Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 12:06 pm BST

PDB ID	:	4C4O
Title	:	Structure of carbonyl reductase CPCR2 from Candida parapsilosis in complex with NADH
Authors	:	Man, H.; Loderer, C.; Ansorge-Schumacher, M.; Grogan, G.
Deposited on	:	2013-09-06
Resolution	:	2.05 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 (i) symbol.

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

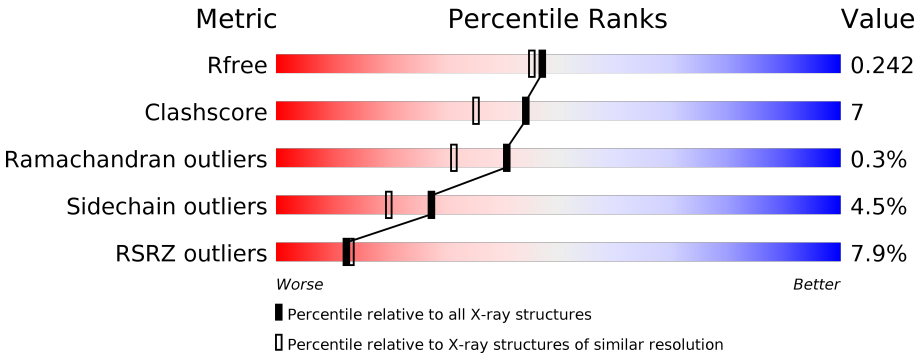
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 on 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	336	7% 86% 9%
1	B	336	86% 11%
1	C	336	13% 78% 10% 10%
1	D	336	9% 70% 9% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	1337	-	-	X	-
4	EDO	C	1337	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9234 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.

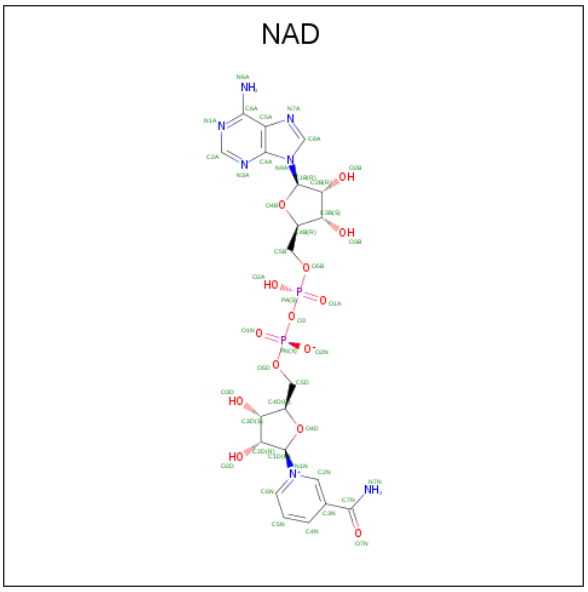
- Molecule 1 is a protein called CARBONYL REDUCTASE CPCR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2318	1468	397	443	10			
1	B	335	Total	C	N	O	S	0	1	0
			2502	1590	424	476	12			
1	C	302	Total	C	N	O	S	0	0	0
			2111	1329	365	407	10			
1	D	270	Total	C	N	O	S	0	0	0
			1855	1165	320	361	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

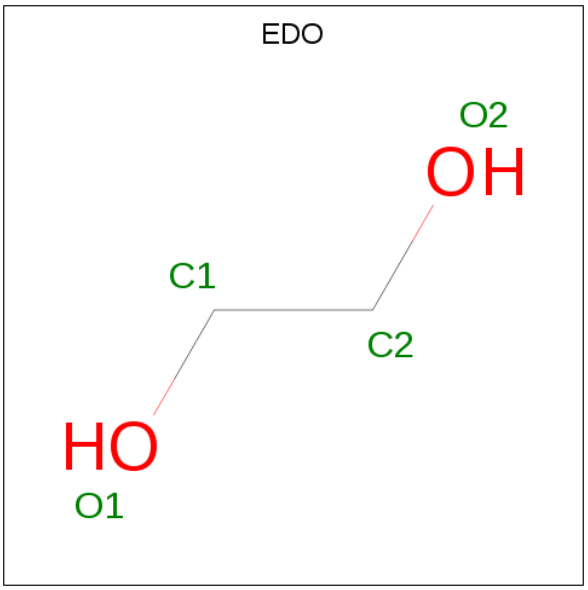
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	6	13	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

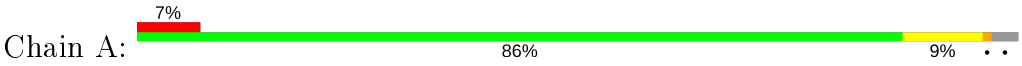
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	102	Total O 102 102	0	0
5	C	44	Total O 44 44	0	0
5	D	34	Total O 34 34	0	0

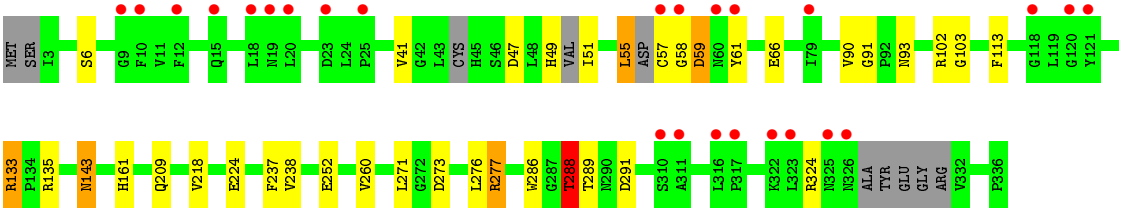
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: CARBONYL REDUCTASE CPCR2

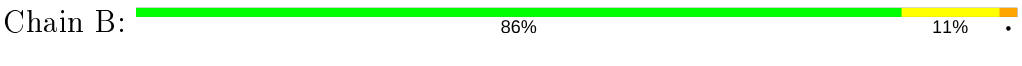
Chain A:

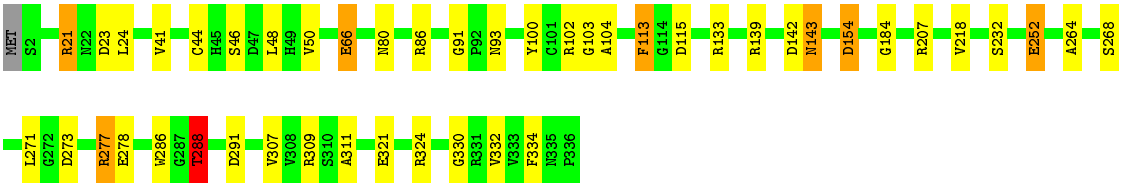




- Molecule 1: CARBONYL REDUCTASE CPCR2

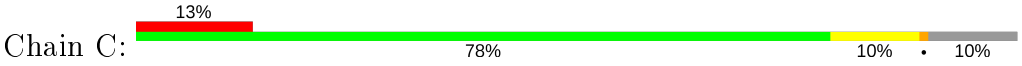
Chain B:

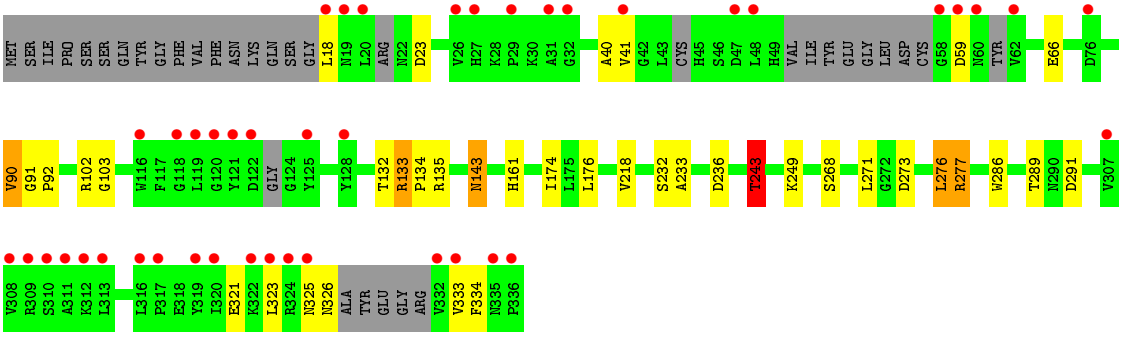




- Molecule 1: CARBONYL REDUCTASE CPCR2

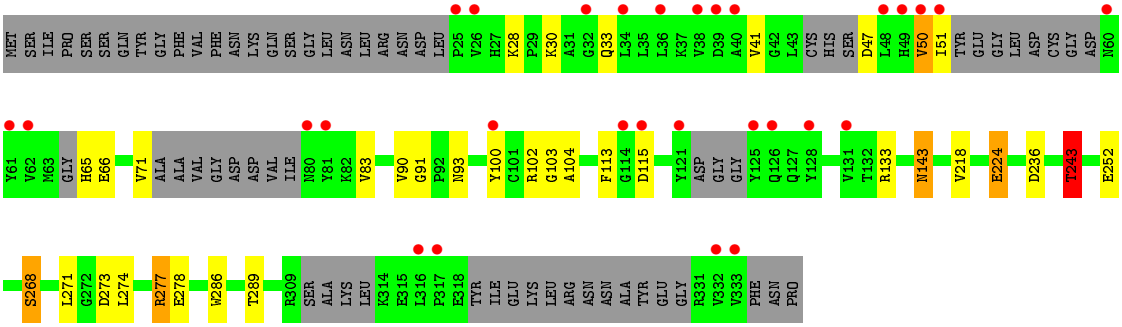
Chain C:





- Molecule 1: CARBONYL REDUCTASE CPCR2

Chain D:


MET SER ILE PRO SER SER GLN TYR GLY PHE VAL PHE ASN LYS GLN SER GLY LEU ASN LEU ARG ASN ASP LEU P25 V26 H27 K28 P29 K30 A31 G32 Q33 L34 L35 L36 K37 V38 D39 A40 V41 G42 L43 CYS HIS SER D47 L48 H49 V50 I51 TYR GLU GLY LEU ASP CYS GLY ASP N60
Y61 V62 M63 GLY H65 E66 V71 ALA ALA VAL GLY ASP ASP VAL ILE N80 Y81 K82 V83 V90 G91 P92 N93 Y100 C101 R102 G103 A104 F113 G114 D115 Y121 ASP GLY GLY Y125 Q126 Q127 Y128 V131 T132 R133 N143 V218 E224 D236 T243 E252
S268 L271 G272 D273 L274 R277 E278 W286 T289 R309 SER ALA LYS LEU K314 E315 L316 P317 E318 TYR ILE GLU LYS LEU ARG ASN ASN ALA TYR GLU GLY R331 V332 V333 PHE ASN PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.72Å 88.84Å 118.20Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	58.13 – 2.05 58.13 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.13-2.05) 99.8 (58.13-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.205 , 0.241 0.213 , 0.242	Depositor DCC
R_{free} test set	4253 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, 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	0.79	0/2359	0.96	8/3211 (0.2%)
1	B	0.94	3/2553 (0.1%)	1.02	15/3467 (0.4%)
1	C	0.78	0/2145	0.95	9/2922 (0.3%)
1	D	1.01	2/1880 (0.1%)	0.97	7/2559 (0.3%)
All	All	0.88	5/8937 (0.1%)	0.98	39/12159 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	VAL	C-N	-26.47	0.73	1.34
1	B	277	ARG	CD-NE	-6.70	1.35	1.46
1	B	66[A]	GLU	CG-CD	6.39	1.61	1.51
1	B	66[B]	GLU	CG-CD	6.39	1.61	1.51
1	D	268	SER	CB-OG	-5.04	1.35	1.42

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	277	ARG	NE-CZ-NH2	-17.62	111.49	120.30
1	A	277	ARG	NE-CZ-NH1	16.65	128.63	120.30
1	C	277	ARG	NE-CZ-NH1	16.33	128.47	120.30
1	A	277	ARG	NE-CZ-NH2	-15.99	112.31	120.30
1	C	277	ARG	NE-CZ-NH2	-15.60	112.50	120.30
1	B	277	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	D	277	ARG	NE-CZ-NH2	-15.23	112.68	120.30
1	D	277	ARG	NE-CZ-NH1	15.11	127.86	120.30
1	A	133	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	154	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	D	50	VAL	O-C-N	7.16	134.15	122.70
1	B	66[A]	GLU	OE1-CD-OE2	-6.88	115.04	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66[B]	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	176	LEU	CB-CG-CD2	6.84	122.62	111.00
1	D	243	THR	N-CA-CB	-6.82	97.34	110.30
1	D	252	GLU	CB-CA-C	-6.76	96.88	110.40
1	A	252	GLU	CB-CA-C	-6.74	96.92	110.40
1	C	132	THR	N-CA-C	-6.48	93.52	111.00
1	C	243	THR	N-CA-CB	-6.47	98.00	110.30
1	A	288	THR	N-CA-CB	-6.46	98.03	110.30
1	B	44	CYS	CB-CA-C	-6.45	97.51	110.40
1	B	277	ARG	CD-NE-CZ	6.35	132.50	123.60
1	C	176	LEU	CA-CB-CG	6.25	129.69	115.30
1	B	288	THR	N-CA-CB	-6.23	98.47	110.30
1	D	277	ARG	CD-NE-CZ	6.04	132.05	123.60
1	B	86	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	135	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	276	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	86	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	252	GLU	CB-CA-C	-5.72	98.96	110.40
1	A	135	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	50	VAL	CA-C-N	-5.60	104.88	117.20
1	B	102	ARG	N-CA-C	5.40	125.58	111.00
1	C	135	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	207	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	277	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	277	ARG	CD-NE-CZ	5.09	130.72	123.60
1	B	66[A]	GLU	CG-CD-OE2	5.00	128.31	118.30
1	B	66[B]	GLU	CG-CD-OE2	5.00	128.31	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	0	2156	25	0
1	B	2502	0	2459	33	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2111	0	1944	34	1
1	D	1855	0	1664	30	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	36	0	20	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	4	0	6	0	0
4	B	12	0	18	9	0
4	C	8	0	12	8	0
5	A	67	0	0	1	0
5	B	102	0	0	2	0
5	C	44	0	0	0	0
5	D	34	0	0	1	0
All	All	9234	0	8357	115	1

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 7.

All (115) 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:50:VAL:CA	1:D:51:ILE:N	1.84	1.39
1:D:50:VAL:C	1:D:51:ILE:CA	1.92	1.36
1:D:47:ASP:O	1:D:51:ILE:HG12	1.34	1.22
1:C:323:LEU:O	1:C:326:ASN:HB2	1.39	1.20
1:D:50:VAL:O	1:D:51:ILE:N	1.81	1.11
1:A:55:LEU:C	1:A:57:CYS:N	2.14	0.99
1:A:58:GLY:HA3	1:A:61:TYR:HE2	1.28	0.97
1:A:58:GLY:HA3	1:A:61:TYR:CE2	1.99	0.96
1:C:323:LEU:O	1:C:326:ASN:CB	2.24	0.85
1:B:113:PHE:CE1	1:B:113:PHE:CE2	2.60	0.83
1:A:288:THR:HG21	5:A:2019:HOH:O	1.81	0.81
1:A:276:LEU:HD21	1:B:113:PHE:CE1	2.16	0.79
1:D:115:ASP:OD2	1:D:133:ARG:NH2	2.16	0.78
1:B:115:ASP:OD2	1:B:133:ARG:NH2	2.17	0.78
1:C:321:GLU:O	1:C:325:ASN:ND2	2.16	0.78
1:D:50:VAL:C	1:D:51:ILE:N	0.73	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:THR:HG22	1:B:291:ASP:H	1.51	0.75
1:B:104:ALA:HA	1:C:102:ARG:O	1.87	0.75
1:D:93:ASN:O	1:D:133:ARG:NH1	2.19	0.74
1:B:184:GLY:HA3	4:B:1337:EDO:H21	1.67	0.73
1:D:224:GLU:CD	1:D:224:GLU:H	1.91	0.73
1:B:93:ASN:O	1:B:133:ARG:NH1	2.21	0.73
1:A:55:LEU:O	1:A:57:CYS:N	2.23	0.72
1:B:288:THR:HG21	5:B:2034:HOH:O	1.89	0.72
1:C:249:LYS:HB2	4:C:1337:EDO:H11	1.72	0.71
1:D:50:VAL:O	1:D:51:ILE:CA	2.32	0.70
1:A:288:THR:HG22	1:A:291:ASP:H	1.56	0.70
1:D:71:VAL:HG12	1:D:83:VAL:HA	1.74	0.69
1:A:58:GLY:O	1:A:59:ASP:HB2	1.92	0.69
1:C:233:ALA:HB2	4:C:1338:EDO:H21	1.75	0.69
1:B:80:ASN:O	1:B:139:ARG:NH2	2.26	0.68
1:B:307:VAL:HG22	1:B:330:GLY:HA3	1.75	0.68
1:C:236:ASP:OD2	1:C:243:THR:HG23	1.95	0.67
1:C:90:VAL:HG11	1:C:289:THR:HA	1.77	0.66
1:D:50:VAL:N	1:D:51:ILE:N	2.44	0.66
1:C:161:HIS:HE1	1:D:278:GLU:OE2	1.78	0.65
1:D:236:ASP:OD2	1:D:243:THR:HG23	1.97	0.65
1:C:233:ALA:HB2	4:C:1338:EDO:C2	2.26	0.65
1:D:90:VAL:HG21	1:D:289:THR:HG22	1.79	0.64
1:C:90:VAL:HG23	1:C:92:PRO:HD2	1.79	0.64
1:A:58:GLY:CA	1:A:61:TYR:HE2	2.08	0.64
1:A:161:HIS:HE1	1:B:278:GLU:OE2	1.81	0.63
1:A:161:HIS:HD2	1:A:291:ASP:OD2	1.81	0.63
1:A:90:VAL:HG21	1:A:289:THR:HG22	1.81	0.62
1:D:50:VAL:CB	1:D:51:ILE:N	2.62	0.62
1:A:237:PHE:CE1	1:A:260:VAL:HG21	2.36	0.61
1:C:90:VAL:HG11	1:C:289:THR:HG22	1.83	0.60
1:C:236:ASP:OD2	1:C:243:THR:CG2	2.50	0.59
1:D:50:VAL:O	1:D:51:ILE:HA	2.02	0.58
1:D:236:ASP:OD2	1:D:243:THR:CG2	2.51	0.58
1:A:47:ASP:O	1:A:51:ILE:CB	2.52	0.58
1:A:161:HIS:CD2	1:A:291:ASP:OD2	2.58	0.57
1:A:102:ARG:O	1:D:104:ALA:HA	2.04	0.57
1:B:113:PHE:CE1	4:B:1339:EDO:H11	2.40	0.56
1:C:161:HIS:CD2	1:C:291:ASP:OD2	2.59	0.56
1:C:249:LYS:HB2	4:C:1337:EDO:C1	2.35	0.56
1:B:113:PHE:CD1	4:B:1339:EDO:H11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:HD2	1:C:291:ASP:OD2	1.90	0.55
1:C:40:ALA:HB1	1:C:333:VAL:HG21	1.90	0.54
1:B:21:ARG:NH1	1:B:23:ASP:OD1	2.40	0.54
1:D:50:VAL:C	1:D:51:ILE:HA	2.13	0.53
1:B:309:ARG:CG	1:B:332:VAL:HG22	2.40	0.52
1:C:236:ASP:CG	1:C:243:THR:HG23	2.30	0.51
1:B:143:ASN:H	1:B:143:ASN:HD22	1.58	0.51
1:A:93:ASN:O	1:A:133:ARG:NH1	2.45	0.50
1:B:330:GLY:HA2	4:B:1337:EDO:C1	2.41	0.50
1:D:47:ASP:O	1:D:51:ILE:CG1	2.30	0.49
1:D:236:ASP:CG	1:D:243:THR:HG23	2.33	0.48
1:D:65:HIS:CE1	5:D:2003:HOH:O	2.66	0.48
1:C:249:LYS:CB	4:C:1337:EDO:H11	2.42	0.48
1:B:309:ARG:HG3	1:B:332:VAL:HG22	1.96	0.48
1:C:40:ALA:HB1	1:C:333:VAL:CG2	2.43	0.48
1:C:91:GLY:HA3	1:C:286:TRP:CZ2	2.49	0.47
1:D:91:GLY:HA3	1:D:286:TRP:CZ2	2.49	0.47
1:A:161:HIS:CE1	1:B:278:GLU:OE2	2.65	0.47
1:C:232:SER:OG	4:C:1338:EDO:H11	2.15	0.47
1:C:90:VAL:CG1	1:C:289:THR:HG22	2.45	0.46
1:B:91:GLY:HA3	1:B:286:TRP:CZ2	2.50	0.46
1:C:102:ARG:N	1:C:103:GLY:HA3	2.31	0.46
1:B:46:SER:O	1:B:50:VAL:HG23	2.15	0.46
1:A:143:ASN:H	1:A:143:ASN:HD22	1.63	0.45
1:A:91:GLY:HA3	1:A:286:TRP:CZ2	2.52	0.45
1:D:30:LYS:HA	1:D:33:GLN:HB2	1.98	0.45
1:B:330:GLY:HA2	4:B:1337:EDO:H11	1.97	0.45
1:C:161:HIS:CE1	1:D:278:GLU:OE2	2.65	0.45
1:A:49:HIS:HB3	1:A:55:LEU:HD23	1.99	0.44
1:C:41:VAL:C	1:C:333:VAL:HG23	2.38	0.44
1:D:41:VAL:HA	1:D:66:GLU:O	2.19	0.43
1:B:273:ASP:OD1	1:B:277:ARG:HD3	2.19	0.43
1:C:41:VAL:HA	1:C:66:GLU:O	2.19	0.43
1:D:143:ASN:H	1:D:143:ASN:HD22	1.64	0.43
1:C:273:ASP:OD1	1:C:277:ARG:HD3	2.19	0.43
1:D:273:ASP:OD1	1:D:277:ARG:HD3	2.18	0.42
1:B:100:TYR:O	1:B:103:GLY:HA3	2.19	0.42
1:B:288:THR:CG2	1:B:291:ASP:H	2.28	0.42
1:B:252:GLU:OE2	4:B:1338:EDO:C2	2.67	0.42
1:C:143:ASN:H	1:C:143:ASN:HD22	1.67	0.42
1:A:90:VAL:HG21	1:A:289:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LYS:N	4:C:1337:EDO:H11	2.35	0.42
1:B:232:SER:HB3	4:B:1338:EDO:C2	2.49	0.41
1:D:100:TYR:O	1:D:103:GLY:HA3	2.20	0.41
1:B:252:GLU:OE2	4:B:1338:EDO:H22	2.20	0.41
1:B:264:ALA:HB2	5:B:2087:HOH:O	2.19	0.41
1:A:41:VAL:HA	1:A:66:GLU:O	2.20	0.41
1:B:66[A]:GLU:HG2	1:B:154:ASP:CB	2.51	0.41
1:A:273:ASP:OD1	1:A:277:ARG:HD3	2.21	0.41
1:C:249:LYS:CA	4:C:1337:EDO:H11	2.51	0.41
1:A:102:ARG:N	1:A:103:GLY:HA3	2.35	0.41
1:D:102:ARG:N	1:D:103:GLY:HA3	2.36	0.41
1:C:133:ARG:N	1:C:134:PRO:HD3	2.36	0.41
1:B:311:ALA:O	1:B:334:PHE:HA	2.21	0.41
1:B:307:VAL:HG13	4:B:1337:EDO:H22	2.02	0.40
1:C:174:ILE:HG21	1:C:174:ILE:HD13	1.81	0.40
1:C:40:ALA:HA	1:C:334:PHE:O	2.22	0.40

All (1) 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)
1:B:142:ASP:OD2	1:C:23:ASP:O[2_545]	2.15	0.05

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	316/336 (94%)	301 (95%)	14 (4%)	1 (0%)	41 31
1	B	334/336 (99%)	320 (96%)	14 (4%)	0	100 100
1	C	288/336 (86%)	274 (95%)	12 (4%)	2 (1%)	22 12
1	D	254/336 (76%)	239 (94%)	14 (6%)	1 (0%)	34 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1192/1344 (89%)	1134 (95%)	54 (4%)	4 (0%)	41 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	C	59	ASP
1	D	28	LYS
1	C	133	ARG

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	222/270 (82%)	211 (95%)	11 (5%)	24 16
1	B	261/270 (97%)	250 (96%)	11 (4%)	30 22
1	C	200/270 (74%)	192 (96%)	8 (4%)	31 24
1	D	168/270 (62%)	160 (95%)	8 (5%)	25 18
All	All	851/1080 (79%)	813 (96%)	38 (4%)	27 20

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	55	LEU
1	A	113	PHE
1	A	143	ASN
1	A	209	GLN
1	A	218	VAL
1	A	224	GLU
1	A	238	VAL
1	A	271	LEU
1	A	288	THR
1	A	324	ARG

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Mol	Chain	Res	Type
1	B	21	ARG
1	B	24	LEU
1	B	48	LEU
1	B	113	PHE
1	B	143	ASN
1	B	218	VAL
1	B	268	SER
1	B	271	LEU
1	B	288	THR
1	B	321	GLU
1	B	324	ARG
1	C	18	LEU
1	C	90	VAL
1	C	143	ASN
1	C	218	VAL
1	C	243	THR
1	C	268	SER
1	C	271	LEU
1	C	276	LEU
1	D	113	PHE
1	D	143	ASN
1	D	218	VAL
1	D	224	GLU
1	D	243	THR
1	D	268	SER
1	D	271	LEU
1	D	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	143	ASN
1	A	161	HIS
1	B	93	ASN
1	B	143	ASN
1	C	143	ASN
1	C	161	HIS
1	C	266	ASN
1	D	143	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	EDO	C	1338	-	3,3,3	0.52	0	2,2,2	0.38	0
4	EDO	B	1337	-	3,3,3	0.64	0	2,2,2	0.39	0
4	EDO	C	1337	-	3,3,3	0.33	0	2,2,2	0.77	0
3	NAD	B	1000	-	42,48,48	0.87	1 (2%)	50,73,73	1.17	4 (8%)
3	NAD	D	1000	-	42,48,48	1.23	6 (14%)	50,73,73	1.46	8 (16%)
3	NAD	A	1000	-	33,39,48	1.06	3 (9%)	38,60,73	1.41	6 (15%)
4	EDO	B	1339	-	3,3,3	1.49	0	2,2,2	1.05	0
3	NAD	C	1000	-	42,48,48	0.97	2 (4%)	50,73,73	1.33	7 (14%)
4	EDO	B	1338	-	3,3,3	0.62	0	2,2,2	0.31	0
4	EDO	A	1337	-	3,3,3	0.44	0	2,2,2	0.42	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
4	EDO	C	1338	-	-	1/1/1/1	-
4	EDO	B	1337	-	-	1/1/1/1	-
4	EDO	C	1337	-	-	1/1/1/1	-
3	NAD	B	1000	-	-	7/26/62/62	0/5/5/5
3	NAD	D	1000	-	-	7/26/62/62	0/5/5/5
3	NAD	A	1000	-	-	3/18/54/62	0/4/4/5
4	EDO	B	1339	-	-	1/1/1/1	-
3	NAD	C	1000	-	-	5/26/62/62	0/5/5/5
4	EDO	B	1338	-	-	1/1/1/1	-
4	EDO	A	1337	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	NAD	O4B-C1B	3.29	1.45	1.41
3	C	1000	NAD	O4D-C1D	3.20	1.45	1.41
3	A	1000	NAD	C2A-N3A	3.12	1.37	1.32
3	A	1000	NAD	C5A-C4A	2.76	1.48	1.40
3	D	1000	NAD	C5A-C4A	2.73	1.48	1.40
3	B	1000	NAD	C2A-N3A	2.72	1.36	1.32
3	D	1000	NAD	C3N-C7N	2.64	1.54	1.50
3	D	1000	NAD	C2A-N1A	2.60	1.38	1.33
3	D	1000	NAD	C2A-N3A	2.43	1.36	1.32
3	D	1000	NAD	C2N-N1N	2.16	1.37	1.35
3	D	1000	NAD	C4A-N3A	2.12	1.38	1.35
3	C	1000	NAD	C2A-N3A	2.00	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1000	NAD	C5A-C6A-N6A	-4.21	113.95	120.35
3	C	1000	NAD	N3A-C2A-N1A	-4.14	122.20	128.68
3	A	1000	NAD	N3A-C2A-N1A	-4.12	122.23	128.68
3	D	1000	NAD	N3A-C2A-N1A	-4.10	122.26	128.68
3	D	1000	NAD	N6A-C6A-N1A	3.71	126.28	118.57
3	B	1000	NAD	N3A-C2A-N1A	-3.56	123.12	128.68
3	C	1000	NAD	C4A-C5A-N7A	-3.11	106.16	109.40
3	C	1000	NAD	O7N-C7N-C3N	2.84	123.03	119.63
3	C	1000	NAD	C6N-N1N-C2N	-2.58	119.63	121.97
3	A	1000	NAD	C3D-C2D-C1D	2.56	106.29	101.42
3	D	1000	NAD	C6N-N1N-C2N	-2.51	119.69	121.97
3	A	1000	NAD	C4A-C5A-N7A	-2.51	106.78	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1000	NAD	O2A-PA-O1A	2.47	124.45	112.24
3	D	1000	NAD	O4B-C1B-C2B	-2.47	103.32	106.93
3	C	1000	NAD	O4B-C1B-C2B	-2.44	103.36	106.93
3	A	1000	NAD	PN-O3-PA	-2.42	124.53	132.83
3	D	1000	NAD	O4D-C1D-C2D	-2.39	103.44	106.93
3	A	1000	NAD	O2A-PA-O1A	2.38	123.99	112.24
3	B	1000	NAD	C5A-C6A-N6A	-2.17	117.05	120.35
3	B	1000	NAD	N6A-C6A-N1A	2.14	123.01	118.57
3	D	1000	NAD	C3N-C7N-N7N	2.13	120.31	117.75
3	A	1000	NAD	O4B-C1B-C2B	-2.10	103.86	106.93
3	C	1000	NAD	C3N-C2N-N1N	2.04	122.42	120.43
3	D	1000	NAD	O3D-C3D-C4D	-2.04	105.15	111.05
3	C	1000	NAD	O7N-C7N-N7N	-2.02	119.70	122.58

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1000	NAD	O4D-C1D-N1N-C2N
3	B	1000	NAD	O4D-C1D-N1N-C6N
3	B	1000	NAD	C2D-C1D-N1N-C2N
3	B	1000	NAD	C2D-C1D-N1N-C6N
3	D	1000	NAD	O4D-C1D-N1N-C2N
3	D	1000	NAD	O4D-C1D-N1N-C6N
3	D	1000	NAD	C2D-C1D-N1N-C2N
3	D	1000	NAD	C2D-C1D-N1N-C6N
3	C	1000	NAD	O4D-C1D-N1N-C2N
3	C	1000	NAD	O4D-C1D-N1N-C6N
3	C	1000	NAD	C2D-C1D-N1N-C2N
3	C	1000	NAD	C2D-C1D-N1N-C6N
4	B	1338	EDO	O1-C1-C2-O2
4	A	1337	EDO	O1-C1-C2-O2
3	D	1000	NAD	PN-O3-PA-O1A
4	C	1338	EDO	O1-C1-C2-O2
4	B	1337	EDO	O1-C1-C2-O2
4	B	1339	EDO	O1-C1-C2-O2
3	B	1000	NAD	O4B-C4B-C5B-O5B
3	C	1000	NAD	O4B-C4B-C5B-O5B
3	D	1000	NAD	PN-O3-PA-O2A
3	A	1000	NAD	PN-O3-PA-O2A
3	B	1000	NAD	PN-O3-PA-O1A
3	A	1000	NAD	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	1000	NAD	O4B-C4B-C5B-O5B
4	C	1337	EDO	O1-C1-C2-O2
3	D	1000	NAD	O4B-C4B-C5B-O5B
3	B	1000	NAD	PN-O3-PA-O2A

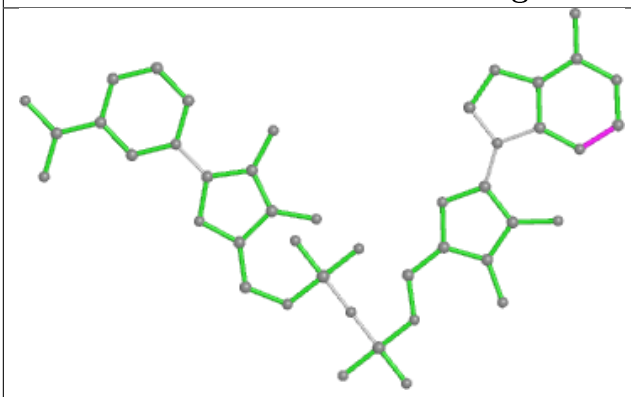
There are no ring outliers.

5 monomers are involved in 17 short contacts:

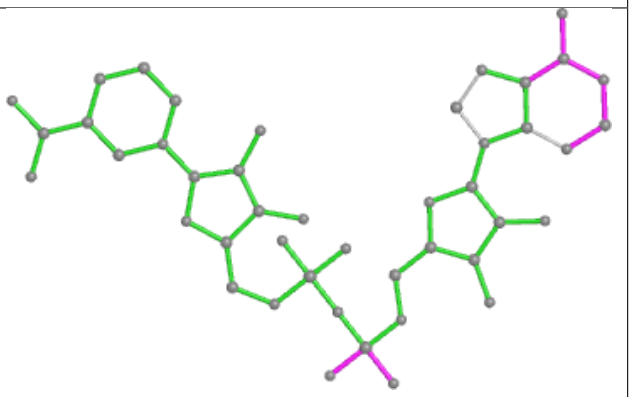
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1338	EDO	3	0
4	B	1337	EDO	4	0
4	C	1337	EDO	5	0
4	B	1339	EDO	2	0
4	B	1338	EDO	3	0

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.

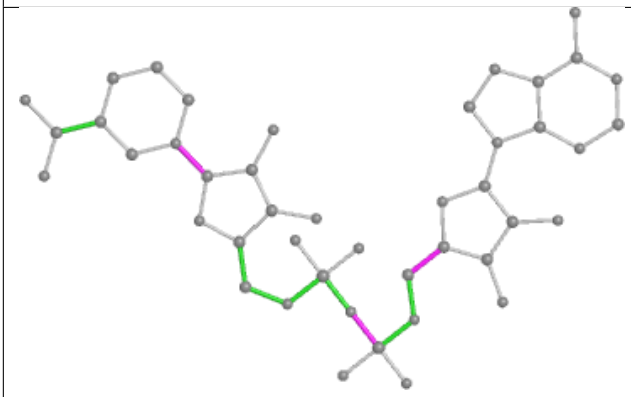
Ligand NAD B 1000



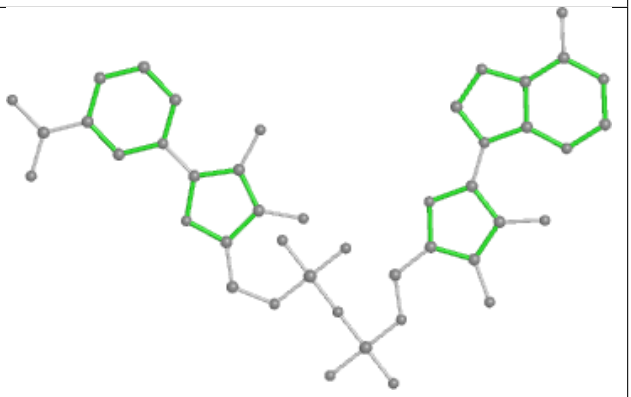
Bond lengths



Bond angles

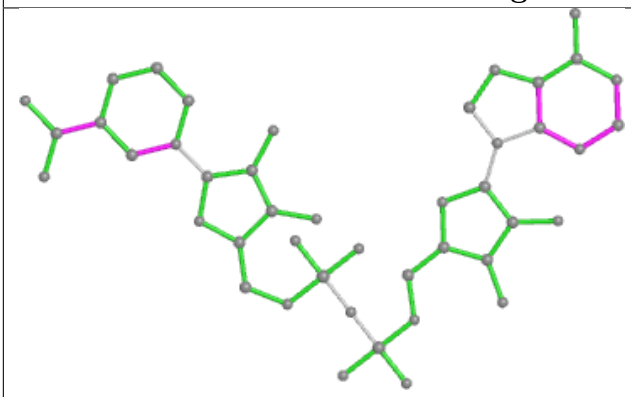


Torsions

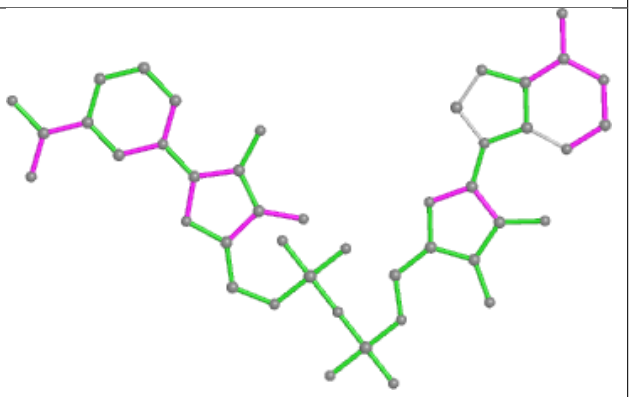


Rings

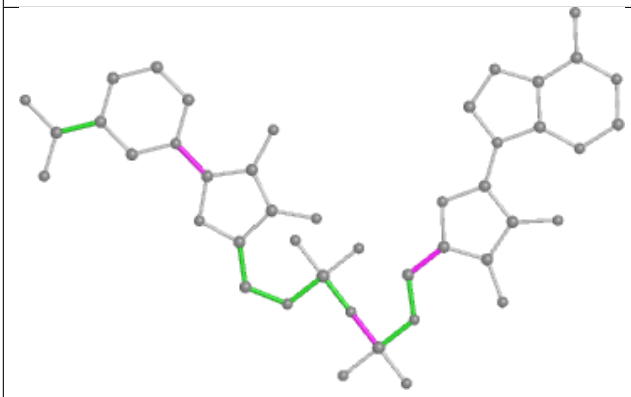
Ligand NAD D 1000



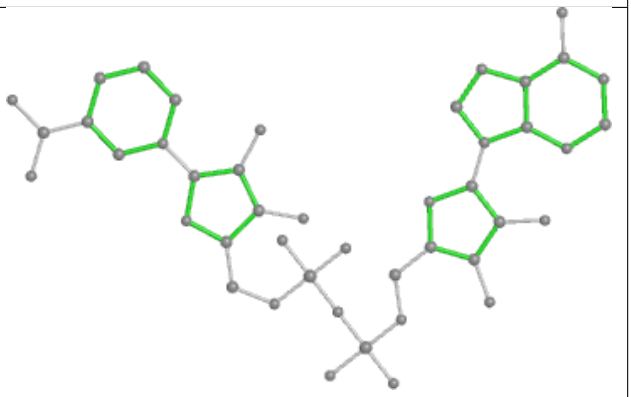
Bond lengths



Bond angles

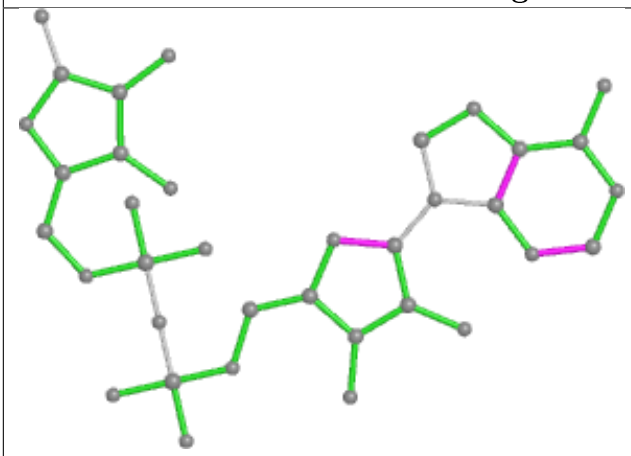


Torsions

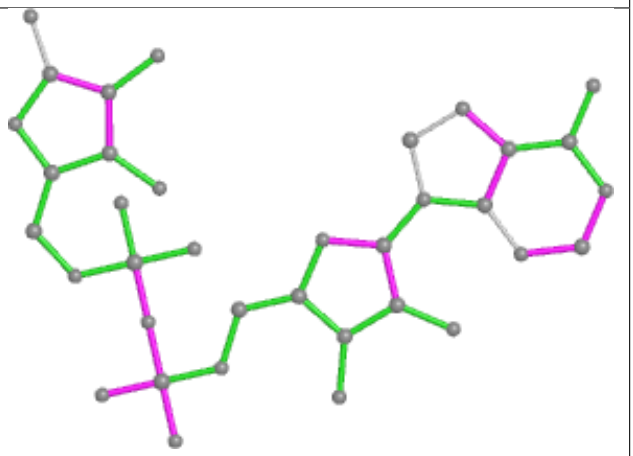


Rings

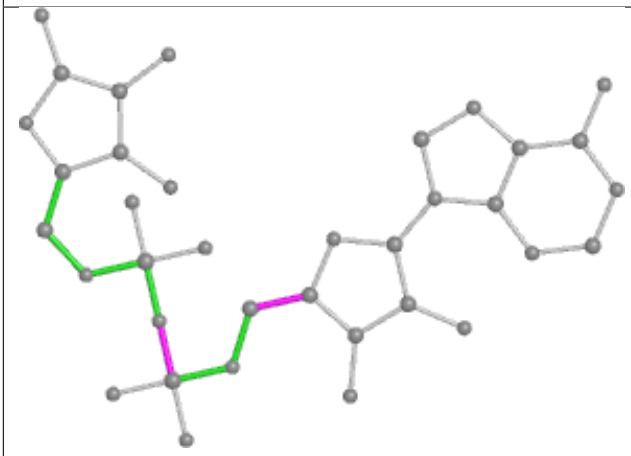
Ligand NAD A 1000



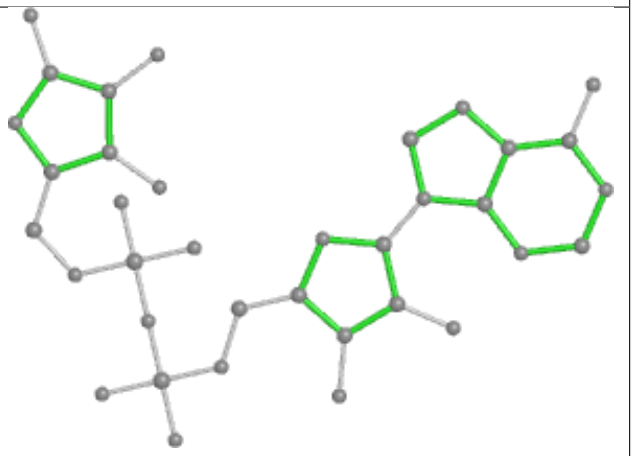
Bond lengths



Bond angles

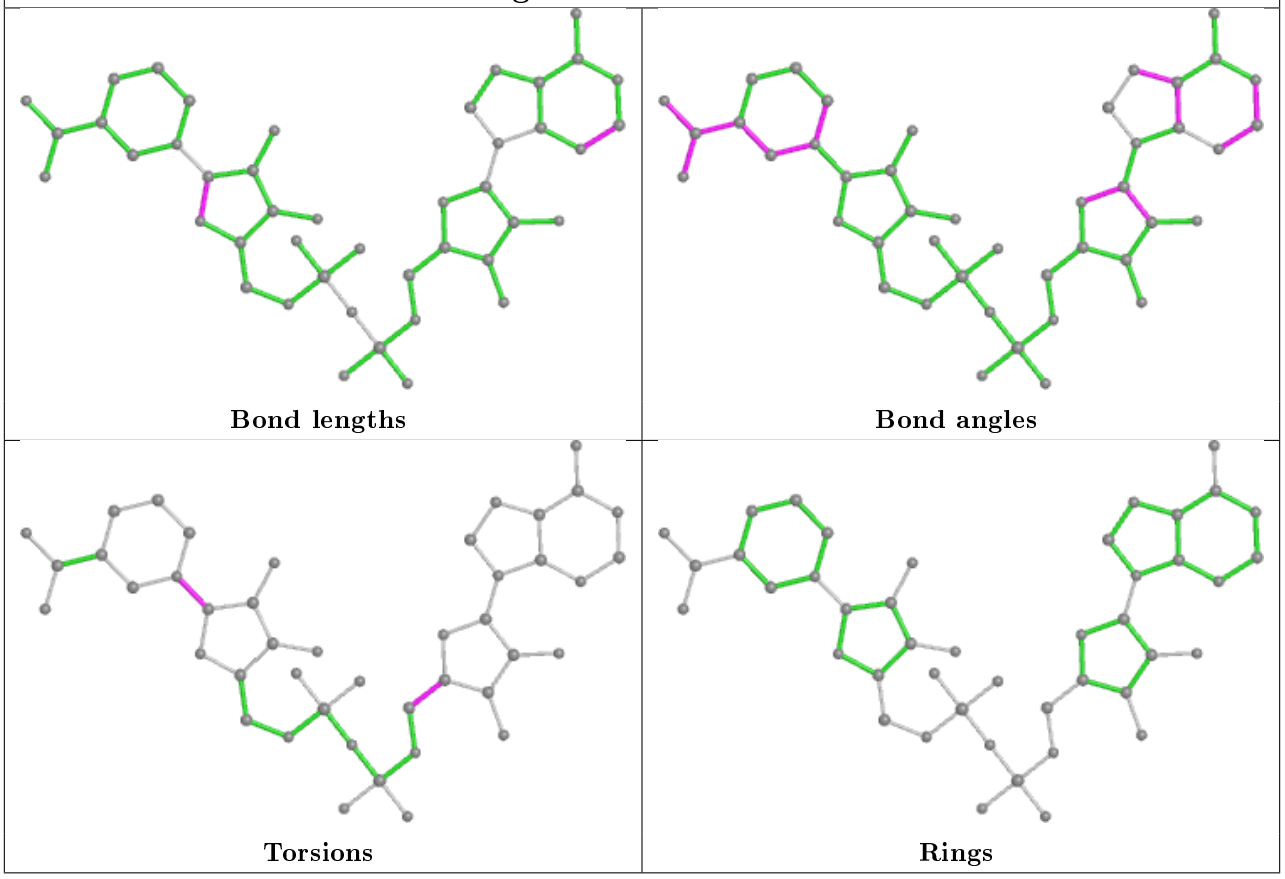


Torsions



Rings

Ligand NAD C 1000



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	50:VAL	C	51:ILE	N	0.73

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, 95^{th} 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	326/336 (97%)	0.27	25 (7%) 13 14	23, 46, 77, 96	0
1	B	335/336 (99%)	-0.09	0 100 100	22, 33, 54, 73	0
1	C	302/336 (89%)	0.50	43 (14%) 2 2	27, 49, 84, 108	0
1	D	270/336 (80%)	0.39	29 (10%) 6 6	25, 47, 93, 110	0
All	All	1233/1344 (91%)	0.26	97 (7%) 12 13	22, 43, 83, 110	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	HIS	6.2
1	D	48	LEU	6.2
1	D	36	LEU	5.8
1	C	48	LEU	5.8
1	D	316	LEU	5.4
1	D	62	VAL	5.3
1	C	333	VAL	5.2
1	C	320	ILE	5.0
1	C	332	VAL	4.8
1	C	308	VAL	4.8
1	C	317	PRO	4.6
1	D	50	VAL	4.6
1	C	319	TYR	4.5
1	C	311	ALA	4.4
1	D	317	PRO	4.3
1	D	51	ILE	4.3
1	A	15	GLN	4.2
1	C	313	LEU	4.0
1	D	114	GLY	3.9
1	D	26	VAL	3.9
1	A	325	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	57	CYS	3.8
1	D	121	TYR	3.8
1	A	326	ASN	3.8
1	C	59	ASP	3.8
1	C	125	TYR	3.7
1	D	61	TYR	3.7
1	D	32	GLY	3.7
1	C	120	GLY	3.7
1	D	332	VAL	3.7
1	D	125	TYR	3.6
1	C	325	ASN	3.6
1	A	60	ASN	3.5
1	C	316	LEU	3.5
1	C	31	ALA	3.4
1	A	120	GLY	3.4
1	A	12	PHE	3.4
1	D	80	ASN	3.3
1	C	32	GLY	3.2
1	C	336	PRO	3.1
1	A	323	LEU	3.1
1	C	41	VAL	3.0
1	C	322	LYS	3.0
1	C	310	SER	3.0
1	C	62	VAL	3.0
1	C	122	ASP	3.0
1	C	128	TYR	2.9
1	D	60	ASN	2.8
1	A	9	GLY	2.8
1	A	18	LEU	2.8
1	C	119	LEU	2.8
1	C	324	ARG	2.8
1	A	10	PHE	2.7
1	A	58	GLY	2.7
1	D	34	LEU	2.7
1	C	27	HIS	2.6
1	C	116	TRP	2.6
1	A	23	ASP	2.6
1	A	121	TYR	2.6
1	A	20	LEU	2.5
1	C	20	LEU	2.5
1	C	323	LEU	2.5
1	C	312	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	307	VAL	2.5
1	A	311	ALA	2.5
1	A	317	PRO	2.4
1	A	310	SER	2.4
1	C	118	GLY	2.4
1	C	76	ASP	2.4
1	C	121	TYR	2.4
1	A	25	PRO	2.4
1	D	81	TYR	2.4
1	A	316	LEU	2.3
1	D	131	VAL	2.3
1	C	19	ASN	2.3
1	D	126	GLN	2.3
1	C	60	ASN	2.3
1	C	309	ARG	2.3
1	A	19	ASN	2.2
1	D	25	PRO	2.2
1	D	38	VAL	2.2
1	C	47	ASP	2.2
1	D	128	TYR	2.2
1	D	39	ASP	2.2
1	A	79	ILE	2.1
1	A	61	TYR	2.1
1	C	18	LEU	2.1
1	D	100	TYR	2.1
1	D	115	ASP	2.1
1	D	333	VAL	2.1
1	A	118	GLY	2.1
1	C	26	VAL	2.1
1	C	29	PRO	2.1
1	C	335	ASN	2.0
1	A	322	LYS	2.0
1	D	40	ALA	2.0
1	C	58	GLY	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 carbohydrates in this entry.

6.4 Ligands (i)

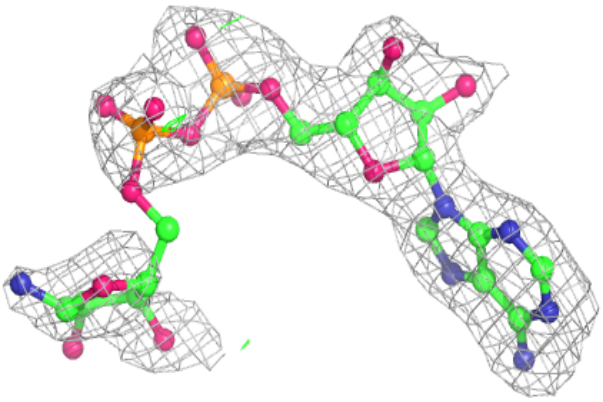
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

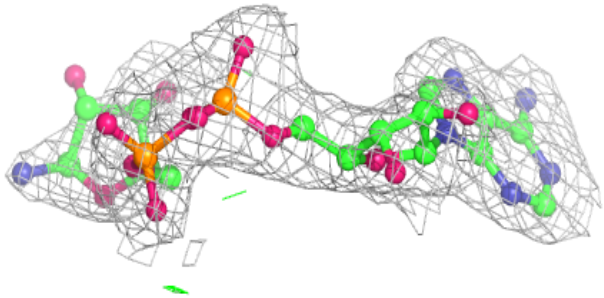
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	1339	4/4	0.71	0.20	46,48,48,56	0
2	ZN	D	500	1/1	0.85	0.07	92,92,92,92	0
2	ZN	B	499	1/1	0.88	0.11	37,37,37,37	1
4	EDO	A	1337	4/4	0.89	0.32	46,53,59,62	0
3	NAD	A	1000	36/44	0.90	0.14	40,58,91,94	0
4	EDO	B	1338	4/4	0.91	0.21	40,41,43,46	0
4	EDO	C	1337	4/4	0.91	0.15	51,51,53,54	0
4	EDO	C	1338	4/4	0.92	0.21	41,43,45,48	0
3	NAD	D	1000	44/44	0.93	0.14	43,51,58,67	0
3	NAD	C	1000	44/44	0.93	0.12	42,55,69,72	0
2	ZN	B	500	1/1	0.95	0.16	28,28,28,28	1
4	EDO	B	1337	4/4	0.96	0.33	38,40,42,47	0
2	ZN	C	500	1/1	0.96	0.04	60,60,60,60	1
2	ZN	C	600	1/1	0.97	0.03	49,49,49,49	0
2	ZN	A	500	1/1	0.98	0.05	45,45,45,45	1
3	NAD	B	1000	44/44	0.98	0.10	23,27,31,32	0
2	ZN	D	600	1/1	0.99	0.04	50,50,50,50	0
2	ZN	B	600	1/1	1.00	0.09	36,36,36,36	0
2	ZN	A	600	1/1	1.00	0.06	38,38,38,38	1

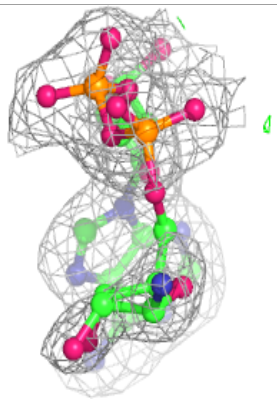
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 1000:

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

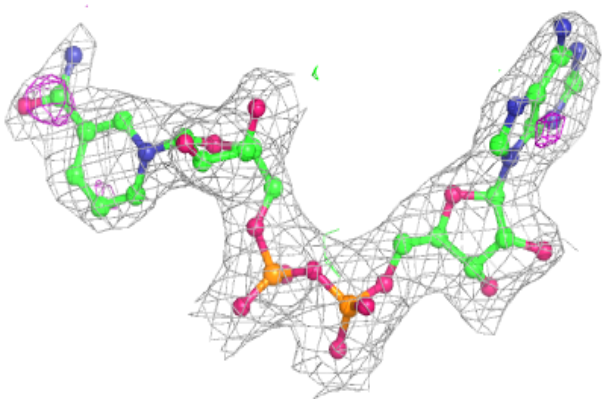


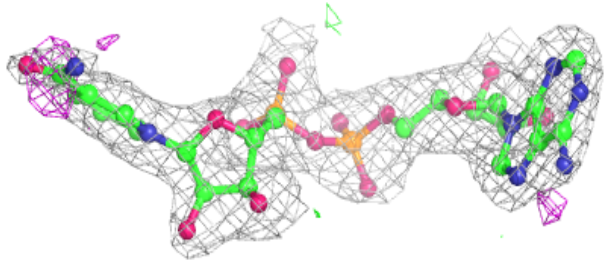


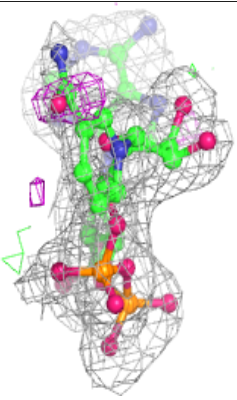


Electron density around NAD D 1000:

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

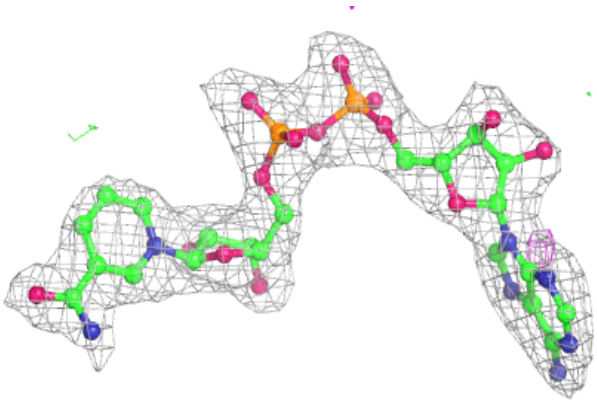


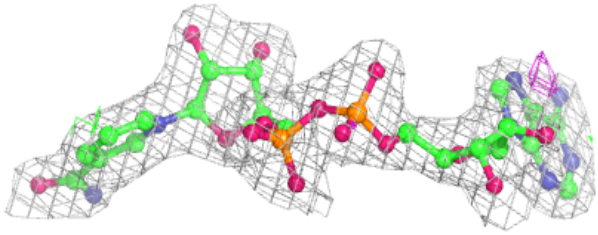


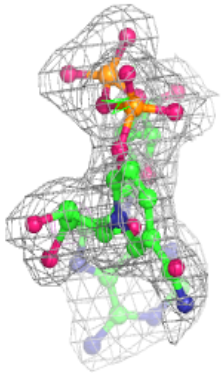


Electron density around NAD C 1000:

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

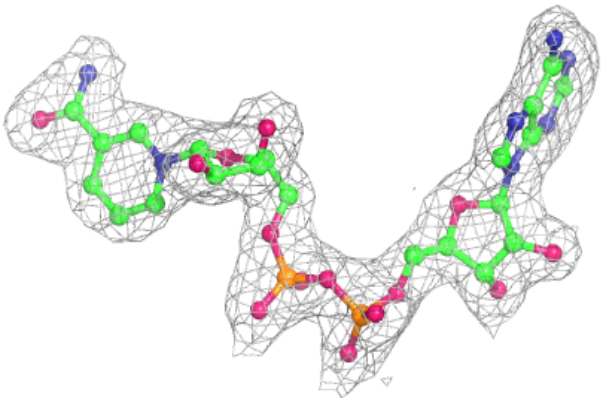


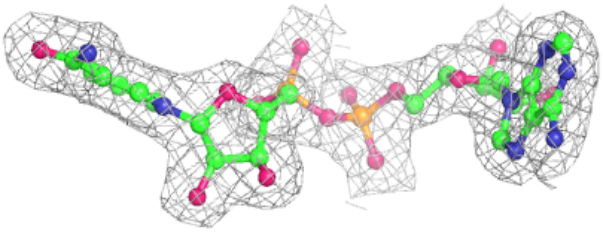


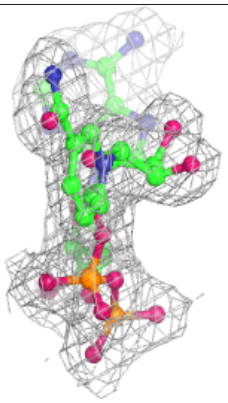


Electron density around NAD B 1000:

$2mF_o$-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.