1:A:232:MET:SD	2.58	0.44
1:B:130:MET:HE3	1:B:130:MET:HB2	1.88	0.43
1:C:130:MET:HE3	1:C:130:MET:HB2	1.88	0.43
1:A:195:ARG:CG	1:A:233:LYS:HA	2.49	0.43
1:B:198:ALA:O	1:B:202:ILE:HG12	2.20	0.41
1:B:232:MET:HE3	1:B:232:MET:HB2	1.99	0.41
1:A:130:MET:HE3	1:A:130:MET:HB2	1.87	0.40
1:A:225:ARG:HD2	1:A:267:GLN:O	2.22	0.40
1:B:199:MET:HG2	3:B:1271:KXU:HC1	2.04	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	258/269 (96%)	248 (96%)	10 (4%)	0	100	100
1	B	264/269 (98%)	254 (96%)	10 (4%)	0	100	100
1	C	245/269 (91%)	235 (96%)	9 (4%)	1 (0%)	30	16
1	D	261/269 (97%)	251 (96%)	10 (4%)	0	100	100
All	All	1028/1076 (96%)	988 (96%)	39 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	ASP

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	189/205 (92%)	187 (99%)	2 (1%)	65	50
1	B	196/205 (96%)	193 (98%)	3 (2%)	57	38
1	C	185/205 (90%)	182 (98%)	3 (2%)	55	35
1	D	190/205 (93%)	187 (98%)	3 (2%)	55	35
All	All	760/820 (93%)	749 (99%)	11 (1%)	57	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	SER
1	A	269	LEU
1	B	50	ILE
1	B	105	ILE
1	B	269	LEU
1	C	20	SER
1	C	170	SER
1	C	269	LEU
1	D	46	LEU
1	D	215	ILE
1	D	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	66	GLN
1	D	66	GLN
1	D	214	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 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
3	KXU	D	1271	-	28,28,28	1.78	7 (25%)	36,38,38	1.51	8 (22%)
2	NAD	B	1270	-	46,48,48	0.51	0	64,73,73	0.67	1 (1%)
3	KXU	B	1271	-	28,28,28	1.87	7 (25%)	36,38,38	1.48	8 (22%)
3	KXU	C	1271	-	28,28,28	2.01	7 (25%)	36,38,38	1.76	11 (30%)
3	KXU	A	1271	-	28,28,28	1.77	7 (25%)	36,38,38	1.59	9 (25%)
2	NAD	A	1270	-	46,48,48	0.60	1 (2%)	64,73,73	0.63	0
2	NAD	D	1270	-	46,48,48	0.74	1 (2%)	64,73,73	0.71	2 (3%)
2	NAD	C	1270	-	46,48,48	0.47	0	64,73,73	0.74	1 (1%)

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	KXU	D	1271	-	-	2/14/14/14	0/3/3/3
2	NAD	B	1270	-	-	7/30/62/62	0/5/5/5
3	KXU	B	1271	-	-	2/14/14/14	0/3/3/3
3	KXU	C	1271	-	-	7/14/14/14	0/3/3/3
3	KXU	A	1271	-	-	2/14/14/14	0/3/3/3
2	NAD	A	1270	-	-	6/30/62/62	0/5/5/5
2	NAD	D	1270	-	-	6/30/62/62	0/5/5/5
2	NAD	C	1270	-	-	5/30/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1271	KXU	C9-N3	5.34	1.42	1.33
3	C	1271	KXU	O-N2	-5.08	1.33	1.42
3	A	1271	KXU	O-N2	-4.69	1.33	1.42
3	D	1271	KXU	O-N2	-4.18	1.34	1.42
3	D	1271	KXU	C9-N3	4.11	1.40	1.33
3	B	1271	KXU	C9-N3	4.08	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1271	KXU	C4-N	3.95	1.40	1.34
3	A	1271	KXU	C9-N3	3.33	1.39	1.33
3	B	1271	KXU	O-N2	-3.13	1.36	1.42
2	D	1270	NAD	O7N-C7N	2.98	1.29	1.24
3	A	1271	KXU	C4-N1	2.66	1.38	1.34
3	C	1271	KXU	C7-C6	2.64	1.38	1.34
3	D	1271	KXU	C1-N1	2.57	1.39	1.34
2	A	1270	NAD	C2N-N1N	2.42	1.37	1.35
3	C	1271	KXU	C4-N1	2.40	1.37	1.34
3	B	1271	KXU	C2-C1	2.39	1.43	1.38
3	D	1271	KXU	C4-N	2.37	1.37	1.34
3	C	1271	KXU	C1-N1	2.37	1.39	1.34
3	C	1271	KXU	C4-N	2.36	1.37	1.34
3	B	1271	KXU	C7-C6	2.35	1.38	1.34
3	A	1271	KXU	C15-C14	2.30	1.43	1.38
3	A	1271	KXU	O-C6	2.24	1.38	1.35
3	B	1271	KXU	O-C6	2.15	1.38	1.35
3	D	1271	KXU	C3-N	2.08	1.38	1.34
3	D	1271	KXU	C14-N4	2.05	1.38	1.34
3	A	1271	KXU	C4-N	2.05	1.37	1.34
3	A	1271	KXU	C14-N4	2.05	1.38	1.34
3	D	1271	KXU	C15-C14	2.02	1.42	1.38
3	B	1271	KXU	C14-N4	2.01	1.38	1.34
3	C	1271	KXU	C15-C14	2.01	1.42	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1271	KXU	C10-N3-C9	4.72	128.82	122.07
3	A	1271	KXU	C11-C15-C14	-4.16	117.24	120.32
3	C	1271	KXU	C6-O-N2	3.81	111.17	108.30
3	D	1271	KXU	C11-C15-C14	-3.67	117.61	120.32
3	B	1271	KXU	C7-C8-N2	-3.30	109.37	112.11
3	D	1271	KXU	C6-O-N2	3.16	110.68	108.30
3	C	1271	KXU	C11-C15-C14	-3.10	118.03	120.32
3	B	1271	KXU	C5-S-C4	2.98	105.48	101.65
3	B	1271	KXU	C11-C15-C14	-2.97	118.13	120.32
3	C	1271	KXU	C11-C10-N3	2.80	118.98	113.07
3	D	1271	KXU	C5-S-C4	2.73	105.16	101.65
3	A	1271	KXU	C5-S-C4	2.63	105.03	101.65
3	D	1271	KXU	C7-C8-N2	-2.62	109.93	112.11
3	B	1271	KXU	O-C6-C5	2.51	120.40	116.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1271	KXU	C8-C7-C6	-2.50	103.15	104.62
3	C	1271	KXU	O-N2-C8	2.48	107.60	104.91
3	A	1271	KXU	C15-C14-N4	2.48	124.03	121.61
3	A	1271	KXU	C6-O-N2	2.45	110.14	108.30
3	A	1271	KXU	O-C6-C5	2.42	120.25	116.04
3	A	1271	KXU	C5-C6-C7	-2.40	130.57	134.14
3	B	1271	KXU	C1-C2-C3	-2.39	115.97	118.80
3	B	1271	KXU	O-N2-C8	2.37	107.48	104.91
3	A	1271	KXU	C11-C10-N3	-2.36	108.09	113.07
3	C	1271	KXU	O1-C9-N3	2.35	127.60	123.35
3	B	1271	KXU	C5-C6-C7	-2.34	130.67	134.14
3	A	1271	KXU	C7-C8-N2	-2.30	110.19	112.11
3	A	1271	KXU	C8-C9-N3	-2.28	112.20	115.56
3	C	1271	KXU	C7-C8-N2	-2.25	110.24	112.11
2	D	1270	NAD	O5B-PA-O1A	2.23	117.79	108.94
3	C	1271	KXU	C1-C2-C3	-2.22	116.17	118.80
3	D	1271	KXU	C11-C10-N3	-2.20	108.44	113.07
3	C	1271	KXU	C5-S-C4	2.17	104.44	101.65
3	C	1271	KXU	O-C6-C7	-2.16	107.73	109.73
3	D	1271	KXU	C1-C2-C3	-2.13	116.27	118.80
3	B	1271	KXU	C-C1-N1	-2.11	113.37	116.56
2	B	1270	NAD	O5B-PA-O1A	2.10	117.25	108.94
2	D	1270	NAD	C4B-O4B-C1B	-2.09	104.86	109.47
3	D	1271	KXU	O-C6-C5	2.04	119.58	116.04
2	C	1270	NAD	C4B-O4B-C1B	-2.03	104.98	109.47
3	D	1271	KXU	C7-C8-C9	-2.03	124.19	127.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1270	NAD	PN-O3-PA-O5B
2	A	1270	NAD	C5D-O5D-PN-O3
2	A	1270	NAD	C5D-O5D-PN-O1N
2	A	1270	NAD	C5D-O5D-PN-O2N
2	A	1270	NAD	O4D-C1D-N1N-C2N
2	A	1270	NAD	O4D-C1D-N1N-C6N
2	B	1270	NAD	C5D-O5D-PN-O3
2	B	1270	NAD	C5D-O5D-PN-O1N
2	B	1270	NAD	C5D-O5D-PN-O2N
2	B	1270	NAD	O4D-C1D-N1N-C2N
2	B	1270	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	C	1270	NAD	C5D-O5D-PN-O3
2	C	1270	NAD	C5D-O5D-PN-O1N
2	C	1270	NAD	C5D-O5D-PN-O2N
2	C	1270	NAD	O4D-C1D-N1N-C2N
2	C	1270	NAD	O4D-C1D-N1N-C6N
2	D	1270	NAD	PN-O3-PA-O5B
2	D	1270	NAD	C5D-O5D-PN-O3
2	D	1270	NAD	C5D-O5D-PN-O1N
2	D	1270	NAD	C5D-O5D-PN-O2N
2	D	1270	NAD	O4D-C1D-N1N-C2N
2	D	1270	NAD	O4D-C1D-N1N-C6N
3	A	1271	KXU	S-C5-C6-C7
3	B	1271	KXU	S-C5-C6-C7
3	B	1271	KXU	S-C5-C6-O
3	C	1271	KXU	C7-C8-C9-O1
3	C	1271	KXU	N2-C8-C9-O1
3	C	1271	KXU	C7-C8-C9-N3
3	C	1271	KXU	N2-C8-C9-N3
3	C	1271	KXU	C11-C10-N3-C9
3	C	1271	KXU	S-C5-C6-C7
3	D	1271	KXU	S-C5-C6-C7
2	B	1270	NAD	PN-O3-PA-O5B
3	A	1271	KXU	S-C5-C6-O
3	C	1271	KXU	S-C5-C6-O
3	D	1271	KXU	S-C5-C6-O
2	B	1270	NAD	O4B-C4B-C5B-O5B

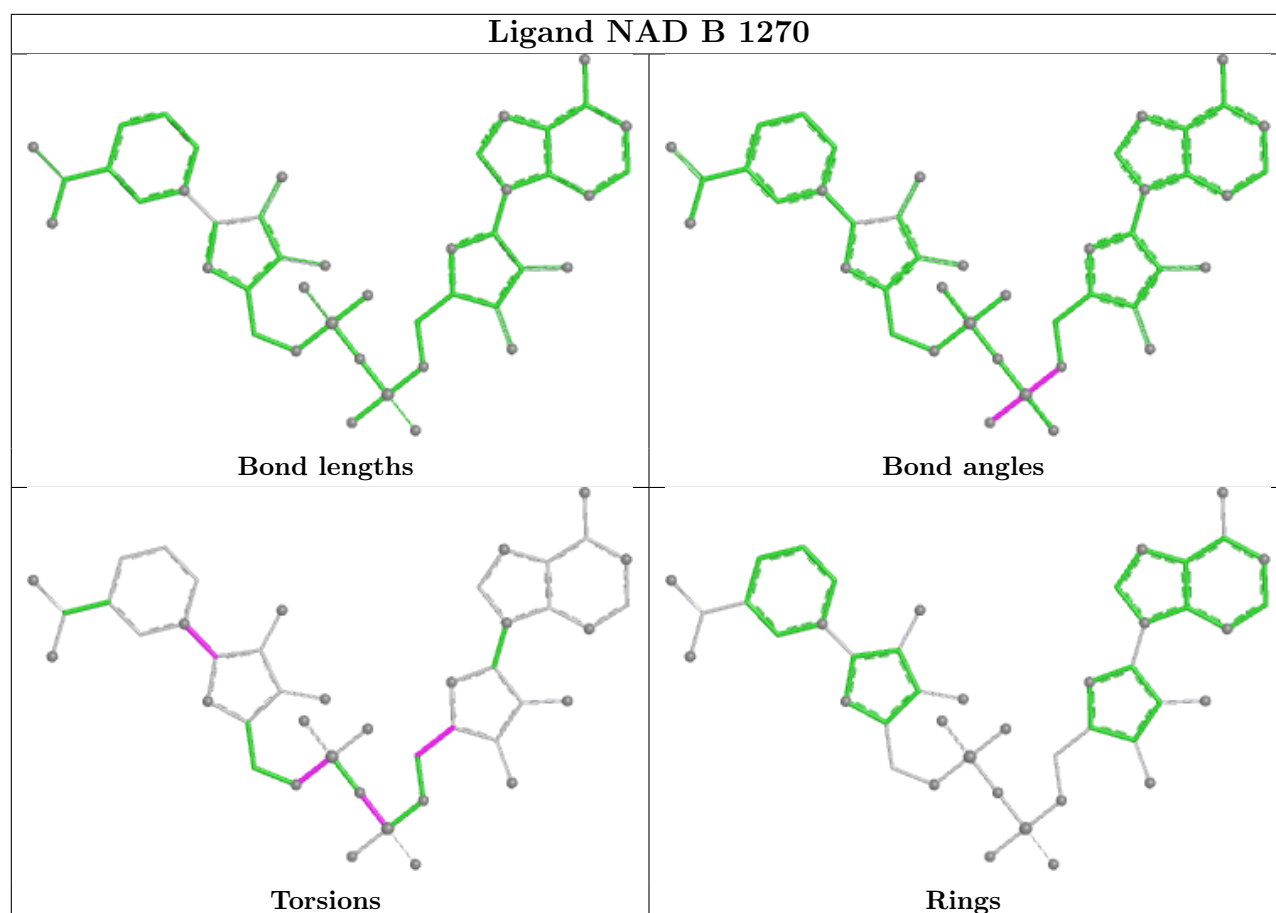
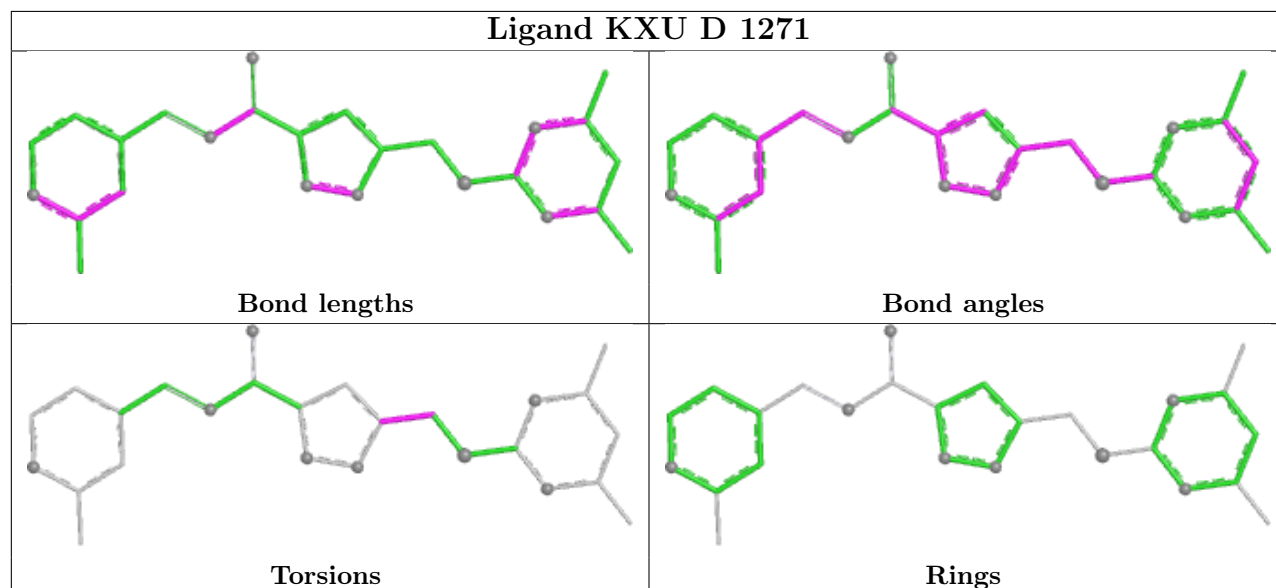
There are no ring outliers.

1 monomer is involved in 1 short contact:

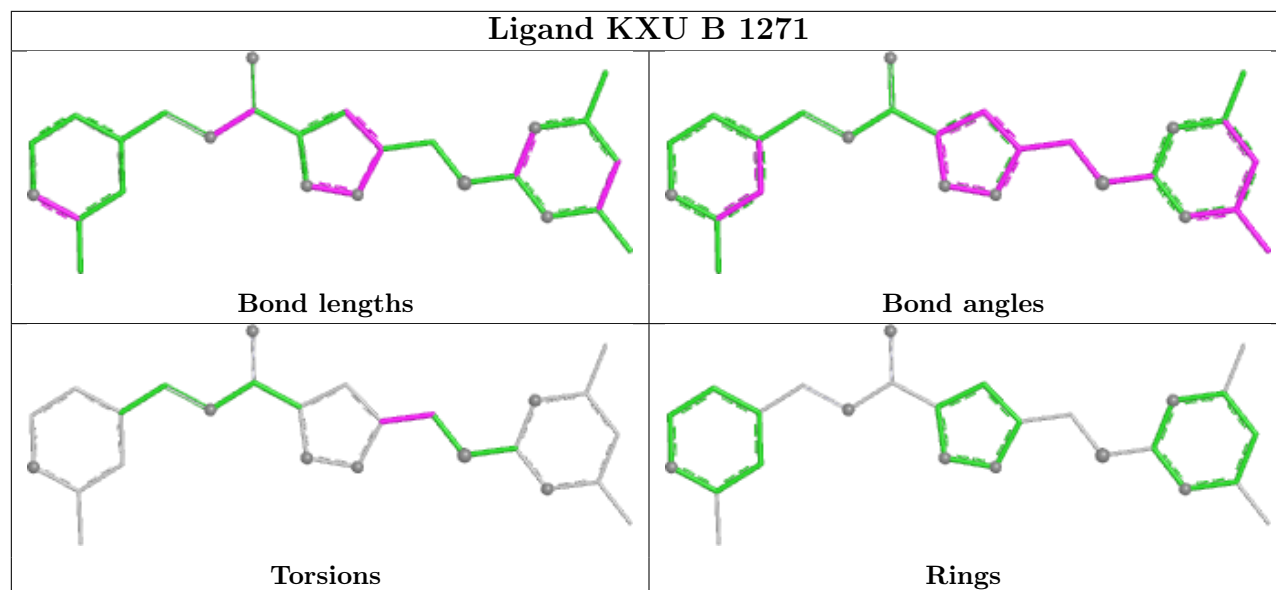
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1271	KXU	1	0

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

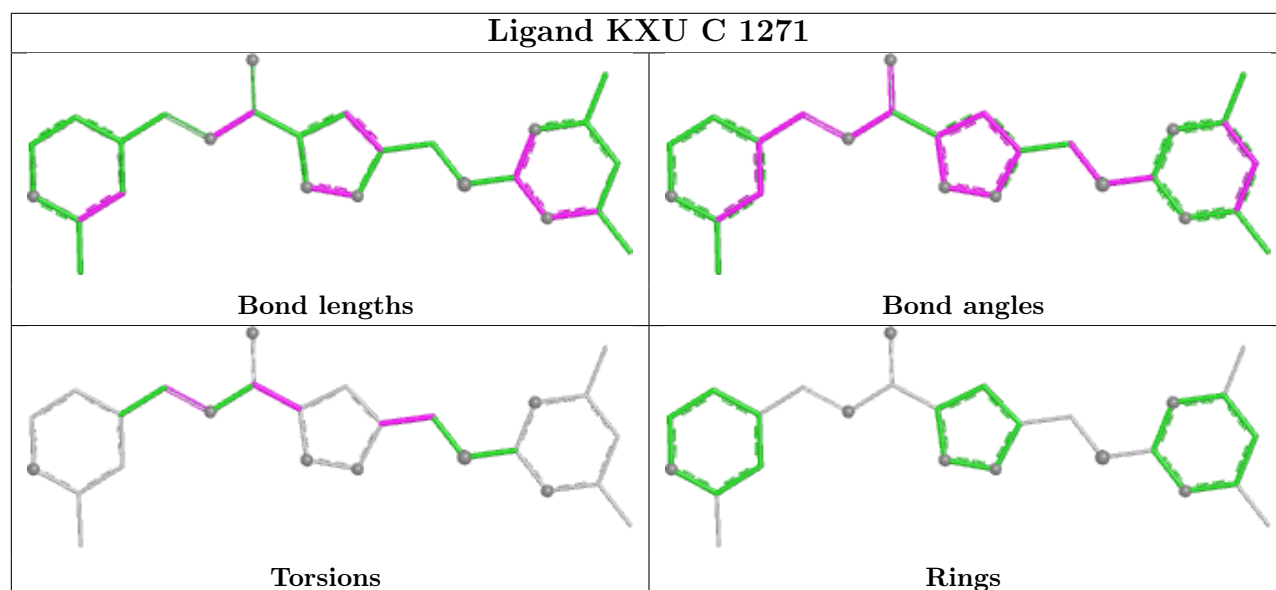
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



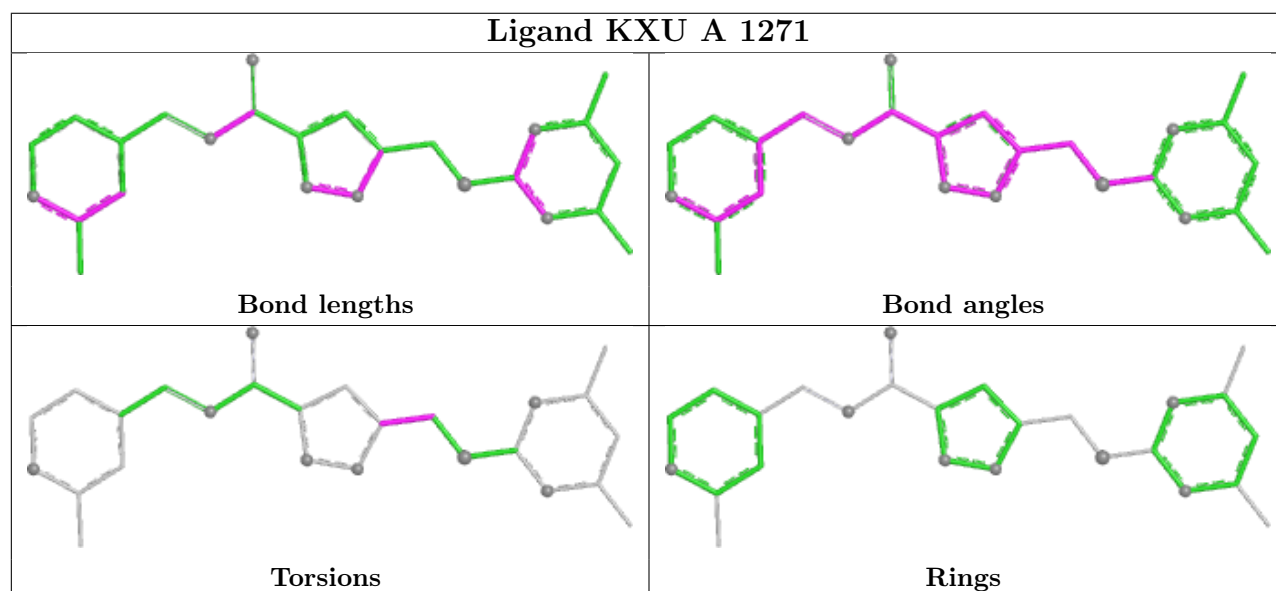
Ligand KXU B 1271

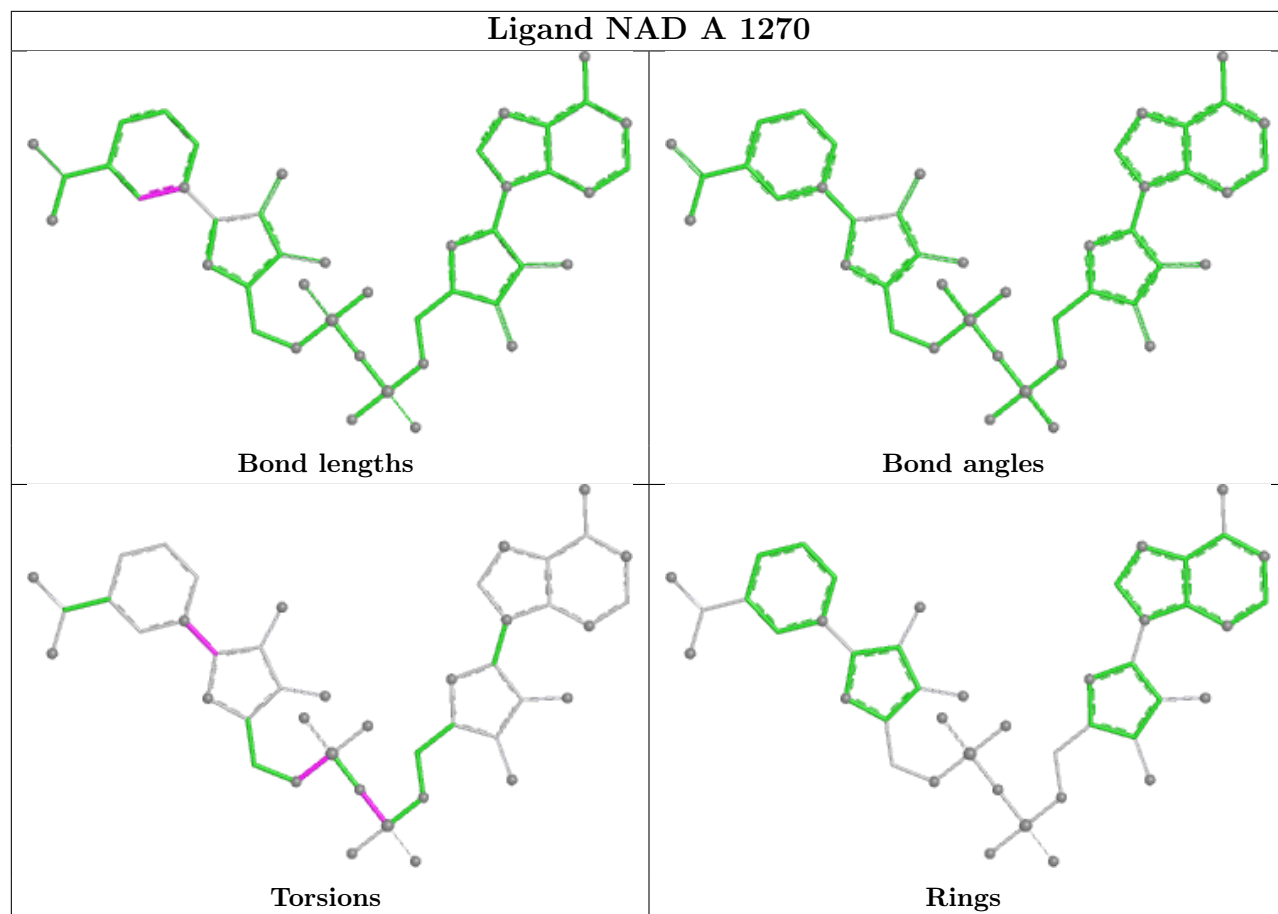


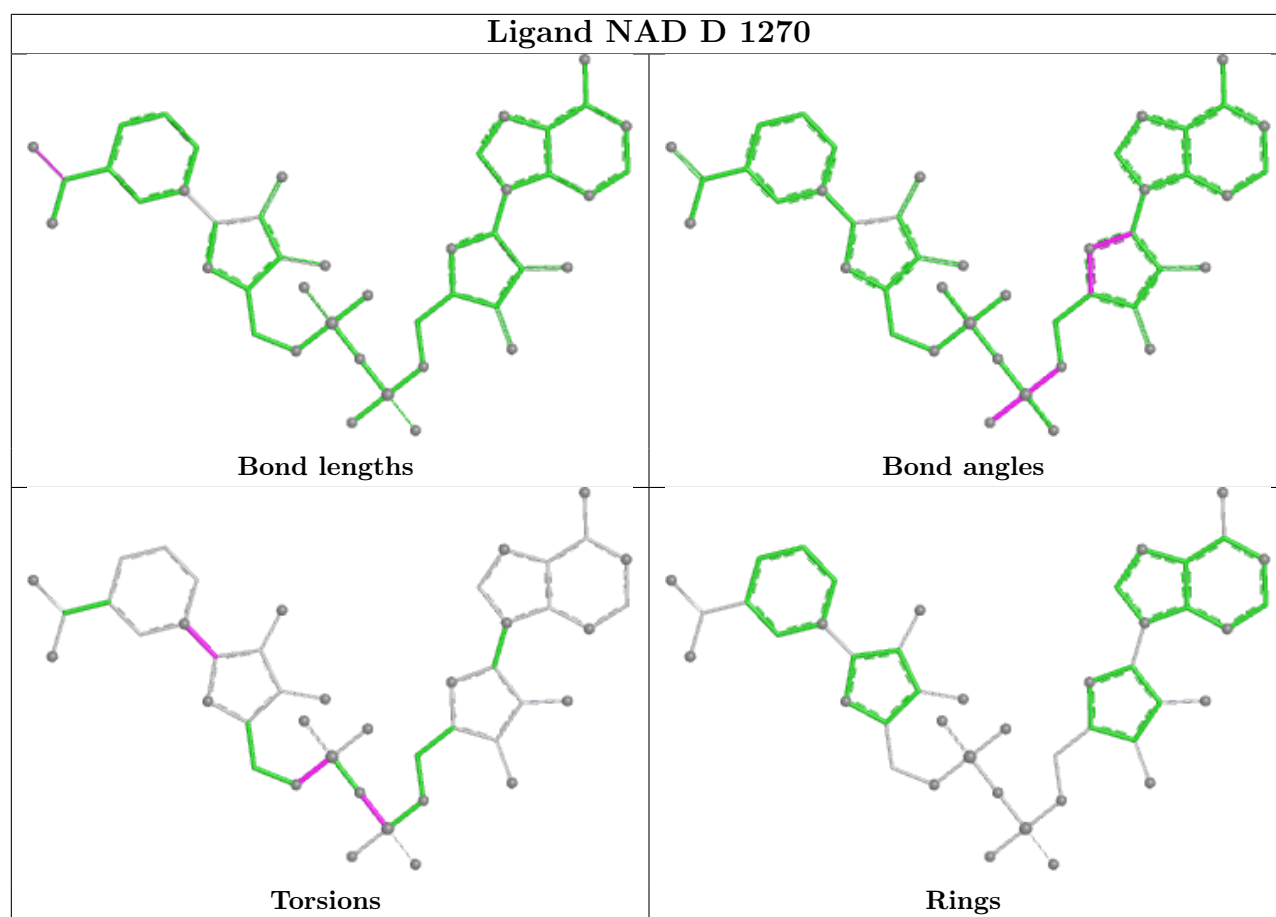
Ligand KXU C 1271

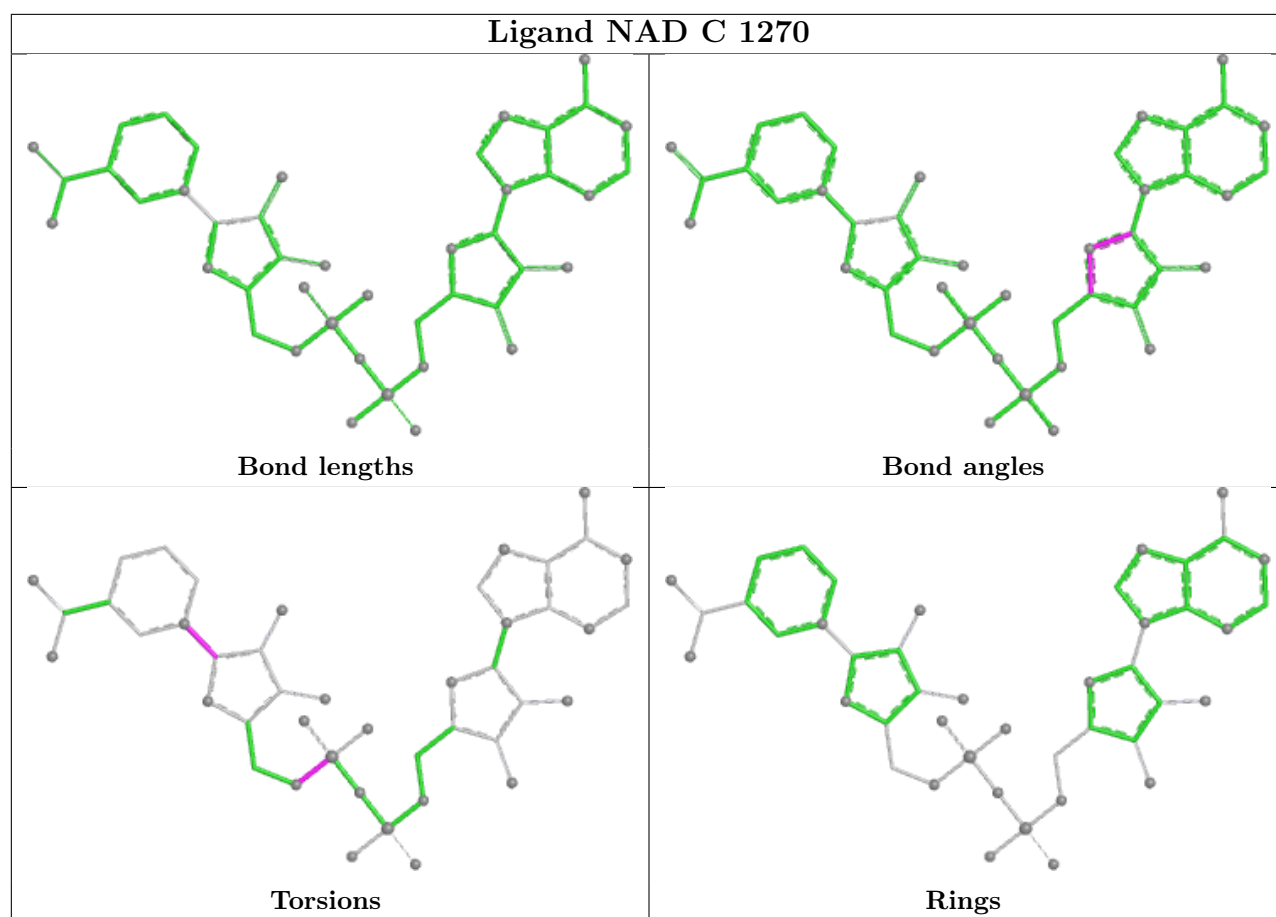


Ligand KXU A 1271









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	261/269 (97%)	-0.03	5 (1%) 66 73	6, 16, 36, 53	1 (0%)
1	B	267/269 (99%)	0.11	17 (6%) 25 31	5, 18, 42, 75	1 (0%)
1	C	249/269 (92%)	-0.00	7 (2%) 55 63	8, 17, 33, 61	0
1	D	264/269 (98%)	0.14	21 (7%) 18 23	5, 17, 42, 62	1 (0%)
All	All	1041/1076 (96%)	0.06	50 (4%) 35 43	5, 17, 39, 75	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	6.7
1	B	206	ALA	5.5
1	C	217	LEU	5.5
1	B	197	LEU	5.3
1	B	202	ILE	4.9
1	B	203	VAL	4.9
1	D	197	LEU	4.8
1	D	2	THR	4.8
1	D	46	LEU	4.6
1	B	105	ILE	4.5
1	D	41	PHE	4.4
1	A	2	THR	4.2
1	D	198	ALA	4.2
1	D	201	ALA	4.1
1	B	200	SER	3.9
1	D	202	ILE	3.8
1	D	196	THR	3.8
1	D	203	VAL	3.7
1	D	204	GLY	3.5
1	C	2	THR	3.4
1	C	216	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	208	GLY	3.2
1	C	218	LEU	3.2
1	C	269	LEU	3.1
1	D	211	ALA	3.1
1	A	85	GLY	3.1
1	D	215	ILE	3.1
1	D	206	ALA	3.0
1	D	199	MET	3.0
1	D	207	LEU	2.9
1	D	200	SER	2.8
1	A	269	LEU	2.8
1	B	213	ALA	2.7
1	D	218	LEU	2.7
1	B	53	ARG	2.6
1	D	269	LEU	2.6
1	B	2	THR	2.6
1	B	104	GLY	2.5
1	A	196	THR	2.5
1	C	196	THR	2.3
1	B	201	ALA	2.3
1	B	199	MET	2.3
1	B	198	ALA	2.3
1	B	269	LEU	2.2
1	B	212	GLY	2.2
1	D	68	GLU	2.1
1	B	215	ILE	2.1
1	D	47	ILE	2.1
1	D	219	GLU	2.0
1	C	219	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

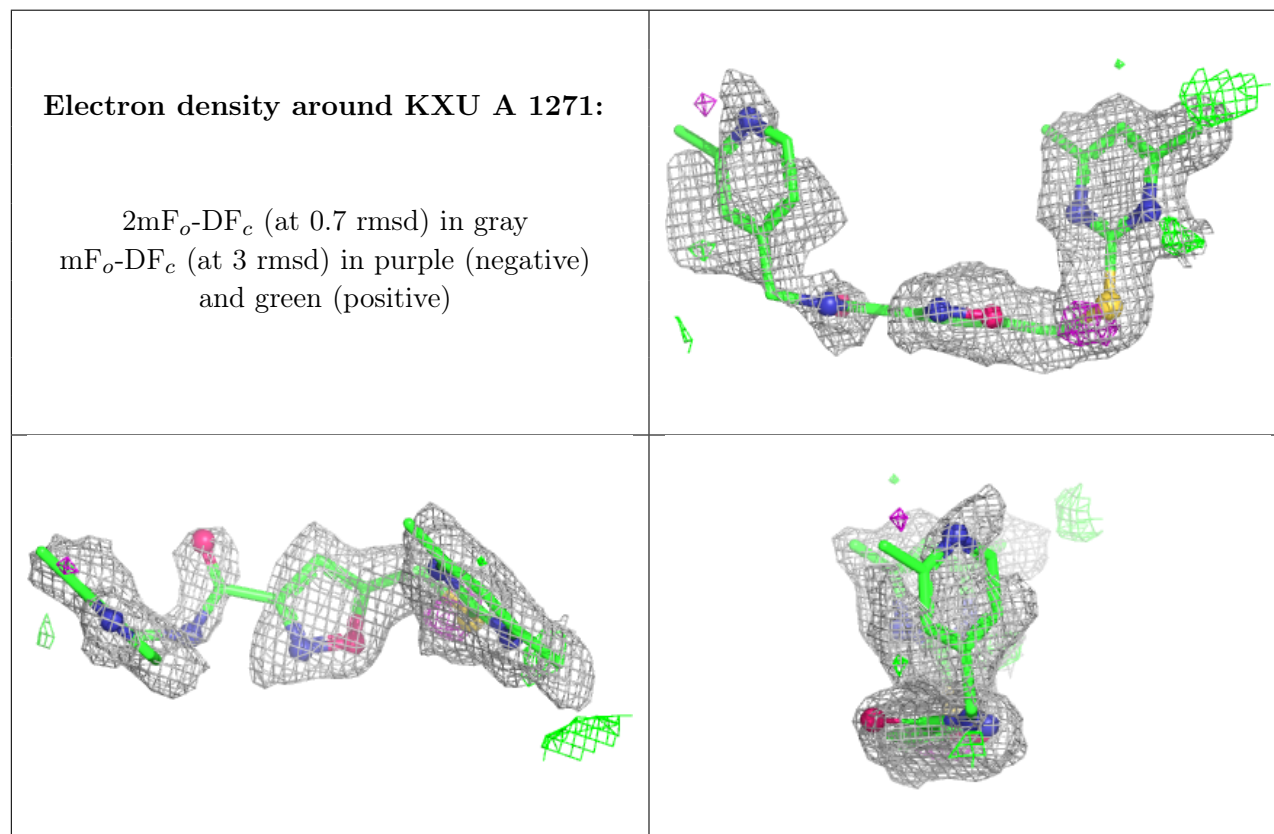
There are no oligosaccharides in this entry.

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, 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.

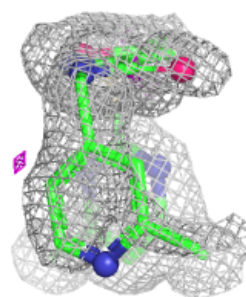
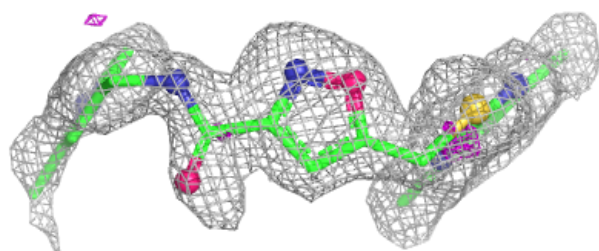
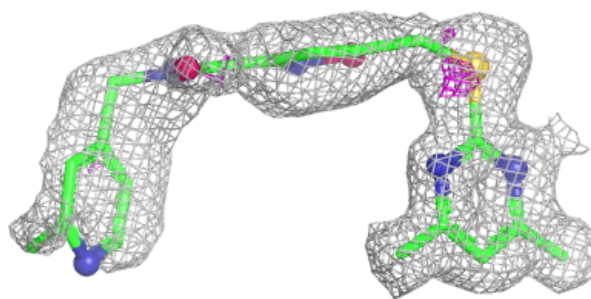
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KXU	A	1271	26/26	0.90	0.13	19,37,52,53	0
3	KXU	D	1271	26/26	0.92	0.12	19,32,49,49	0
3	KXU	C	1271	26/26	0.93	0.14	13,33,57,58	0
3	KXU	B	1271	26/26	0.95	0.10	13,28,50,52	0
2	NAD	D	1270	44/44	0.97	0.06	11,15,18,22	0
2	NAD	C	1270	44/44	0.98	0.05	10,14,15,16	0
2	NAD	A	1270	44/44	0.98	0.05	9,13,16,17	0
2	NAD	B	1270	44/44	0.98	0.05	9,13,17,19	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.

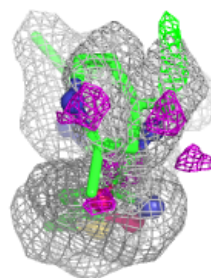
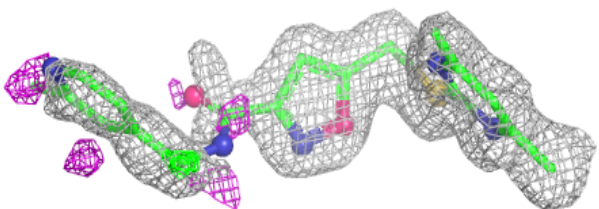
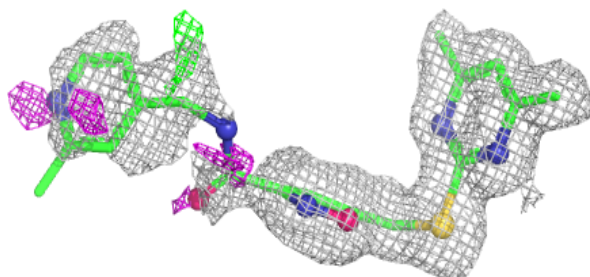


Electron density around KXU D 1271:

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

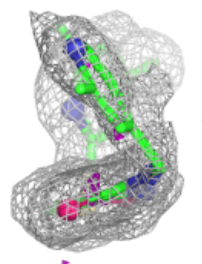
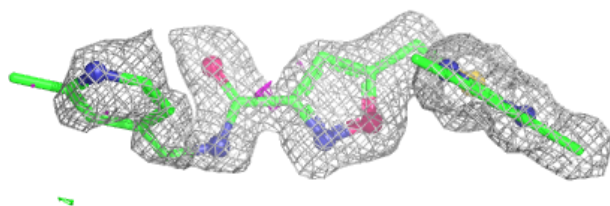
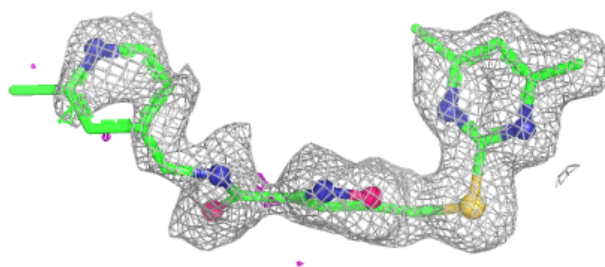
**Electron density around KXU C 1271:**

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

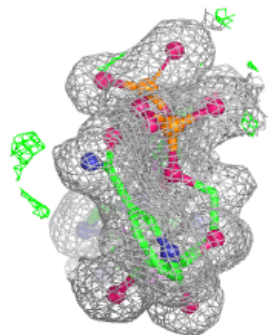
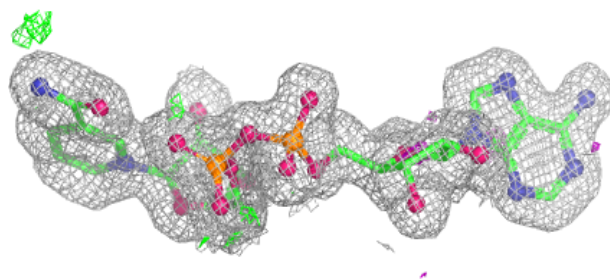
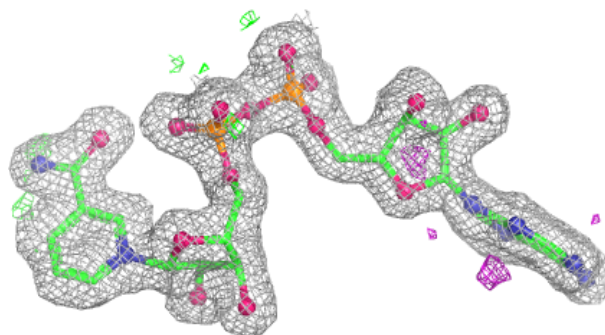


Electron density around KXU B 1271:

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

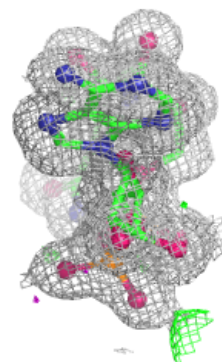
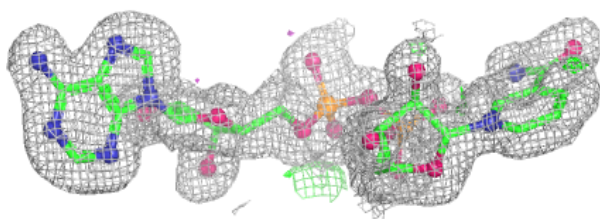
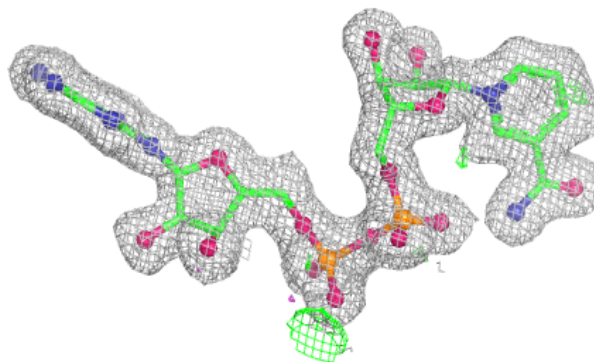
**Electron density around NAD D 1270:**

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

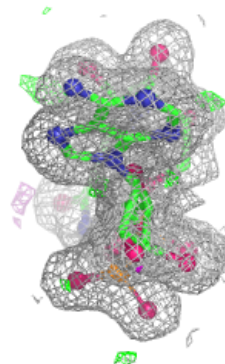
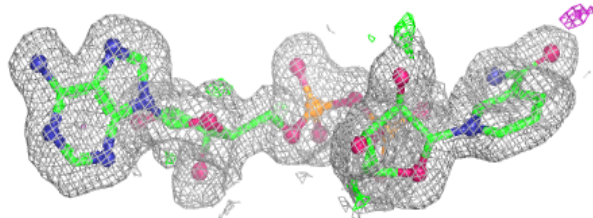
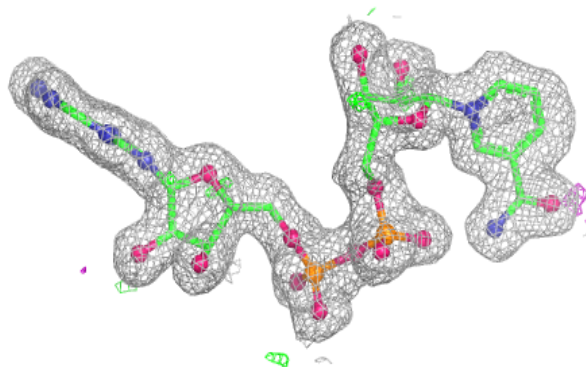


Electron density around NAD C 1270:

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

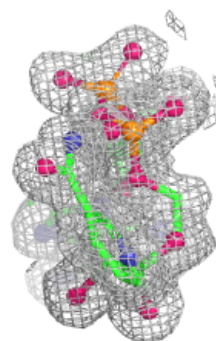
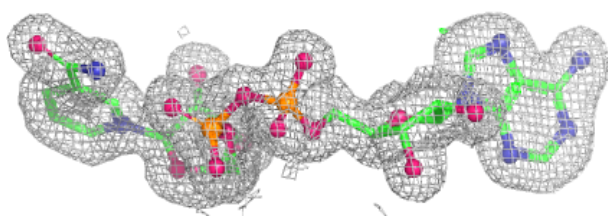
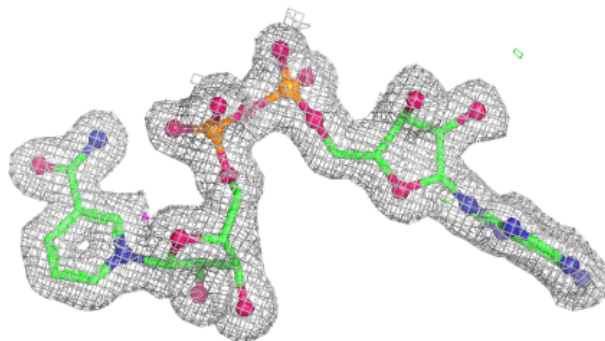
**Electron density around NAD A 1270:**

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



Electron density around NAD B 1270:

$2mF_o-DF_c$ (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.