WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2024 – 12:39 AM EST

PDB ID : 1ORR

Title : Crystal Structure of CDP-Tyvelose 2-Epimerase complexed with NAD and CDP

Authors : Koropatkin, N.M.; Liu, H.; Holden, H.M.

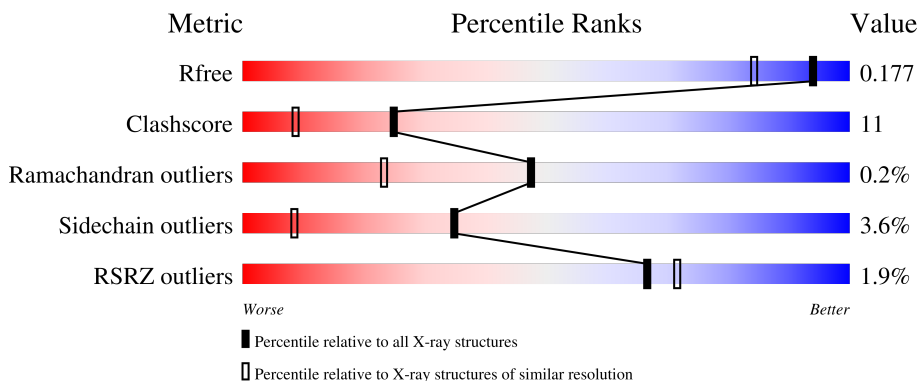Deposited on : 2003-03-14

Resolution : 1.50 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
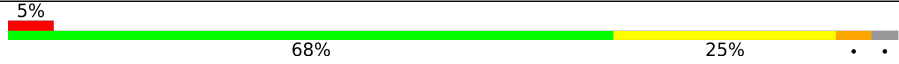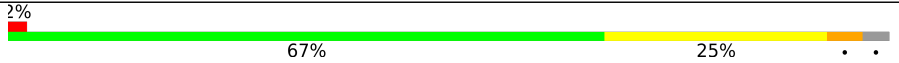*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	Percentile Ranks	Value
Rfree		0.177
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		3.6%
RSRZ outliers		1.9%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	72% 23% · ·
1	B	347	.% 76% 18% · ·
1	C	347	5% 68% 25% · ·
1	D	347	2% 67% 25% · ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12059 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 CDP-tyvelose-2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	11	0
			2706	1712	458	520	16			
1	B	338	Total	C	N	O	S	0	4	0
			2676	1695	451	514	16			
1	C	335	Total	C	N	O	S	0	6	0
			2661	1686	448	511	16			
1	D	336	Total	C	N	O	S	0	5	0
			2661	1685	450	510	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P14169
A	2	ALA	-	cloning artifact	UNP P14169
A	340	LEU	-	expression tag	UNP P14169
A	341	GLU	-	expression tag	UNP P14169
A	342	HIS	-	expression tag	UNP P14169
A	343	HIS	-	expression tag	UNP P14169
A	344	HIS	-	expression tag	UNP P14169
A	345	HIS	-	expression tag	UNP P14169
A	346	HIS	-	expression tag	UNP P14169
A	347	HIS	-	expression tag	UNP P14169
B	1	MET	-	cloning artifact	UNP P14169
B	2	ALA	-	cloning artifact	UNP P14169
B	340	LEU	-	expression tag	UNP P14169
B	341	GLU	-	expression tag	UNP P14169
B	342	HIS	-	expression tag	UNP P14169
B	343	HIS	-	expression tag	UNP P14169
B	344	HIS	-	expression tag	UNP P14169
B	345	HIS	-	expression tag	UNP P14169
B	346	HIS	-	expression tag	UNP P14169
B	347	HIS	-	expression tag	UNP P14169
C	1	MET	-	cloning artifact	UNP P14169

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	cloning artifact	UNP P14169
C	340	LEU	-	expression tag	UNP P14169
C	341	GLU	-	expression tag	UNP P14169
C	342	HIS	-	expression tag	UNP P14169
C	343	HIS	-	expression tag	UNP P14169
C	344	HIS	-	expression tag	UNP P14169
C	345	HIS	-	expression tag	UNP P14169
C	346	HIS	-	expression tag	UNP P14169
C	347	HIS	-	expression tag	UNP P14169
D	1	MET	-	cloning artifact	UNP P14169
D	2	ALA	-	cloning artifact	UNP P14169
D	340	LEU	-	expression tag	UNP P14169
D	341	GLU	-	expression tag	UNP P14169
D	342	HIS	-	expression tag	UNP P14169
D	343	HIS	-	expression tag	UNP P14169
D	344	HIS	-	expression tag	UNP P14169
D	345	HIS	-	expression tag	UNP P14169
D	346	HIS	-	expression tag	UNP P14169
D	347	HIS	-	expression tag	UNP P14169

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
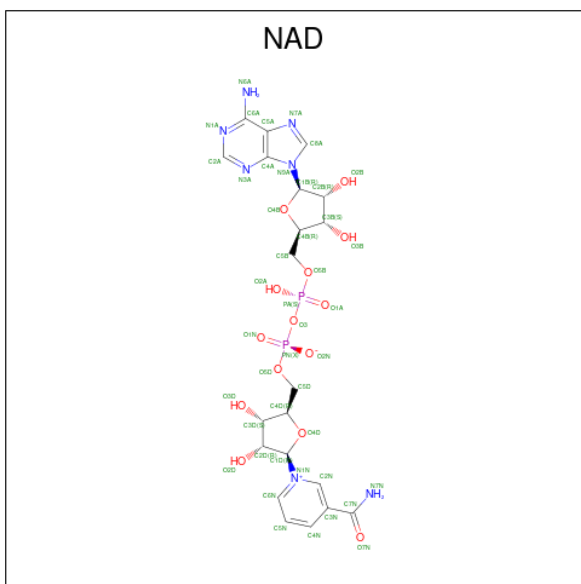
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0

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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 CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).
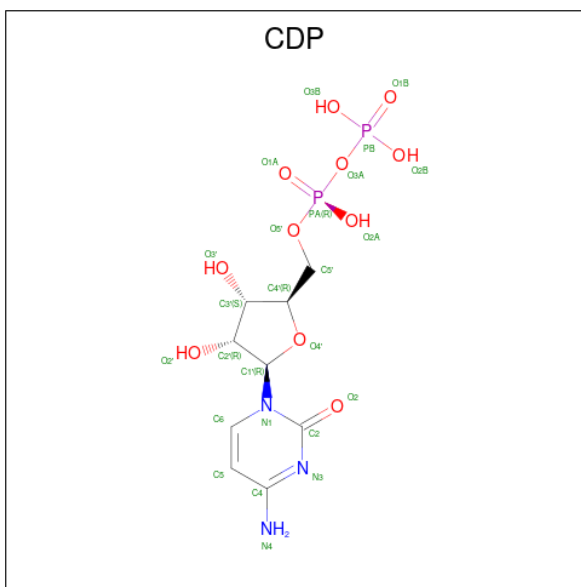
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	277	Total	O	0	0
			277	277		

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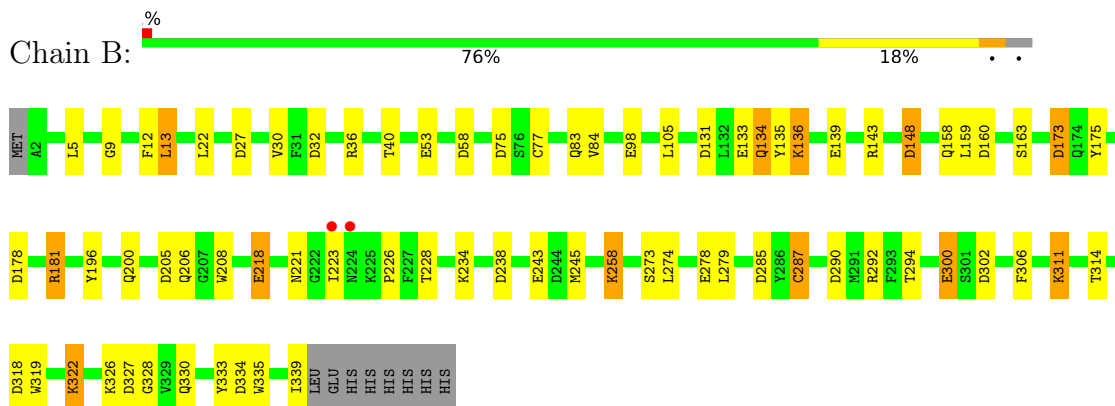| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	259	Total 259	O 259	0	0
4	D	233	Total 233	O 233	0	0

3 Residue-property plots ⓘ

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.
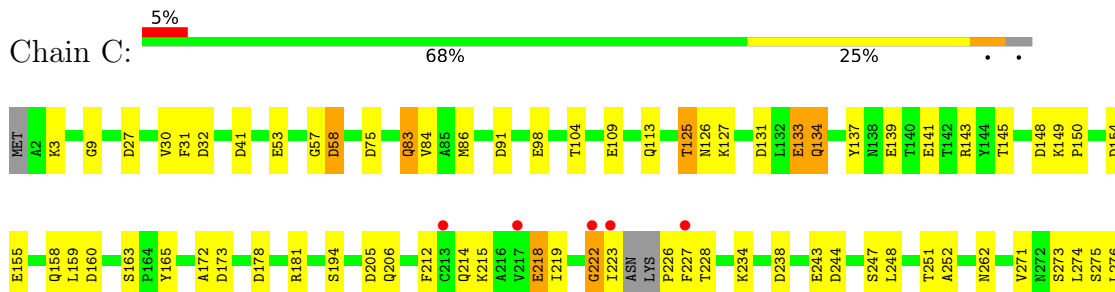
• Molecule 1: CDP-tyvelose-2-epimerase
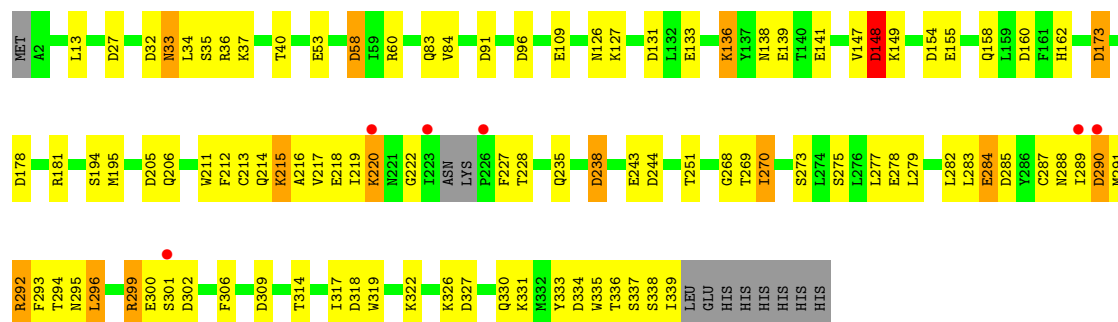
Chain A:

• Molecule 1: CDP-tyvelose-2-epimerase

Chain B:

• Molecule 1: CDP-tyvelose-2-epimerase

Chain C:

L277 E278 L279 F280 K281 L282 L283 E284 D285 Y286 C287 N288 I289 D290 M291 R292 F293 T294 N295 L296 R299 E300 SER D302 F306 D309 T314 I317 D318 W319 K326 D327 Q330 K331 M332 Y333 D334 W335 T336 S337 S338 I339 LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: CDP-tyvelose-2-epimerase

Chain D:

2%

67%   25%

MET A2 L13 D27 D32 N33 L34 S35 R36 K37 T40 E53 D58 I59 R60 Q83 V84 D91 D96 E109 N126 K127 D131 L132 E133 K136 Y137 N138 E139 T140 E141 V147 D148 K149 D154 E155 Q158 L159 D160 F161 H162 D173

D178 R181 S194 M195 D205 Q206 W211 F212 C213 Q214 K215 A216 V217 E218 I219 K220 N221 G222 I223 ASN LYS P226 F227 T228 Q235 D238 E243 D244 T251 G268 T269 I270 S273 L274 S275 L276 L277 E278 L279 L282 L283 E284 D285 Y286 C287 N288 I289 D290 M291

R292 F293 T294 N295 L296 R299 E300 S301 D302 F306 D309 T314 I317 D318 W319 K322 K326 D327 Q330 K331 M332 Y333 D334 W335 T336 S337 S338 I339 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.00Å 168.10Å 89.60Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 47.01 – 1.46	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.50) 95.4 (47.01-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 1.46Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.178 , 0.229 0.175 , 0.177	Depositor DCC
R_{free} test set	22493 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 80.5	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, 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	0.87	10/2828 (0.4%)	1.31	43/3830 (1.1%)
1	B	0.88	8/2761 (0.3%)	1.30	32/3738 (0.9%)
1	C	0.87	12/2757 (0.4%)	1.32	42/3729 (1.1%)
1	D	0.90	10/2740 (0.4%)	1.32	42/3704 (1.1%)
All	All	0.88	40/11086 (0.4%)	1.31	159/15001 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
All	All	2	0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	GLU	CD-OE2	7.30	1.33	1.25
1	D	278	GLU	CD-OE2	7.02	1.33	1.25
1	C	155	GLU	CD-OE2	6.87	1.33	1.25
1	C	284	GLU	CD-OE2	6.69	1.33	1.25
1	D	133	GLU	CD-OE2	6.65	1.32	1.25

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	292	ARG	NE-CZ-NH1	9.43	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	A	302	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	96	ASP	CB-CG-OD2	-8.21	110.91	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	300	GLU	CA
1	C	299	ARG	CA

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	2706	0	2639	67	0
1	B	2676	0	2612	49	0
1	C	2661	0	2592	68	0
1	D	2661	0	2584	60	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
3	A	25	0	12	0	0
3	B	25	0	12	0	0
3	C	25	0	12	1	0
3	D	25	0	12	1	0
4	A	310	0	0	12	0
4	B	277	0	0	5	0
4	C	259	0	0	4	0
4	D	233	0	0	6	0
All	All	12059	0	10579	233	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 11.

The worst 5 of 233 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:C:125[C]:THR:HG22	1:C:127:LYS:H	1.00	1.11
1:C:218:GLU:HA	1:C:223:ILE:HD12	1.34	1.05
1:C:218:GLU:HB3	1:C:223:ILE:HB	1.42	0.99
1:B:134:GLN:HE21	1:B:134:GLN:H	1.14	0.94
1:C:125[C]:THR:HG22	1:C:127:LYS:N	1.85	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	350/347 (101%)	339 (97%)	11 (3%)	0	100	100
1	B	342/347 (99%)	332 (97%)	10 (3%)	0	100	100
1	C	337/347 (97%)	325 (96%)	11 (3%)	1 (0%)	41	18
1	D	337/347 (97%)	319 (95%)	17 (5%)	1 (0%)	41	18
All	All	1366/1388 (98%)	1315 (96%)	49 (4%)	2 (0%)	47	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	GLY
1	D	301	SER

5.3.2 Protein sidechains ⓘ

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	306/301 (102%)	300 (98%)	6 (2%)	55	25
1	B	298/301 (99%)	289 (97%)	9 (3%)	41	12
1	C	297/301 (99%)	284 (96%)	13 (4%)	28	5
1	D	294/301 (98%)	278 (95%)	16 (5%)	22	3
All	All	1195/1204 (99%)	1151 (96%)	44 (4%)	35	8

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	ASN
1	D	215	LYS
1	D	83	GLN
1	D	173	ASP
1	D	270	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	200	GLN
1	D	113	GLN
1	D	138	ASN
1	D	126	ASN
1	B	134	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	1400	-	42,48,48	2.00	7 (16%)	50,73,73	1.57	7 (14%)
3	CDP	C	1401	-	24,26,26	1.38	3 (12%)	37,40,40	1.25	5 (13%)
3	CDP	A	1201	-	24,26,26	1.35	3 (12%)	37,40,40	1.33	5 (13%)
2	NAD	A	1200	-	42,48,48	1.81	8 (19%)	50,73,73	1.89	7 (14%)
3	CDP	B	1301	-	24,26,26	1.28	3 (12%)	37,40,40	1.32	6 (16%)
3	CDP	D	1501	-	24,26,26	1.36	3 (12%)	37,40,40	1.31	5 (13%)
2	NAD	D	1500	-	42,48,48	1.83	6 (14%)	50,73,73	1.60	6 (12%)
2	NAD	B	1300	-	42,48,48	1.82	7 (16%)	50,73,73	1.81	10 (20%)

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	C	1400	-	-	4/26/62/62	0/5/5/5
3	CDP	C	1401	-	-	1/16/32/32	0/2/2/2
3	CDP	A	1201	-	-	0/16/32/32	0/2/2/2
2	NAD	A	1200	-	-	7/26/62/62	0/5/5/5
3	CDP	B	1301	-	-	0/16/32/32	0/2/2/2
3	CDP	D	1501	-	-	0/16/32/32	0/2/2/2
2	NAD	D	1500	-	-	1/26/62/62	0/5/5/5
2	NAD	B	1300	-	-	5/26/62/62	0/5/5/5

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1400	NAD	C4N-C3N	6.94	1.51	1.39
2	D	1500	NAD	C4N-C3N	6.72	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1400	NAD	C2N-C3N	6.32	1.48	1.39
2	D	1500	NAD	C5N-C4N	5.53	1.50	1.38
2	A	1200	NAD	C4N-C3N	5.47	1.48	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1200	NAD	C5N-C4N-C3N	-8.73	110.01	120.34
2	B	1300	NAD	C5N-C4N-C3N	-6.90	112.18	120.34
2	C	1400	NAD	C5N-C4N-C3N	-6.67	112.45	120.34
2	D	1500	NAD	C3N-C7N-N7N	6.28	125.29	117.75
2	A	1200	NAD	C6N-N1N-C2N	-5.68	116.80	121.97

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1200	NAD	C5B-O5B-PA-O1A
2	A	1200	NAD	C5D-O5D-PN-O2N
2	B	1300	NAD	C5D-O5D-PN-O2N
2	A	1200	NAD	C5B-O5B-PA-O3
2	B	1300	NAD	C5D-O5D-PN-O3

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1400	NAD	3	0
3	C	1401	CDP	1	0
2	A	1200	NAD	4	0
3	D	1501	CDP	1	0
2	D	1500	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

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

Ligand NAD C 1400

Bond lengths

Bond angles

Torsions

Rings

Ligand CDP C 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand CDP A 1201

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 1200

Bond lengths

Bond angles

Torsions

Rings

Ligand CDP B 1301

Bond lengths

Bond angles

Torsions

Rings

Ligand CDP D 1501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD D 1500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 1300

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	338/347 (97%)	-0.63	1 (0%)	94	95	11, 18, 48, 75	0
1	B	338/347 (97%)	-0.66	2 (0%)	89	91	11, 19, 50, 95	0
1	C	335/347 (96%)	-0.20	17 (5%)	28	30	11, 21, 57, 95	0
1	D	336/347 (96%)	-0.34	6 (1%)	68	73	11, 20, 58, 90	0
All	All	1347/1388 (97%)	-0.46	26 (1%)	66	71	11, 19, 55, 95	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	ILE	7.0
1	D	289	ILE	5.1
1	C	333	TYR	4.1
1	C	339	ILE	3.8
1	C	282	LEU	3.6

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CDP	C	1401	25/25	0.95	0.08	19,25,100,100	0
3	CDP	D	1501	25/25	0.96	0.07	15,22,62,100	0
3	CDP	A	1201	25/25	0.97	0.07	14,21,45,100	0
3	CDP	B	1301	25/25	0.97	0.06	15,23,32,100	0
2	NAD	A	1200	44/44	0.99	0.05	11,15,24,37	0
2	NAD	B	1300	44/44	0.99	0.05	12,15,28,95	0
2	NAD	C	1400	44/44	0.99	0.05	11,16,26,100	0
2	NAD	D	1500	44/44	0.99	0.05	11,15,18,23	0

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

Electron density around CDP C 1401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
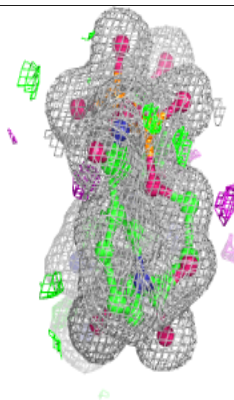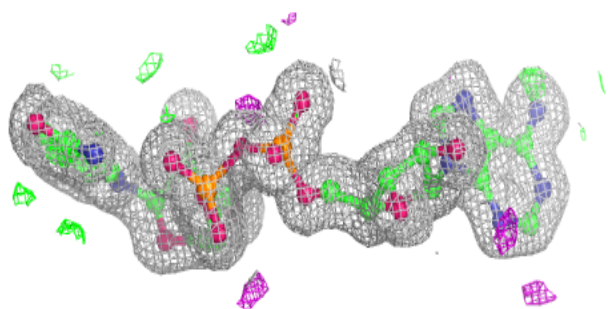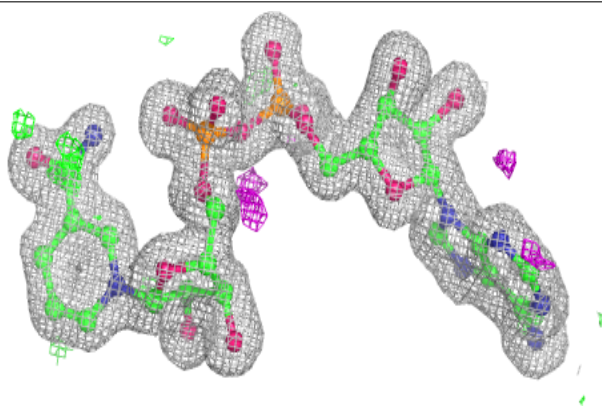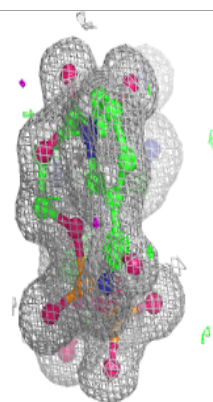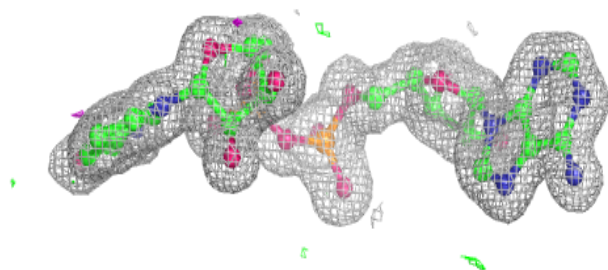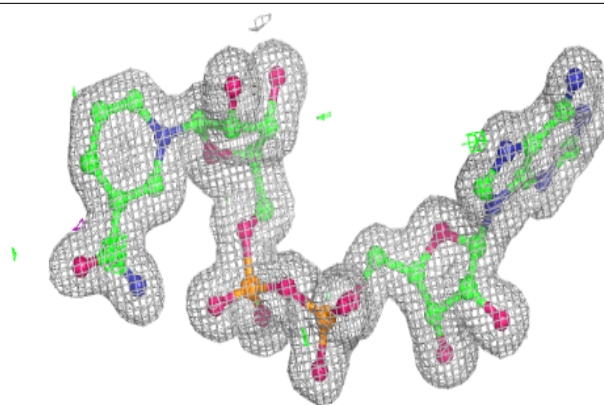mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
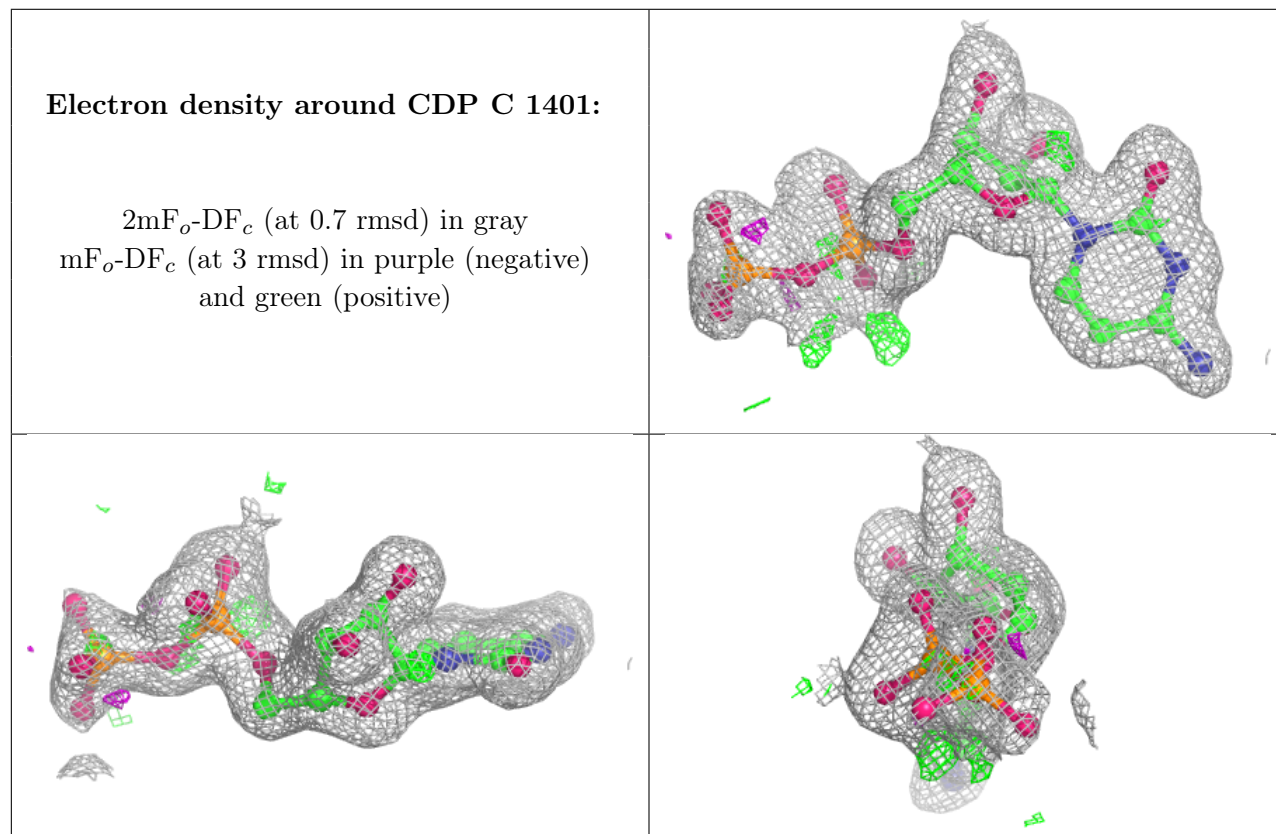
Electron density around CDP D 1501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
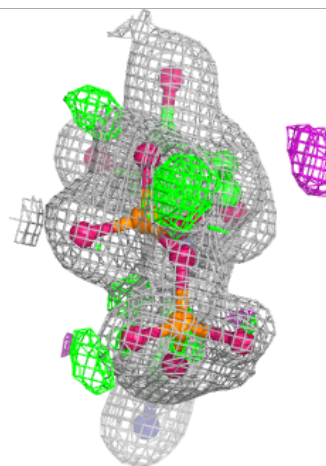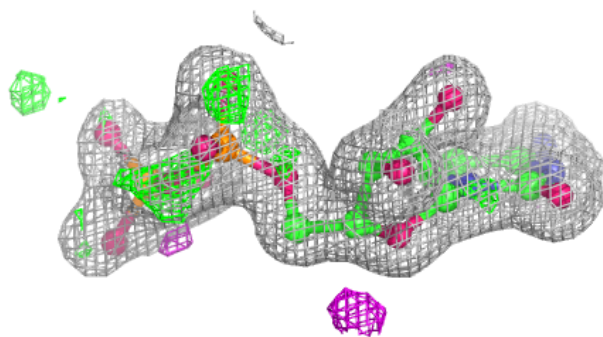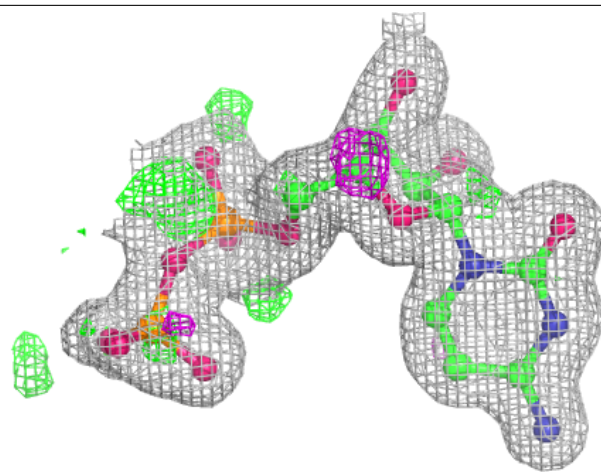
Electron density around CDP A 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
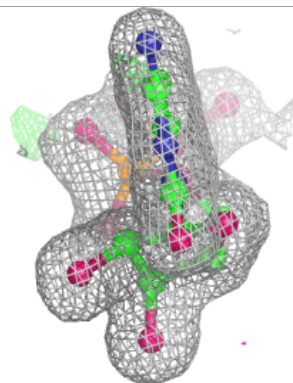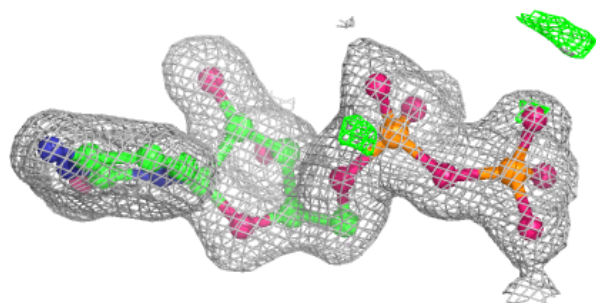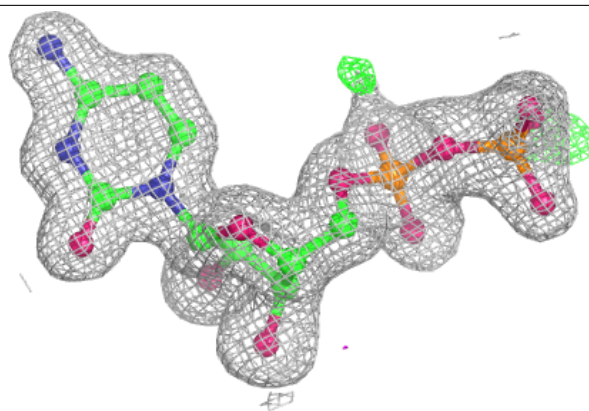
Electron density around CDP B 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
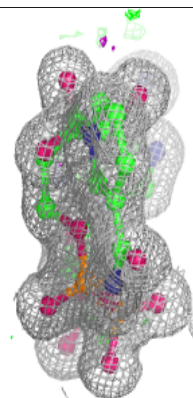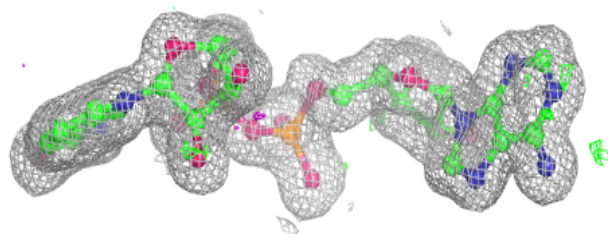and green (positive)
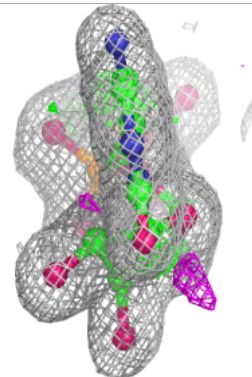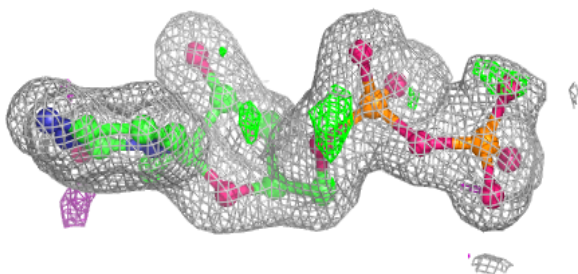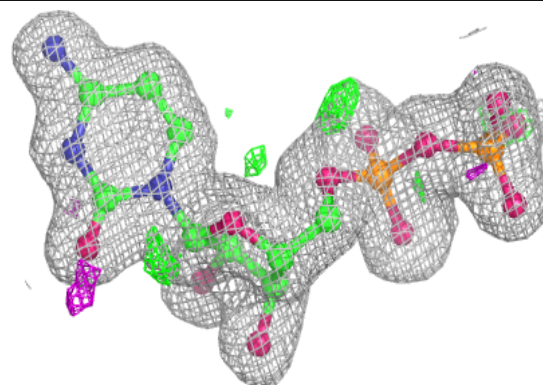
Electron density around NAD A 1200:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
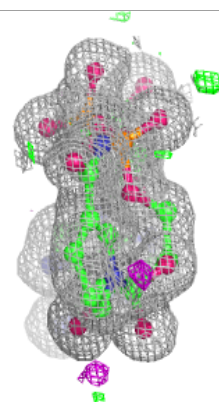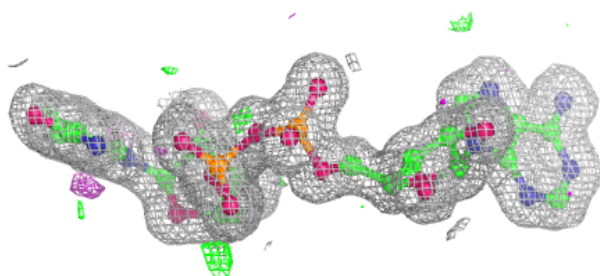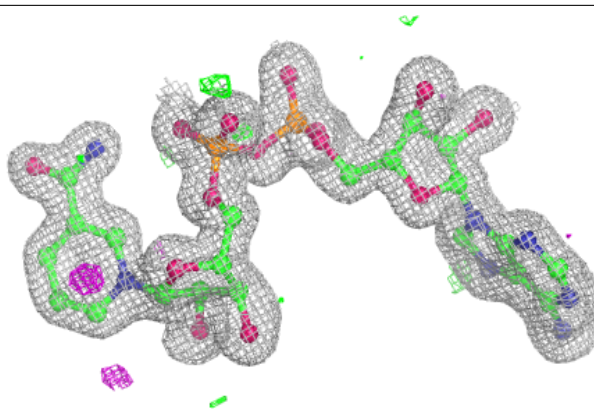
Electron density around NAD B 1300:

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

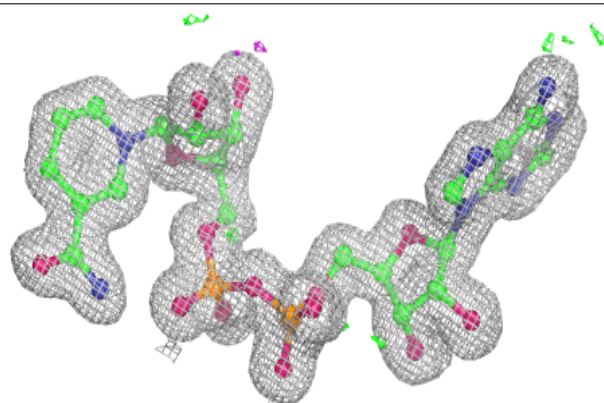**Electron density around NAD C 1400:**

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 1500:

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 ⓘ

There are no such residues in this entry.