



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2022 – 06:33 pm GMT

PDB ID : 5MH6
Title : D-2-hydroxyacid dehydrogenases (D2-HDH) from *Haloferax mediterranei* in complex with 2-ketohexanoic acid and NAD⁺ (1.35 Å resolution)
Authors : Bisson, C.; Baker, P.J.; Domenech Perez, J.; Pramanpol, N.; Harding, S.E.; Rice, D.W.; Ferrer, J.
Deposited on : 2016-11-23
Resolution : 1.35 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

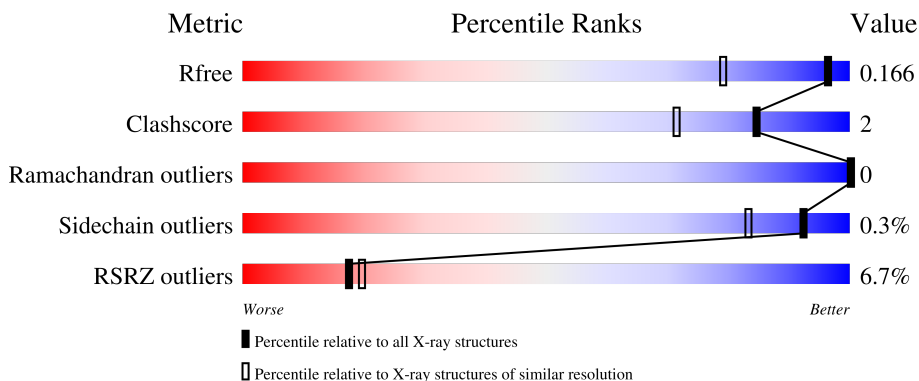
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

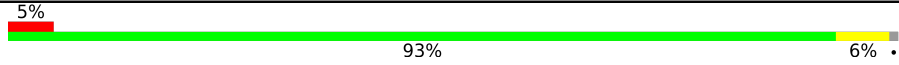
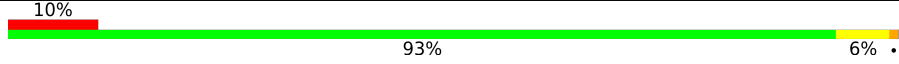
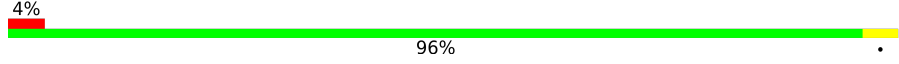
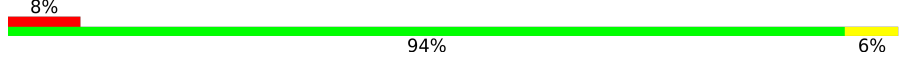
The reported resolution of this entry is 1.35 Å.

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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	308	
1	B	308	
1	C	308	
1	D	308	

2 Entry composition [i](#)

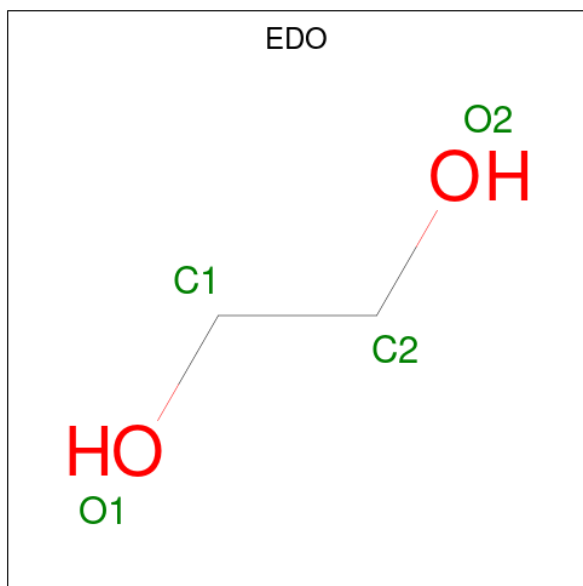
There are 8 unique types of molecules in this entry. The entry contains 11624 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-2-hydroxyacid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	Total 2380	C 1493	N 404	O 476	S 7	0	9	0
1	B	306	Total 2375	C 1489	N 405	O 474	S 7	0	8	0
1	C	308	Total 2375	C 1488	N 405	O 474	S 8	0	5	0
1	D	308	Total 2380	C 1491	N 408	O 473	S 8	0	6	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

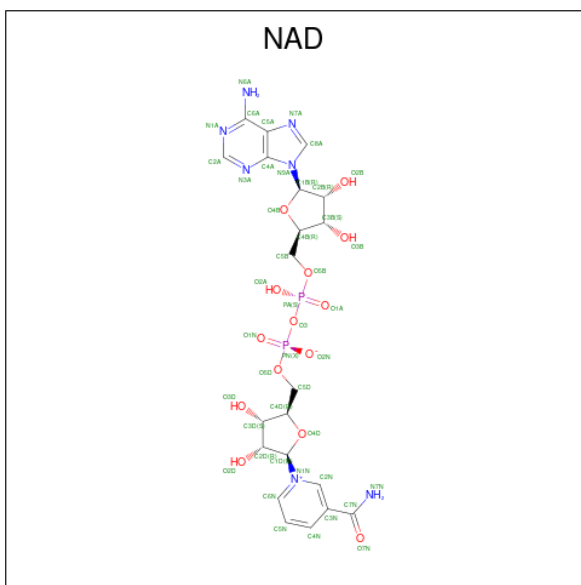


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

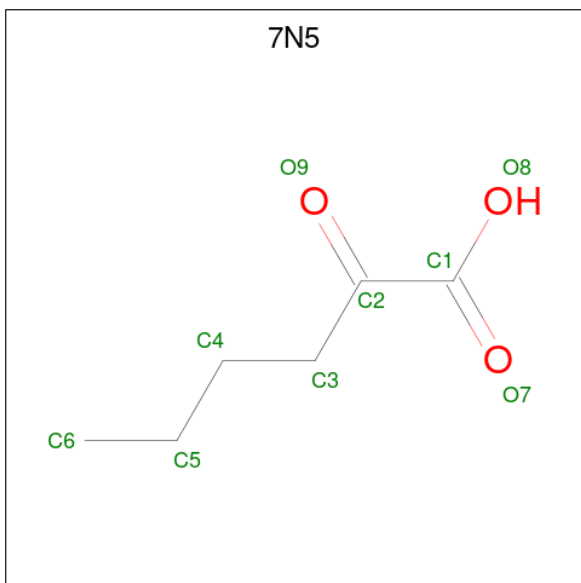
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total Mg 8 8	0	0
4	B	5	Total Mg 5 5	0	0
4	C	6	Total Mg 6 6	0	0
4	D	5	Total Mg 5 5	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 6 is 2-Ketohexanoic acid (three-letter code: 7N5) (formula: C₆H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	B	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	465	Total	O	0	12
			477	477		
8	B	413	Total	O	0	9
			422	422		
8	C	464	Total	O	0	3
			467	467		
8	D	396	Total	O	0	6
			402	402		

3 Residue-property plots [i](#)

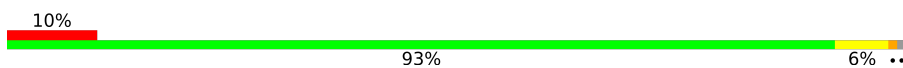
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: D-2-hydroxyacid dehydrogenase

Chain A: 



- Molecule 1: D-2-hydroxyacid dehydrogenase

Chain B: 

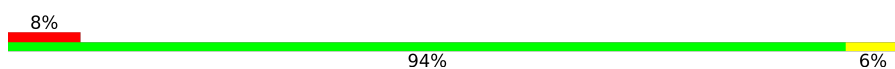


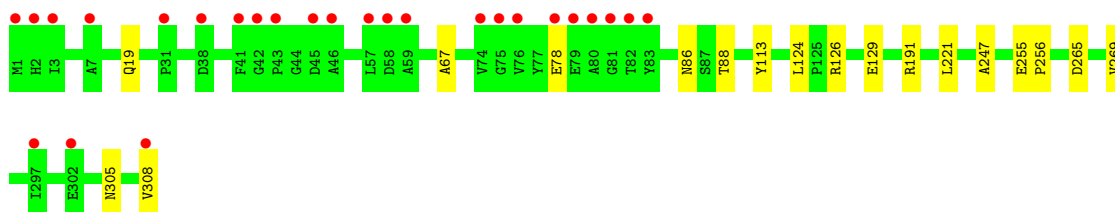
- Molecule 1: D-2-hydroxyacid dehydrogenase

Chain C: 



- Molecule 1: D-2-hydroxyacid dehydrogenase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 75.01Å 77.56Å 109.11° 107.55° 95.91°	Depositor
Resolution (Å)	46.54 – 1.35 41.64 – 1.35	Depositor EDS
% Data completeness (in resolution range)	80.2 (46.54-1.35) 92.9 (41.64-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.35Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.126 , 0.162 0.131 , 0.166	Depositor DCC
R_{free} test set	13634 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11624	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4346e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 7N5, EDO, NAD, NA, SO4, MG

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	0.56	1/2458 (0.0%)	0.81	4/3353 (0.1%)
1	B	0.52	0/2447	0.79	3/3338 (0.1%)
1	C	0.52	0/2441	0.78	4/3330 (0.1%)
1	D	0.51	0/2449	0.75	1/3340 (0.0%)
All	All	0.53	1/9795 (0.0%)	0.79	12/13361 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLU	CD-OE2	-5.03	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260[A]	ASP	CB-CG-OD1	11.24	128.42	118.30
1	A	260[B]	ASP	CB-CG-OD1	11.24	128.42	118.30
1	B	165	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	191	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	165	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	165	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	191	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	165	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	165	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	D	265	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	201	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	165	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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	2380	0	2285	12	0
1	B	2375	0	2280	13	0
1	C	2375	0	2274	8	0
1	D	2380	0	2285	13	0
2	A	24	0	36	0	0
2	B	24	0	36	1	0
2	C	24	0	36	1	1
2	D	16	0	24	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	8	0	0	0	0
4	B	5	0	0	0	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
5	A	44	0	26	0	0
5	B	44	0	26	0	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
6	A	9	0	0	0	0
6	B	9	0	0	0	0
6	C	9	0	0	0	0
6	D	9	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	477	0	0	2	0
8	B	422	0	0	3	4
8	C	467	0	0	2	1
8	D	402	0	0	3	2
All	All	11624	0	9360	45	4

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 2.

All (45) 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:88[B]:THR:HG21	8:D:637[B]:HOH:O	1.69	0.93
1:C:88[B]:THR:HG21	8:C:659:HOH:O	1.68	0.92
1:B:86[B]:ASN:OD1	1:B:88[B]:THR:HG23	1.77	0.83
1:D:191[A]:ARG:NH2	8:D:501:HOH:O	2.11	0.81
1:B:86[A]:ASN:OD1	1:B:88[A]:THR:HG22	1.85	0.75
1:D:191[B]:ARG:NH2	8:D:502:HOH:O	2.21	0.67
1:B:20[B]:ARG:NH1	8:B:501:HOH:O	2.19	0.66
1:A:20[A]:ARG:NH2	8:A:501:HOH:O	2.05	0.66
1:B:137:ARG:NH2	1:B:160:GLU:OE1	2.32	0.62
1:A:191[B]:ARG:NH2	8:A:502:HOH:O	2.29	0.58
1:A:297:ILE:HG13	1:A:303:LEU:HD21	1.87	0.57
1:A:165:ARG:HG2	1:A:177[A]:VAL:CG1	2.36	0.56
1:B:191[A]:ARG:NH2	8:B:502:HOH:O	2.34	0.54
1:C:86[A]:ASN:OD1	1:C:305:ASN:HB3	2.09	0.53
1:C:205:GLY:HA3	2:C:406:EDO:H11	1.91	0.53
1:B:126:ARG:HB2	1:B:129:GLU:HG3	1.94	0.50
1:A:255:GLU:HA	1:A:256:PRO:C	2.34	0.48
1:B:57[B]:LEU:CD1	1:B:57[B]:LEU:N	2.78	0.46
1:D:19:GLN:HB3	2:D:403:EDO:H11	1.96	0.46
1:B:86[B]:ASN:ND2	1:B:305:ASN:HB3	2.31	0.45
1:D:255:GLU:HA	1:D:256:PRO:C	2.36	0.45
1:D:126:ARG:HB2	1:D:129:GLU:HG3	1.99	0.45
1:D:86[A]:ASN:OD1	1:D:305:ASN:HB3	2.18	0.44
1:A:86:ASN:OD1	1:A:88[B]:THR:HG22	2.17	0.44
1:A:78:GLU:HB2	1:A:308:VAL:HG21	2.00	0.43
1:A:165:ARG:HG2	1:A:177[A]:VAL:HG11	1.99	0.43
1:B:57[B]:LEU:HD21	1:B:76:VAL:HG12	2.00	0.43
1:D:78:GLU:HB2	1:D:308:VAL:HG21	2.00	0.43
1:A:20[A]:ARG:HG2	1:A:283:HIS:CD2	2.54	0.43
1:A:113:TYR:CZ	1:B:275:VAL:HG21	2.54	0.43
1:C:67:ALA:HB1	1:C:88[B]:THR:HG22	2.01	0.43
1:B:74:VAL:HG13	1:B:308:VAL:HB	2.00	0.42
1:C:255:GLU:HA	1:C:256:PRO:C	2.40	0.42
1:D:221:LEU:O	1:D:247:ALA:HA	2.20	0.42
2:B:406:EDO:H21	8:B:579:HOH:O	2.21	0.41
1:B:255:GLU:HA	1:B:256:PRO:C	2.40	0.41
1:A:165:ARG:HD3	1:A:169:ASP:O	2.20	0.41
1:C:128:GLU:HG2	8:C:811:HOH:O	2.19	0.41
1:D:67:ALA:HB1	1:D:88[B]:THR:HG22	2.02	0.41
1:C:39:GLU:HG2	1:C:41:PHE:CZ	2.56	0.41
1:D:247:ALA:O	1:D:269:VAL:HA	2.20	0.41
1:D:124:LEU:HD21	2:D:405:EDO:H22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ALA:O	1:B:269:VAL:HA	2.21	0.40
1:A:67:ALA:HB1	1:A:88[A]:THR:HG22	2.03	0.40
1:C:275:VAL:HG21	1:D:113:TYR:CZ	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:505:HOH:O	8:D:821:HOH:O[1_545]	1.99	0.21
8:B:807:HOH:O	8:D:519:HOH:O[1_556]	2.08	0.12
2:C:407:EDO:O1	8:B:665:HOH:O[1_565]	2.12	0.08
8:B:878:HOH:O	8:C:897:HOH:O[1_556]	2.14	0.06

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	313/308 (102%)	308 (98%)	5 (2%)	0	100	100
1	B	312/308 (101%)	305 (98%)	7 (2%)	0	100	100
1	C	311/308 (101%)	306 (98%)	5 (2%)	0	100	100
1	D	312/308 (101%)	307 (98%)	5 (2%)	0	100	100
All	All	1248/1232 (101%)	1226 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	252/245 (103%)	251 (100%)	1 (0%)	91	81
1	B	251/245 (102%)	248 (99%)	3 (1%)	71	42
1	C	250/245 (102%)	250 (100%)	0	100	100
1	D	251/245 (102%)	251 (100%)	0	100	100
All	All	1004/980 (102%)	1000 (100%)	4 (0%)	92	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	THR
1	B	57[A]	LEU
1	B	57[B]	LEU
1	B	308	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 26 are monoatomic - leaving 34 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	403	-	3,3,3	0.50	0	2,2,2	0.10	0
2	EDO	D	402	-	3,3,3	0.38	0	2,2,2	0.27	0
3	SO4	D	406	-	4,4,4	0.29	0	6,6,6	0.44	0
2	EDO	C	406	-	3,3,3	0.55	0	2,2,2	0.53	0
2	EDO	C	404	-	3,3,3	0.60	0	2,2,2	0.45	0
6	7N5	A	416	-	8,8,8	2.07	1 (12%)	9,9,9	1.13	1 (11%)
2	EDO	C	405	-	3,3,3	0.55	0	2,2,2	0.21	0
2	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	B	404	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	A	402	-	3,3,3	0.48	0	2,2,2	0.21	0
3	SO4	B	407	-	4,4,4	0.32	0	6,6,6	0.79	0
2	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	B	401	-	3,3,3	0.43	0	2,2,2	0.29	0
6	7N5	C	416	-	8,8,8	2.06	1 (12%)	9,9,9	1.31	2 (22%)
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.09	0
5	NAD	D	412	7	42,48,48	0.93	2 (4%)	50,73,73	1.29	3 (6%)
6	7N5	D	413	-	8,8,8	2.24	1 (12%)	9,9,9	1.27	2 (22%)
2	EDO	A	401	-	3,3,3	0.52	0	2,2,2	0.13	0
5	NAD	B	413	-	42,48,48	0.78	1 (2%)	50,73,73	1.34	7 (14%)
5	NAD	C	415	7	42,48,48	0.79	1 (2%)	50,73,73	1.41	7 (14%)
2	EDO	B	405	-	3,3,3	0.57	0	2,2,2	0.36	0
3	SO4	A	407	-	4,4,4	0.08	0	6,6,6	0.36	0
2	EDO	D	405	-	3,3,3	0.49	0	2,2,2	0.48	0
5	NAD	A	415	-	42,48,48	0.83	1 (2%)	50,73,73	1.22	6 (12%)
2	EDO	B	406	-	3,3,3	0.58	0	2,2,2	0.25	0
2	EDO	D	403	-	3,3,3	1.00	0	2,2,2	0.83	0
2	EDO	C	402	-	3,3,3	0.56	0	2,2,2	0.09	0
2	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.42	0
2	EDO	C	403	-	3,3,3	0.47	0	2,2,2	0.12	0
2	EDO	A	405	-	3,3,3	0.54	0	2,2,2	0.42	0
6	7N5	B	414	-	8,8,8	2.13	1 (12%)	9,9,9	1.20	2 (22%)
2	EDO	A	403	-	3,3,3	0.46	0	2,2,2	0.23	0
2	EDO	D	404	-	3,3,3	0.46	0	2,2,2	0.29	0
3	SO4	C	408	-	4,4,4	0.34	0	6,6,6	0.72	0

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	EDO	B	403	-	-	1/1/1/1	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
6	7N5	A	416	-	-	2/8/8/8	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
6	7N5	C	416	-	-	1/8/8/8	-
2	EDO	C	407	-	-	1/1/1/1	-
5	NAD	D	412	7	-	2/26/62/62	0/5/5/5
6	7N5	D	413	-	-	0/8/8/8	-
2	EDO	A	401	-	-	1/1/1/1	-
5	NAD	B	413	-	-	1/26/62/62	0/5/5/5
5	NAD	C	415	7	-	1/26/62/62	0/5/5/5
2	EDO	B	405	-	-	1/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
5	NAD	A	415	-	-	1/26/62/62	0/5/5/5
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	A	406	-	-	0/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-
6	7N5	B	414	-	-	1/8/8/8	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	404	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	413	7N5	C2-C1	-5.98	1.45	1.53
6	B	414	7N5	C2-C1	-5.72	1.45	1.53
6	C	416	7N5	C2-C1	-5.59	1.46	1.53
6	A	416	7N5	C2-C1	-5.35	1.46	1.53
5	A	415	NAD	C5A-C4A	2.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	415	NAD	C5A-C4A	2.44	1.47	1.40
5	D	412	NAD	C2B-C1B	-2.27	1.50	1.53
5	D	412	NAD	C5A-C4A	2.23	1.46	1.40
5	B	413	NAD	C5A-C4A	2.23	1.46	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	415	NAD	N3A-C2A-N1A	-4.77	121.22	128.68
5	D	412	NAD	N3A-C2A-N1A	-4.61	121.47	128.68
5	D	412	NAD	C1B-N9A-C4A	-4.60	118.57	126.64
5	B	413	NAD	N3A-C2A-N1A	-3.93	122.53	128.68
5	B	413	NAD	C4A-C5A-N7A	-3.86	105.37	109.40
5	A	415	NAD	N3A-C2A-N1A	-3.75	122.82	128.68
5	C	415	NAD	C1B-N9A-C4A	-3.42	120.63	126.64
5	B	413	NAD	C3D-C2D-C1D	3.24	105.86	100.98
5	D	412	NAD	O4B-C1B-C2B	-2.87	102.74	106.93
5	C	415	NAD	C2A-N1A-C6A	2.82	123.58	118.75
5	C	415	NAD	O4B-C4B-C3B	2.71	110.47	105.11
5	C	415	NAD	C3D-C2D-C1D	2.69	105.03	100.98
5	A	415	NAD	C2A-N1A-C6A	2.68	123.34	118.75
5	B	413	NAD	O4B-C4B-C3B	2.63	110.31	105.11
6	C	416	7N5	O7-C1-C2	-2.47	118.42	121.72
5	C	415	NAD	PN-O3-PA	-2.46	124.37	132.83
5	B	413	NAD	PN-O3-PA	-2.45	124.41	132.83
5	A	415	NAD	C1B-N9A-C4A	-2.41	122.40	126.64
5	A	415	NAD	N6A-C6A-N1A	2.39	123.53	118.57
6	D	413	7N5	O8-C1-C2	2.24	120.09	113.97
5	A	415	NAD	O4B-C4B-C3B	2.23	109.52	105.11
6	B	414	7N5	O7-C1-C2	-2.23	118.75	121.72
5	A	415	NAD	C3N-C7N-N7N	2.21	120.40	117.75
5	B	413	NAD	C5B-C4B-C3B	-2.20	106.92	115.18
6	A	416	7N5	C3-C2-C1	2.20	120.05	115.97
6	D	413	7N5	O7-C1-C2	-2.19	118.79	121.72
6	B	414	7N5	O8-C1-C2	2.10	119.72	113.97
5	B	413	NAD	O2A-PA-O1A	2.05	122.36	112.24
5	C	415	NAD	O2N-PN-O1N	2.05	122.36	112.24
6	C	416	7N5	O8-C1-C2	2.03	119.51	113.97

There are no chirality outliers.

All (18) torsion outliers are listed below:

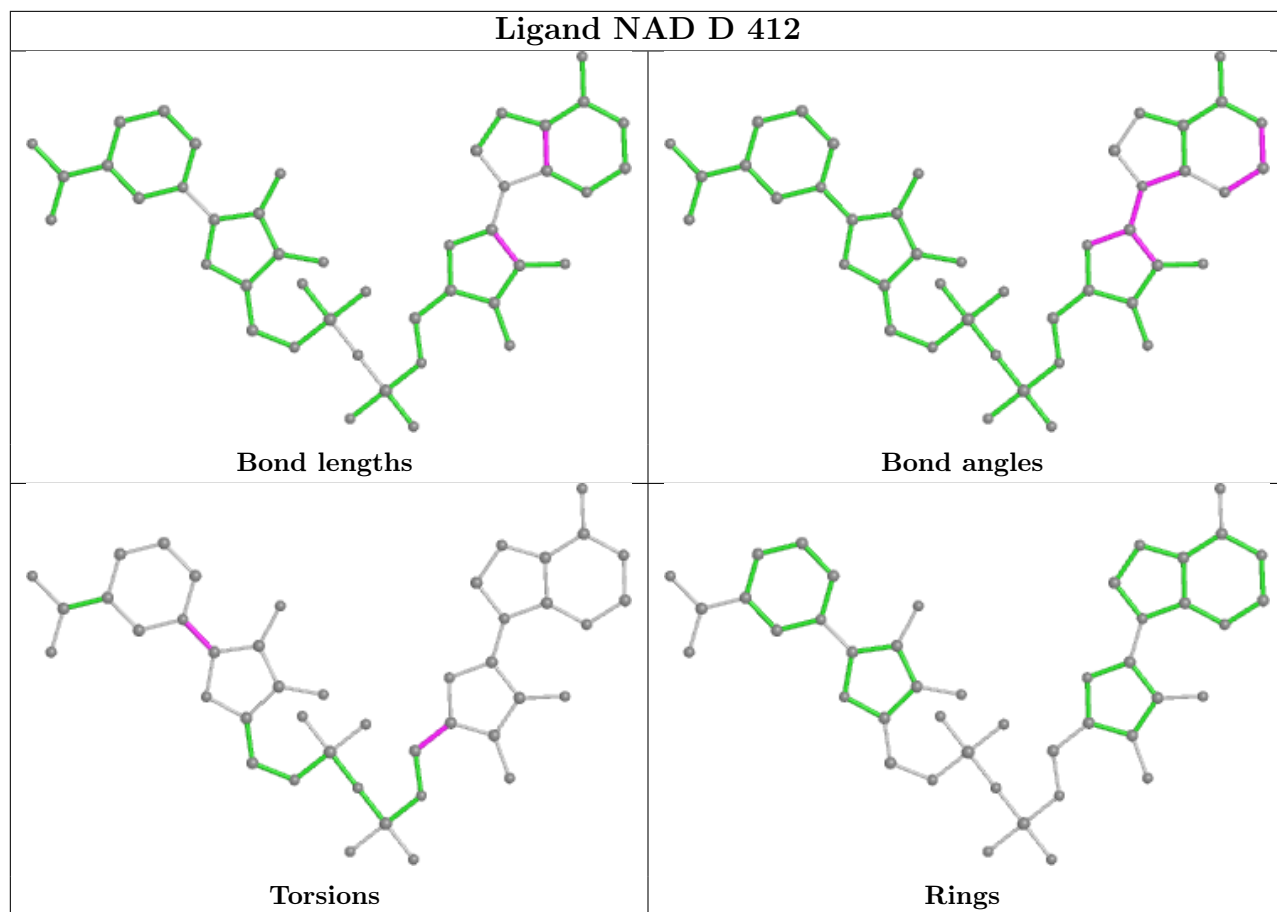
Mol	Chain	Res	Type	Atoms
5	D	412	NAD	O4D-C1D-N1N-C6N
2	A	405	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	D	405	EDO	O1-C1-C2-O2
6	A	416	7N5	C3-C4-C5-C6
2	B	406	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
6	A	416	7N5	O8-C1-C2-O9
6	C	416	7N5	O8-C1-C2-O9
2	A	401	EDO	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2
5	A	415	NAD	O4B-C4B-C5B-O5B
2	C	403	EDO	O1-C1-C2-O2
6	B	414	7N5	C3-C4-C5-C6
5	C	415	NAD	O4B-C4B-C5B-O5B
5	B	413	NAD	O4B-C4B-C5B-O5B
5	D	412	NAD	O4B-C4B-C5B-O5B
2	C	407	EDO	O1-C1-C2-O2

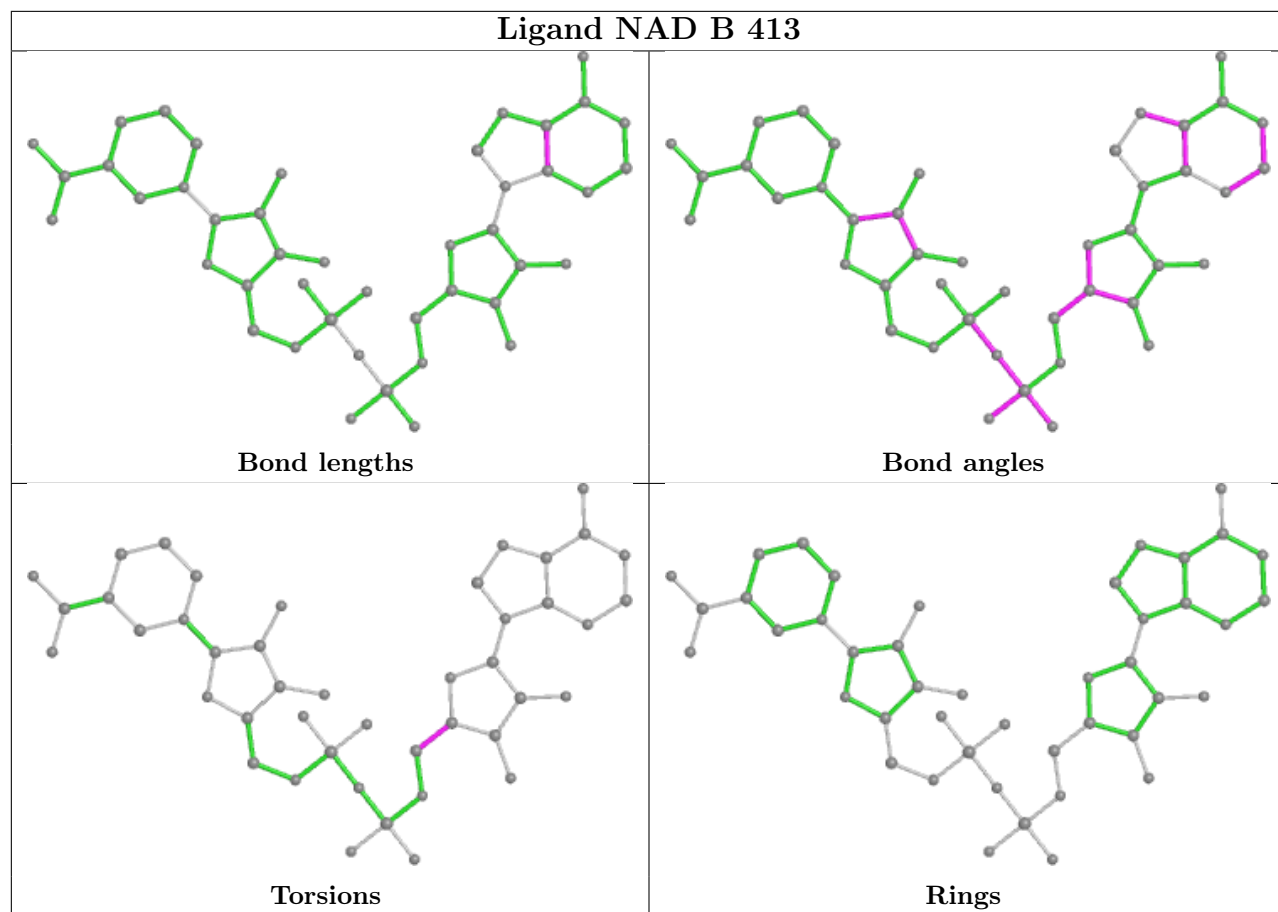
There are no ring outliers.

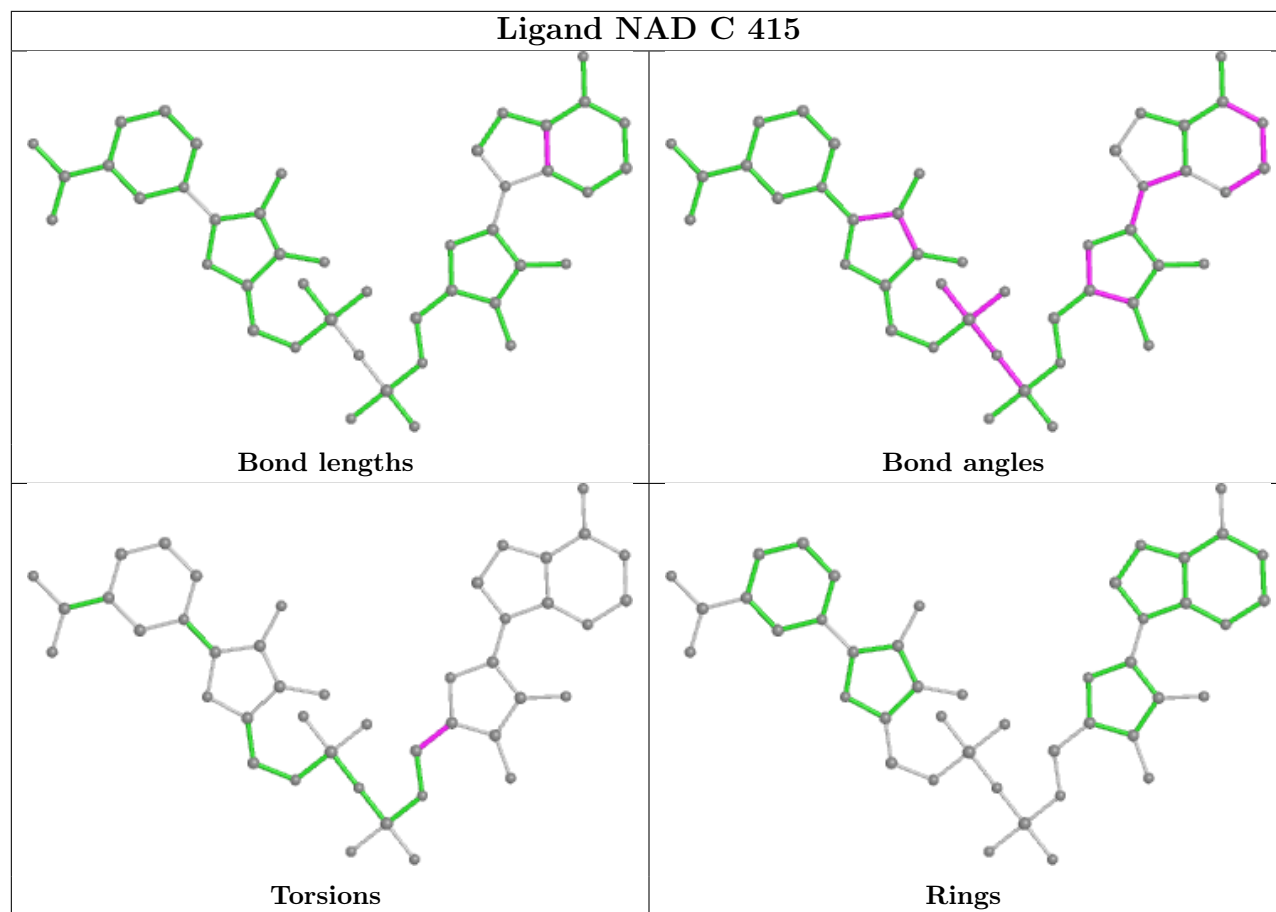
5 monomers are involved in 5 short contacts:

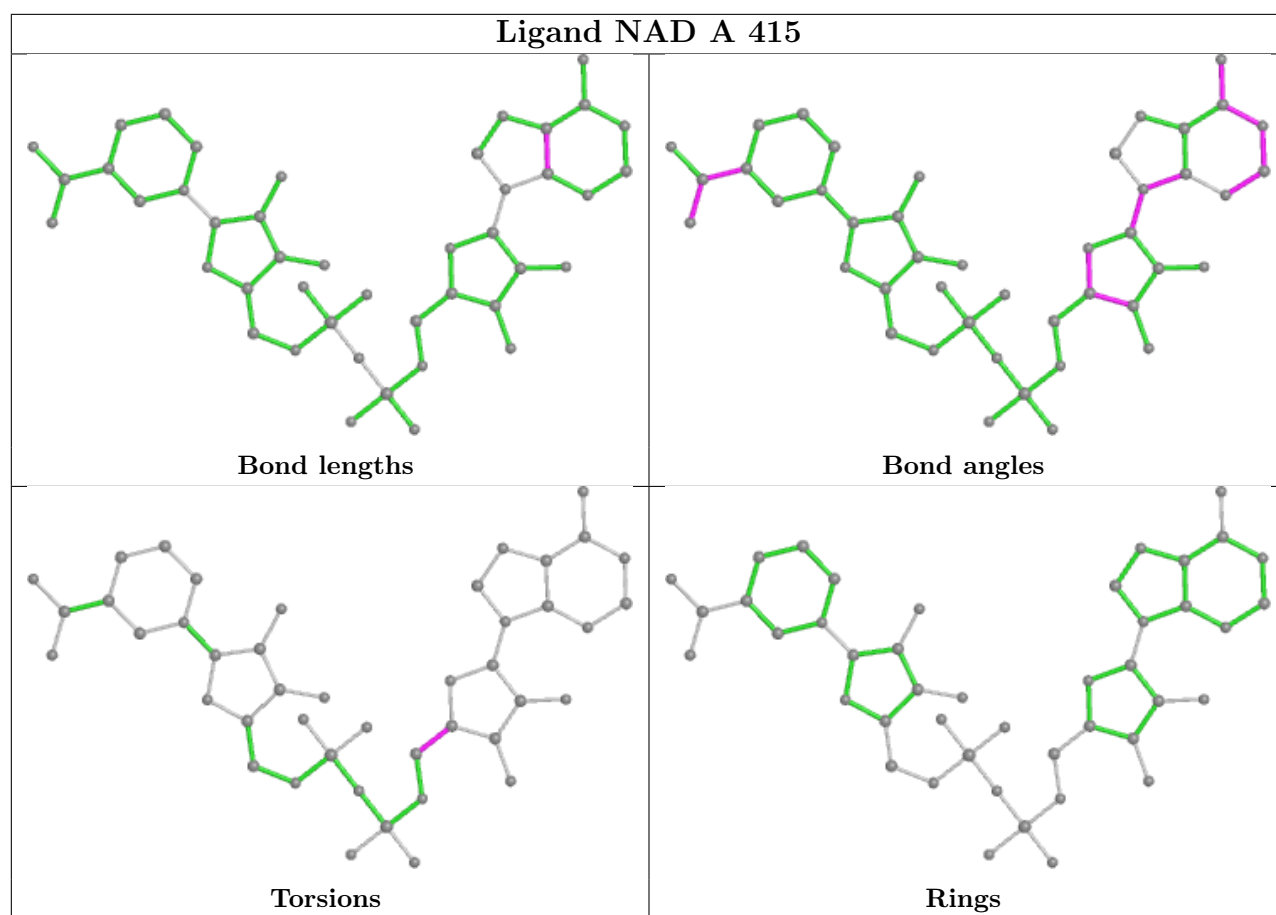
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	406	EDO	1	0
2	C	407	EDO	0	1
2	D	405	EDO	1	0
2	B	406	EDO	1	0
2	D	403	EDO	1	0

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.









5.7 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	306/308 (99%)	0.25	14 (4%) 32 37	4, 11, 30, 70	0
1	B	306/308 (99%)	0.45	31 (10%) 7 8	4, 11, 39, 88	0
1	C	308/308 (100%)	0.18	11 (3%) 42 48	4, 11, 31, 74	0
1	D	308/308 (100%)	0.49	26 (8%) 11 12	5, 12, 34, 76	0
All	All	1228/1232 (99%)	0.34	82 (6%) 17 20	4, 11, 35, 88	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57[A]	LEU	6.4
1	B	308	VAL	6.1
1	B	76	VAL	5.7
1	D	308	VAL	5.6
1	B	74	VAL	5.0
1	D	43	PRO	4.7
1	B	79	GLU	4.6
1	B	75	GLY	4.5
1	B	38	ASP	4.4
1	D	2	HIS	4.3
1	D	41	PHE	4.1
1	C	308	VAL	4.0
1	A	308	VAL	4.0
1	A	79	GLU	4.0
1	D	83	TYR	3.9
1	D	78	GLU	3.9
1	B	77	TYR	3.8
1	A	83	TYR	3.7
1	D	76	VAL	3.7
1	B	42	GLY	3.7
1	D	82	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.6
1	B	56	PHE	3.6
1	B	43	PRO	3.6
1	B	83	TYR	3.6
1	D	57	LEU	3.5
1	B	40	GLN	3.4
1	A	76	VAL	3.4
1	B	300	GLY	3.4
1	B	54	ASP	3.4
1	D	79	GLU	3.3
1	B	55	ALA	3.3
1	B	41	PHE	3.3
1	D	74	VAL	3.2
1	D	58	ASP	3.2
1	A	168	GLY	3.1
1	D	42	GLY	3.0
1	D	80	ALA	3.0
1	D	81	GLY	3.0
1	B	297	ILE	3.0
1	A	78	GLU	2.9
1	A	75	GLY	2.9
1	D	3	ILE	2.9
1	D	297	ILE	2.9
1	B	36	GLY	2.9
1	B	80	ALA	2.9
1	C	38	ASP	2.8
1	C	76	VAL	2.8
1	B	302	GLU	2.7
1	B	59	ALA	2.7
1	C	75	GLY	2.7
1	D	46	ALA	2.7
1	D	38	ASP	2.7
1	C	54	ASP	2.6
1	A	80	ALA	2.6
1	B	37	GLU	2.5
1	B	78	GLU	2.5
1	D	31	PRO	2.5
1	B	301	ASP	2.5
1	B	81	GLY	2.5
1	C	1	MET	2.5
1	D	59	ALA	2.5
1	A	302	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	75	GLY	2.4
1	C	79	GLU	2.4
1	A	81	GLY	2.4
1	A	74	VAL	2.3
1	B	52	HIS	2.3
1	A	43	PRO	2.2
1	D	7	ALA	2.2
1	B	73	PRO	2.2
1	C	302	GLU	2.2
1	A	3	ILE	2.2
1	B	303	LEU	2.2
1	B	39	GLU	2.2
1	D	302	GLU	2.1
1	A	77	TYR	2.1
1	C	299	THR	2.1
1	C	40	GLN	2.1
1	C	55	ALA	2.0
1	B	82	THR	2.0
1	D	45	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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	EDO	D	403	4/4	0.84	0.16	16,24,25,26	0
2	EDO	B	403	4/4	0.85	0.12	24,28,37,42	0
2	EDO	A	405	4/4	0.85	0.13	24,29,35,37	0
2	EDO	A	403	4/4	0.87	0.11	28,29,30,34	0

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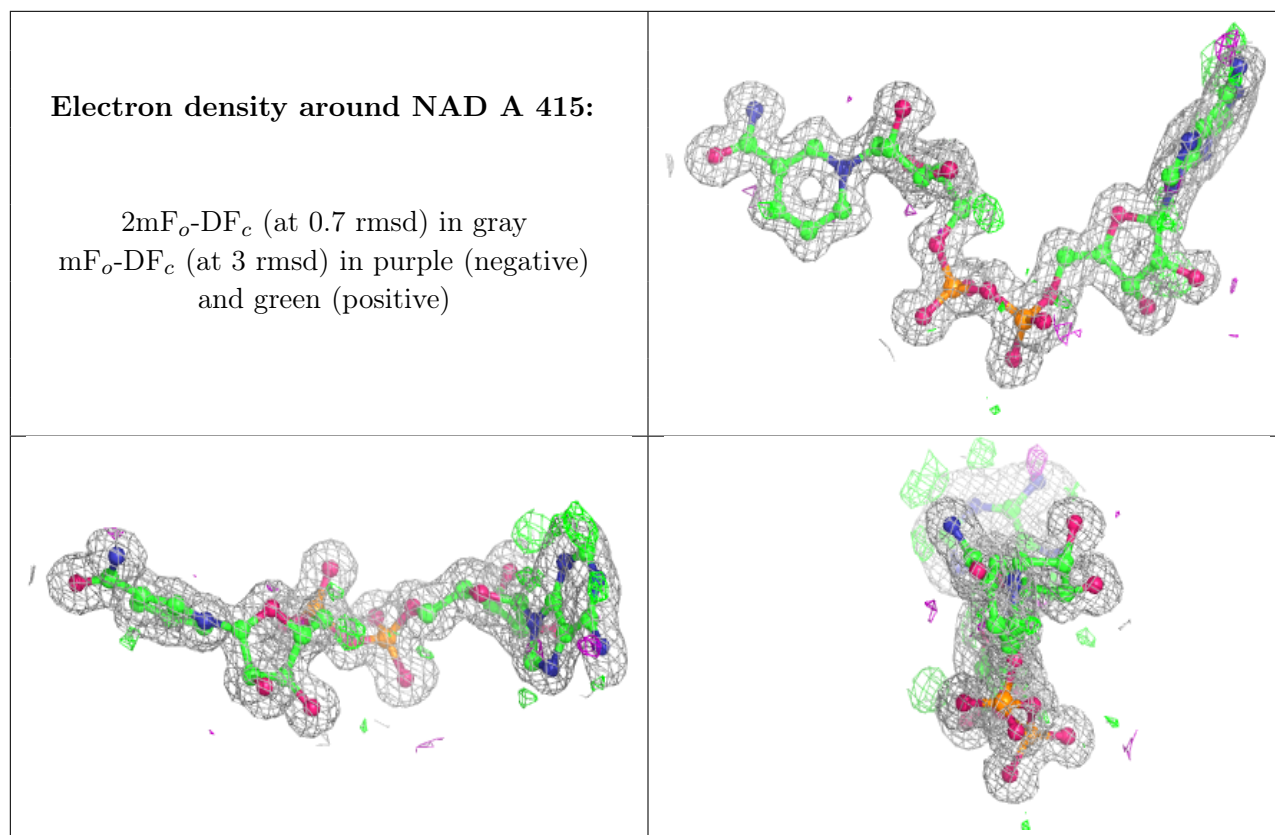
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	C	406	4/4	0.88	0.15	16,19,21,29	0
2	EDO	C	407	4/4	0.88	0.26	26,35,40,51	0
2	EDO	C	403	4/4	0.88	0.17	29,44,45,46	0
2	EDO	A	404	4/4	0.89	0.19	35,39,53,81	0
2	EDO	B	406	4/4	0.89	0.28	17,29,42,57	0
2	EDO	A	406	4/4	0.89	0.13	30,30,31,33	0
3	SO4	D	406	5/5	0.89	0.13	10,12,15,17	5
2	EDO	B	405	4/4	0.90	0.19	22,23,24,26	0
2	EDO	C	402	4/4	0.91	0.09	19,23,27,30	0
3	SO4	B	407	5/5	0.92	0.13	18,19,22,27	5
2	EDO	B	401	4/4	0.92	0.08	16,22,22,24	0
2	EDO	D	402	4/4	0.93	0.13	16,23,31,39	0
2	EDO	C	404	4/4	0.93	0.17	15,18,19,24	0
4	MG	D	410	1/1	0.93	0.06	51,51,51,51	0
2	EDO	A	401	4/4	0.94	0.10	19,24,33,71	0
3	SO4	C	408	5/5	0.94	0.13	12,16,16,21	5
2	EDO	D	404	4/4	0.94	0.09	25,29,33,36	0
2	EDO	D	405	4/4	0.94	0.23	18,23,40,50	0
2	EDO	B	402	4/4	0.95	0.11	23,23,23,23	0
2	EDO	C	405	4/4	0.95	0.11	14,19,26,28	0
2	EDO	B	404	4/4	0.95	0.12	12,17,20,22	0
6	7N5	A	416	9/9	0.96	0.11	10,14,47,54	0
7	NA	C	401	1/1	0.96	0.19	31,31,31,31	0
4	MG	D	409	1/1	0.97	0.37	43,43,43,43	0
2	EDO	A	402	4/4	0.97	0.10	21,23,25,26	0
4	MG	A	417	1/1	0.97	0.17	26,26,26,26	0
6	7N5	C	416	9/9	0.97	0.09	9,15,29,32	0
6	7N5	D	413	9/9	0.97	0.09	10,18,40,40	0
4	MG	C	411	1/1	0.97	0.19	26,26,26,26	0
7	NA	D	401	1/1	0.97	0.21	27,27,27,27	0
5	NAD	A	415	44/44	0.98	0.07	4,9,16,23	0
5	NAD	B	413	44/44	0.98	0.07	6,10,18,21	0
5	NAD	C	415	44/44	0.98	0.07	5,10,21,31	0
5	NAD	D	412	44/44	0.98	0.07	5,11,15,16	0
4	MG	A	410	1/1	0.98	0.13	16,16,16,16	1
6	7N5	B	414	9/9	0.98	0.08	11,16,26,28	0
4	MG	C	412	1/1	0.98	0.25	17,17,17,17	1
4	MG	C	413	1/1	0.98	0.15	28,28,28,28	0
4	MG	A	414	1/1	0.98	0.34	33,33,33,33	0
3	SO4	A	407	5/5	0.98	0.08	8,9,12,13	5
4	MG	A	409	1/1	0.99	0.07	14,14,14,14	0
4	MG	A	411	1/1	0.99	0.30	31,31,31,31	0

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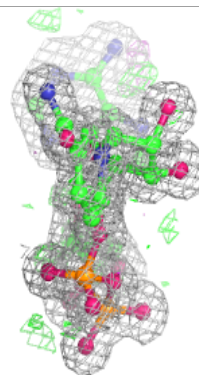
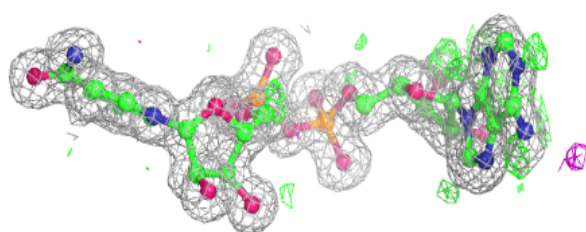
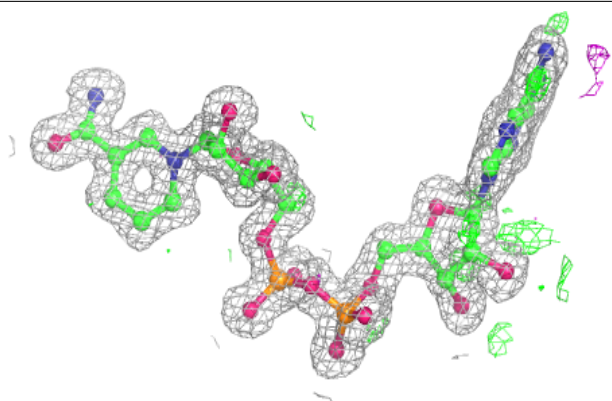
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	409	1/1	0.99	0.08	9,9,9,9	1
4	MG	B	410	1/1	0.99	0.38	36,36,36,36	0
4	MG	B	411	1/1	0.99	0.27	25,25,25,25	0
4	MG	C	410	1/1	0.99	0.08	11,11,11,11	1
4	MG	A	412	1/1	0.99	0.20	25,25,25,25	0
4	MG	B	408	1/1	1.00	0.06	8,8,8,8	0
4	MG	B	412	1/1	1.00	0.06	10,10,10,10	0
4	MG	C	414	1/1	1.00	0.05	11,11,11,11	0
4	MG	D	407	1/1	1.00	0.06	8,8,8,8	0
4	MG	D	408	1/1	1.00	0.05	11,11,11,11	0
4	MG	C	409	1/1	1.00	0.07	7,7,7,7	0
4	MG	A	408	1/1	1.00	0.07	7,7,7,7	0
4	MG	D	411	1/1	1.00	0.05	13,13,13,13	0
4	MG	A	413	1/1	1.00	0.05	11,11,11,11	0

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

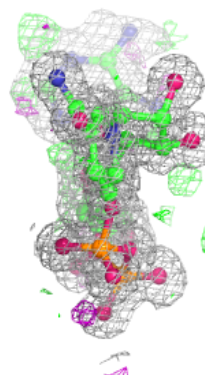
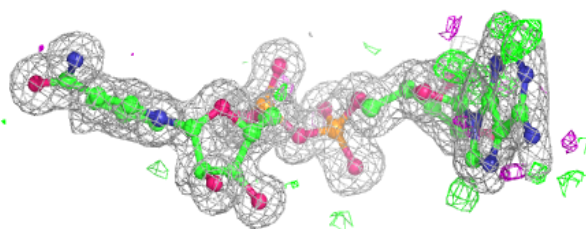
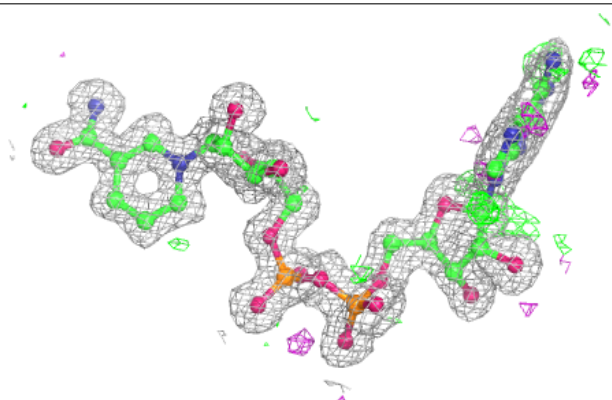


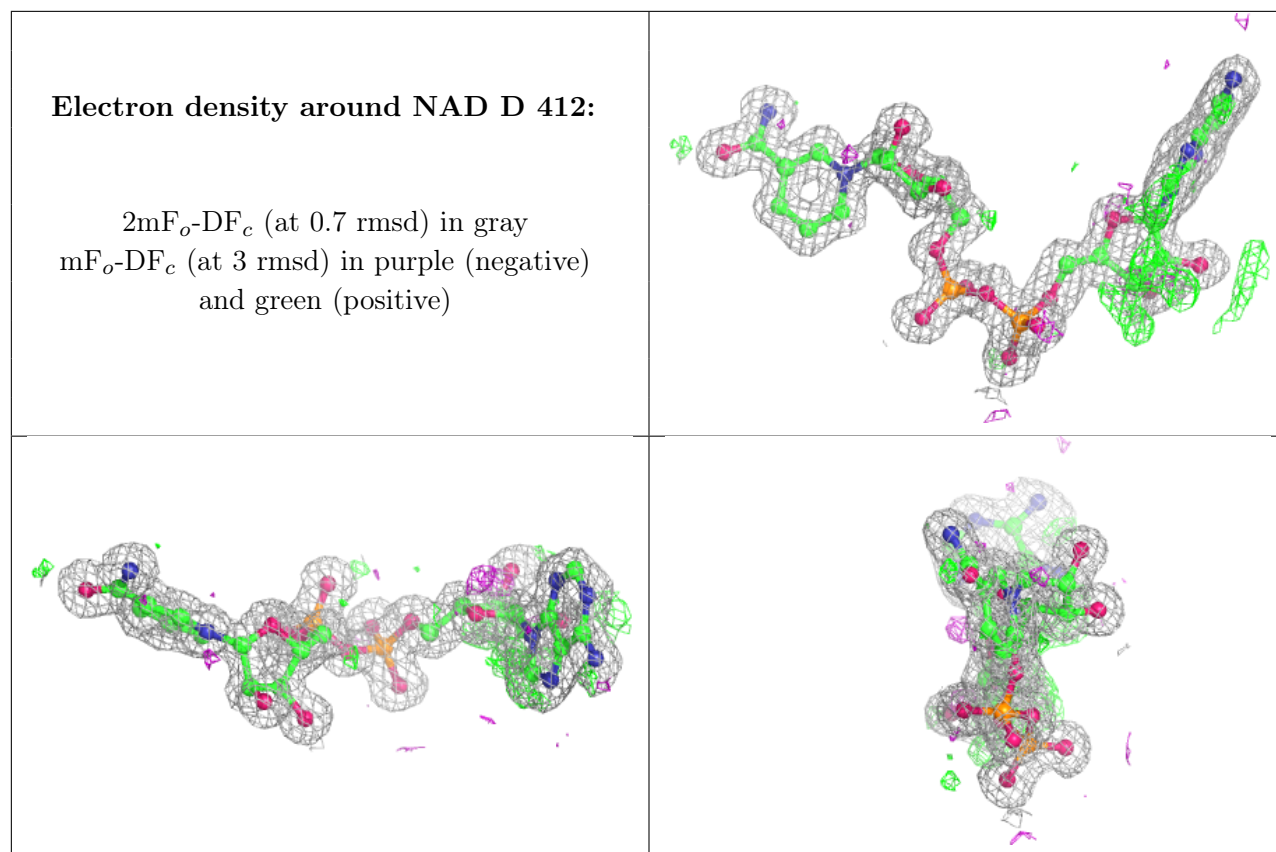
Electron density around NAD B 413:

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

**Electron density around NAD C 415:**

$2mF_o-DF_c$ (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.