Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 07:40 PM JST

PDB ID	:	4YRB
Title	:	mouse TDH mutant R180K with NAD+ bound
Authors	:	He, C.; Li, F.
Deposited on	:	2015-03-14
Resolution	:	3.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

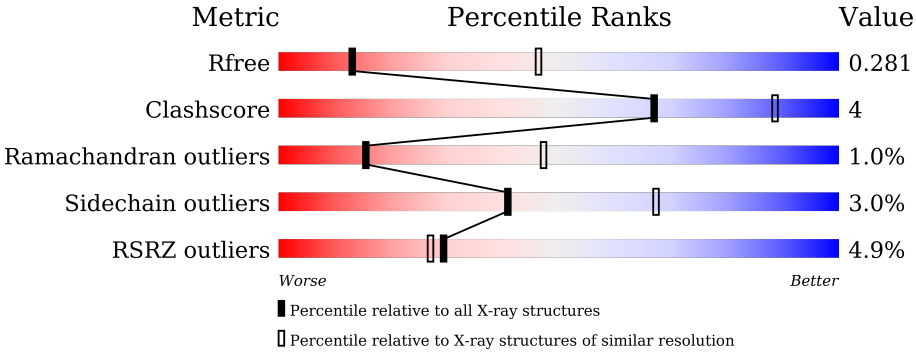
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	329	5% 56% 6% • 37%
1	B	329	2% 57% 9% 35%
1	C	329	5% 63% 12% • 24%
1	D	329	3% 64% 7% 29%
1	E	329	2% 56% 11% • 32%
1	F	329	3% 54% 9% 37%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10856 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 L-threonine 3-dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1645	1060	288	290	7	0	0	0
			Total	C	N	O	S			
1	B	215	1704	1098	294	303	9	0	0	0
			Total	C	N	O	S			
1	C	249	1966	1262	343	350	11	0	0	0
			Total	C	N	O	S			
1	D	232	1844	1186	321	328	9	0	0	0
			Total	C	N	O	S			
1	E	223	1765	1138	307	311	9	0	0	0
			Total	C	N	O	S			
1	F	208	1668	1074	291	296	7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	HIS	-	expression tag	UNP Q8K3F7
A	46	MET	-	expression tag	UNP Q8K3F7
A	180	LYS	ARG	engineered mutation	UNP Q8K3F7
B	45	HIS	-	expression tag	UNP Q8K3F7
B	46	MET	-	expression tag	UNP Q8K3F7
B	180	LYS	ARG	engineered mutation	UNP Q8K3F7
C	45	HIS	-	expression tag	UNP Q8K3F7
C	46	MET	-	expression tag	UNP Q8K3F7
C	180	LYS	ARG	engineered mutation	UNP Q8K3F7
D	45	HIS	-	expression tag	UNP Q8K3F7
D	46	MET	-	expression tag	UNP Q8K3F7
D	180	LYS	ARG	engineered mutation	UNP Q8K3F7
E	45	HIS	-	expression tag	UNP Q8K3F7
E	46	MET	-	expression tag	UNP Q8K3F7
E	180	LYS	ARG	engineered mutation	UNP Q8K3F7
F	45	HIS	-	expression tag	UNP Q8K3F7
F	46	MET	-	expression tag	UNP Q8K3F7

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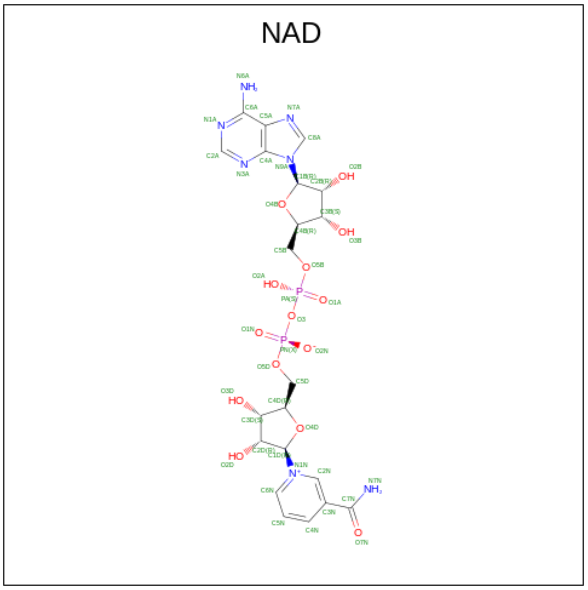
Chain	Residue	Modelled	Actual	Comment	Reference
F	180	LYS	ARG	engineered mutation	UNP Q8K3F7

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



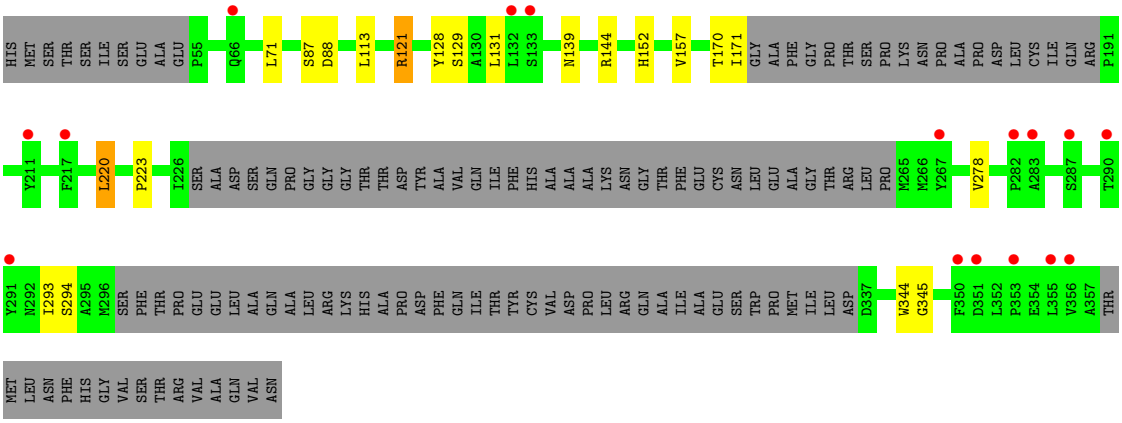
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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.

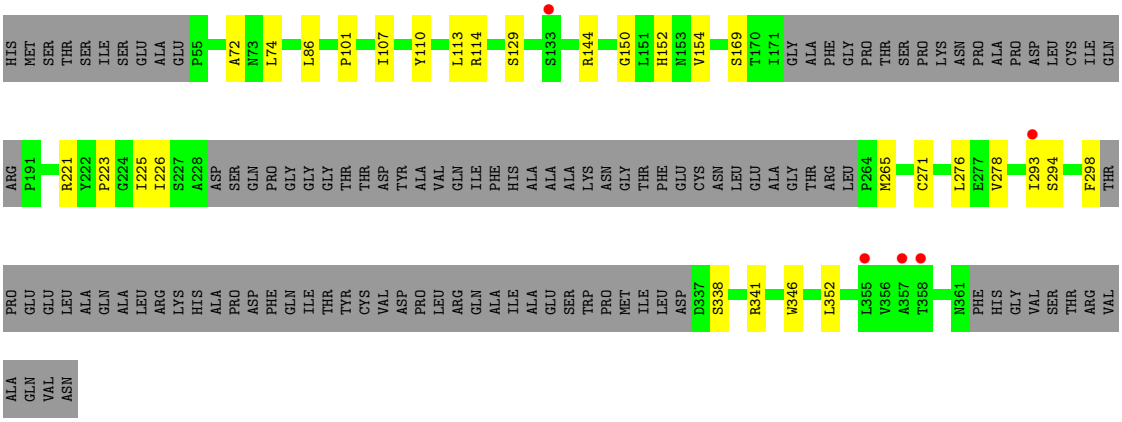
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain A:



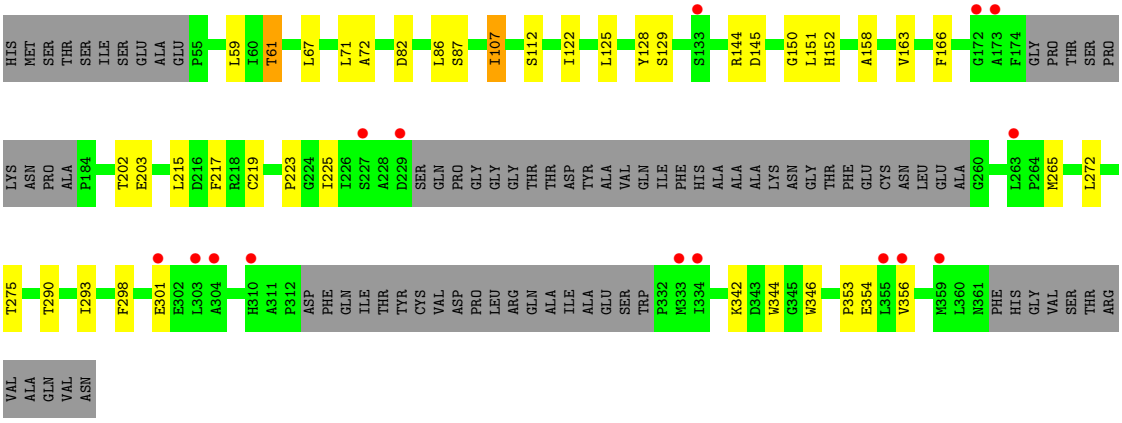
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain B:



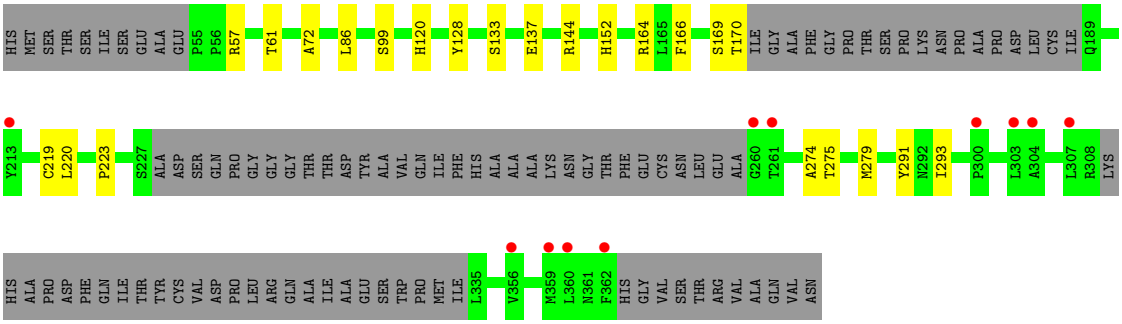
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain C:



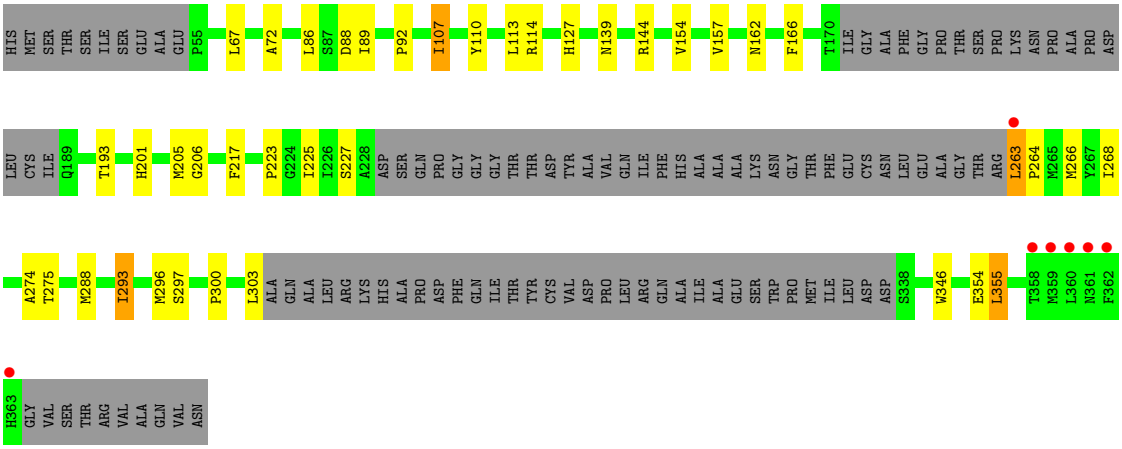
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain D:



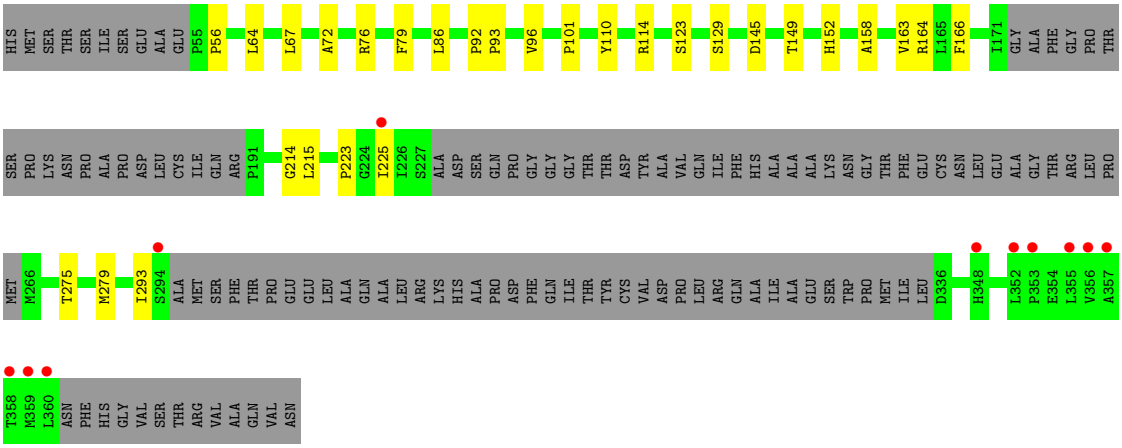
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain E:



• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain F:


HIS MET SER THR SER ILE SER GLU ALA GLU P55 P56 L64 L67 A72 R76 F79 L86 P92 P93 V96 P101 Y110 R114 S123 S129 D145 T149 H152 A158 V163 R164 L165 F166 I171 GLY ALA PHE GLY PRO THR
SER PRO LYS ASN PRO ALA PRO ASP LEU CYS ILE GLN ARG P191 G214 L215 P223 G224 I225 I226 S227 ALA ASP SER GLN PRO GLY GLY GLY THR THR ASP TYR ALA VAL GLN ILE PHE HIS ALA ALA ALA LYS ASN GLY THR PHE GLU CYS ASN LEU GLU ALA GLY THR ARG LEU PRO
MET M266 T275 M279 I293 S294 ALA MET SER PHE THR PRO GLU GLU LEU ALA GLN ALA LEU ARG LYS HIS ALA PRO ASP PHE GLN ILE THR TYR CYS VAL ASP PRO LEU ARG GLN ALA ILE ALA GLU SER TRP PRO MET ILE LEU D336 H348 L352 P353 E354 L355 V356 A357
T358 M359 L360 ASN PHE HIS GLY VAL SER THR ARG VAL ALA GLN VAL ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.24Å 154.05Å 199.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.25 47.12 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.12-3.25) 97.0 (47.12-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.228 , 0.285 0.226 , 0.281	Depositor DCC
R_{free} test set	1772 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	70.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10856	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/1684	0.52	0/2283
1	B	0.31	0/1745	0.53	0/2367
1	C	0.32	0/2013	0.55	0/2729
1	D	0.33	0/1887	0.54	0/2559
1	E	0.32	0/1808	0.54	0/2454
1	F	0.31	0/1707	0.51	0/2313
All	All	0.32	0/10844	0.53	0/14705

There are no bond length outliers.

There are no bond angle outliers.

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	1645	0	1638	11	0
1	B	1704	0	1688	16	0
1	C	1966	0	1955	21	0
1	D	1844	0	1835	11	0
1	E	1765	0	1752	17	0
1	F	1668	0	1669	15	0
2	A	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
All	All	10856	0	10693	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (85) 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:F:164:ARG:NH2	1:F:279:MET:O	2.09	0.86
1:A:121:ARG:NH2	1:E:92:PRO:O	2.17	0.76
1:D:164:ARG:NH2	1:D:279:MET:O	2.29	0.66
1:E:107:ILE:HD11	1:E:154:VAL:HG23	1.81	0.62
1:C:144:ARG:HD2	1:D:152:HIS:CD2	2.37	0.58
1:C:152:HIS:CD2	1:D:144:ARG:HD2	2.39	0.58
1:B:226:ILE:HD11	1:B:265:MET:SD	2.45	0.57
1:A:220:LEU:HD21	1:A:278:VAL:HG11	1.88	0.56
1:D:57:ARG:NH1	1:D:120:HIS:O	2.37	0.56
1:C:107:ILE:HG23	1:C:150:GLY:HA2	1.88	0.56
1:B:225:ILE:CD1	1:B:271:CYS:SG	2.94	0.56
1:E:67:LEU:HD21	1:E:225:ILE:HG21	1.88	0.55
1:B:74:LEU:HD21	1:B:276:LEU:HD22	1.88	0.55
1:B:110:TYR:CE2	1:B:114:ARG:HD2	2.43	0.53
1:F:158:ALA:HA	1:F:163:VAL:HB	1.92	0.51
1:E:107:ILE:HD11	1:E:154:VAL:CG2	2.41	0.50
1:C:344:TRP:CZ3	1:C:346:TRP:HB2	2.47	0.49
1:E:127:HIS:ND1	1:E:154:VAL:HG21	2.28	0.49
1:F:72:ALA:HB2	1:F:86:LEU:HD13	1.94	0.48
1:A:152:HIS:CD2	1:B:144:ARG:HD2	2.48	0.48
1:B:225:ILE:HD13	1:B:271:CYS:SG	2.53	0.48
1:D:61:THR:O	1:D:128:TYR:HB2	2.13	0.48
1:A:71:LEU:HD22	1:A:128:TYR:CE2	2.48	0.48
1:F:129:SER:HB2	2:F:1001:NAD:C4A	2.43	0.48
1:B:129:SER:HB2	2:B:1001:NAD:N3A	2.28	0.48
1:E:88:ASP:OD1	1:E:89:ILE:N	2.47	0.47
1:A:293:ILE:HD11	1:A:344:TRP:CZ2	2.50	0.47
1:C:151:LEU:CD2	1:C:202:THR:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:PHE:CZ	1:D:275:THR:HG23	2.49	0.47
1:D:169:SER:HB2	1:D:219:CYS:SG	2.56	0.46
1:A:113:LEU:HB3	1:A:157:VAL:HG21	1.97	0.46
1:C:265:MET:HG3	1:C:298:PHE:CZ	2.51	0.46
1:C:166:PHE:CZ	1:C:275:THR:HG23	2.51	0.45
1:B:107:ILE:HD13	1:B:113:LEU:HD21	1.98	0.45
1:E:274:ALA:HB2	1:E:346:TRP:CZ3	2.52	0.45
1:C:215:LEU:O	1:C:217:PHE:N	2.49	0.45
1:A:144:ARG:HD2	1:B:152:HIS:CD2	2.52	0.45
1:D:133:SER:O	1:D:137:GLU:HG2	2.17	0.45
1:E:206:GLY:HA3	1:E:217:PHE:CZ	2.52	0.45
1:E:296:MET:HE1	1:E:355:LEU:HD13	1.98	0.45
1:F:145:ASP:O	1:F:149:THR:HB	2.16	0.45
1:C:71:LEU:HA	1:C:272:LEU:HD22	1.97	0.45
1:C:219:CYS:SG	1:C:290:THR:HG23	2.57	0.45
1:D:220:LEU:HD23	1:D:291:TYR:HB2	1.99	0.45
1:C:72:ALA:HB2	1:C:86:LEU:HD13	1.98	0.44
1:C:107:ILE:HB	2:C:1001:NAD:N1A	2.32	0.44
1:F:166:PHE:CZ	1:F:275:THR:HG23	2.52	0.44
1:B:341:ARG:HG2	1:B:346:TRP:O	2.17	0.44
1:A:129:SER:HB2	2:A:1001:NAD:C4A	2.47	0.44
1:E:110:TYR:CE2	1:E:114:ARG:HD2	2.53	0.44
1:C:158:ALA:HA	1:C:163:VAL:HB	2.00	0.44
1:A:170:THR:O	1:A:171:ILE:C	2.56	0.43
1:C:71:LEU:HD22	1:C:128:TYR:CZ	2.53	0.43
1:E:201:HIS:CE1	1:E:205:MET:CG	3.01	0.43
1:F:67:LEU:HD21	1:F:225:ILE:HG21	2.00	0.43
1:F:76:ARG:NH2	1:F:101:PRO:O	2.51	0.43
1:B:169:SER:HB3	1:B:221:ARG:HG2	2.00	0.43
1:C:59:LEU:HB3	1:C:122:ILE:HG21	1.99	0.43
1:D:274:ALA:CB	1:D:293:ILE:CD1	2.97	0.43
1:B:265:MET:HG3	1:B:298:PHE:CZ	2.54	0.43
1:C:203:GLU:OE1	1:C:290:THR:HG21	2.18	0.43
1:A:88:ASP:OD1	2:A:1001:NAD:O2B	2.24	0.43
1:E:144:ARG:HD2	1:F:152:HIS:CD2	2.53	0.43
1:F:92:PRO:HB2	1:F:96:VAL:HG23	2.00	0.43
1:A:170:THR:CG2	2:A:1001:NAD:H6N	2.49	0.43
1:E:72:ALA:HB2	1:E:86:LEU:HD13	2.00	0.42
1:F:110:TYR:CE2	1:F:114:ARG:HD2	2.54	0.42
1:B:72:ALA:HB2	1:B:86:LEU:HD13	2.02	0.42
1:B:150:GLY:O	1:B:154:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HB2	1:C:163:VAL:HG11	2.02	0.42
1:C:61:THR:HG22	1:C:129:SER:HB3	2.02	0.41
1:F:56:PRO:HD2	1:F:79:PHE:CD1	2.55	0.41
1:F:64:LEU:HD21	1:F:92:PRO:HB3	2.03	0.41
1:E:113:LEU:HB2	1:E:157:VAL:HG21	2.01	0.41
1:E:227:SER:HB3	1:E:268:ILE:HB	2.02	0.41
1:B:129:SER:HB2	2:B:1001:NAD:C4A	2.51	0.41
1:C:151:LEU:HD22	1:C:202:THR:HA	2.03	0.41
1:B:352:LEU:HD23	1:B:352:LEU:C	2.41	0.41
1:F:92:PRO:HB2	1:F:96:VAL:CG2	2.51	0.41
1:E:166:PHE:CZ	1:E:275:THR:HG23	2.56	0.41
1:F:214:GLY:O	1:F:215:LEU:C	2.59	0.41
1:D:72:ALA:HB2	1:D:86:LEU:HD13	2.01	0.41
1:C:67:LEU:HD21	1:C:225:ILE:HG21	2.03	0.40
1:C:353:PRO:O	1:C:356:VAL:HG12	2.21	0.40
1:E:263:LEU:HG	1:E:264:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	198/329 (60%)	183 (92%)	13 (7%)	2 (1%)	15 47
1	B	207/329 (63%)	189 (91%)	16 (8%)	2 (1%)	15 47
1	C	241/329 (73%)	220 (91%)	20 (8%)	1 (0%)	34 67
1	D	224/329 (68%)	209 (93%)	14 (6%)	1 (0%)	34 67
1	E	215/329 (65%)	197 (92%)	13 (6%)	5 (2%)	6 29
1	F	200/329 (61%)	184 (92%)	14 (7%)	2 (1%)	15 47
All	All	1285/1974 (65%)	1182 (92%)	90 (7%)	13 (1%)	15 47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	300	PRO
1	A	345	GLY
1	E	162	ASN
1	E	223	PRO
1	A	223	PRO
1	C	223	PRO
1	D	223	PRO
1	E	266	MET
1	E	293	ILE
1	F	223	PRO
1	B	101	PRO
1	B	223	PRO
1	F	93	PRO

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	175/277 (63%)	169 (97%)	6 (3%)	37	64
1	B	182/277 (66%)	178 (98%)	4 (2%)	52	74
1	C	209/277 (76%)	199 (95%)	10 (5%)	25	56
1	D	197/277 (71%)	195 (99%)	2 (1%)	76	85
1	E	188/277 (68%)	178 (95%)	10 (5%)	22	53
1	F	180/277 (65%)	178 (99%)	2 (1%)	73	84
All	All	1131/1662 (68%)	1097 (97%)	34 (3%)	41	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	121	ARG
1	A	131	LEU
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	220	LEU
1	A	294	SER
1	B	278	VAL
1	B	293	ILE
1	B	294	SER
1	B	338	SER
1	C	61	THR
1	C	82	ASP
1	C	87	SER
1	C	107	ILE
1	C	112	SER
1	C	145	ASP
1	C	293	ILE
1	C	301	GLU
1	C	342	LYS
1	C	354	GLU
1	D	99	SER
1	D	170	THR
1	E	107	ILE
1	E	139	ASN
1	E	193	THR
1	E	263	LEU
1	E	288	MET
1	E	293	ILE
1	E	297	SER
1	E	303	LEU
1	E	354	GLU
1	E	355	LEU
1	F	123	SER
1	F	293	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	152	HIS
1	A	153	ASN
1	A	339	ASN
1	B	83	ASN
1	B	153	ASN
1	C	120	HIS
1	C	153	ASN

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Mol	Chain	Res	Type
1	D	83	ASN
1	D	95	HIS
1	D	153	ASN
1	E	153	ASN
1	E	201	HIS
1	F	153	ASN

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)

6 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	D	1001	-	42,48,48	0.82	1 (2%)	50,73,73	1.30	5 (10%)
2	NAD	A	1001	-	42,48,48	0.79	1 (2%)	50,73,73	1.29	7 (14%)
2	NAD	C	1001	-	42,48,48	0.81	1 (2%)	50,73,73	1.33	7 (14%)
2	NAD	E	1001	-	42,48,48	0.79	1 (2%)	50,73,73	1.44	7 (14%)
2	NAD	F	1001	-	42,48,48	0.77	2 (4%)	50,73,73	1.32	5 (10%)
2	NAD	B	1001	-	42,48,48	0.83	2 (4%)	50,73,73	1.28	5 (10%)

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	D	1001	-	-	5/26/62/62	0/5/5/5
2	NAD	A	1001	-	-	2/26/62/62	0/5/5/5
2	NAD	C	1001	-	-	8/26/62/62	0/5/5/5
2	NAD	E	1001	-	-	4/26/62/62	0/5/5/5
2	NAD	F	1001	-	-	8/26/62/62	0/5/5/5
2	NAD	B	1001	-	-	4/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	NAD	C5A-C4A	2.43	1.47	1.40
2	D	1001	NAD	C5A-C4A	2.39	1.47	1.40
2	C	1001	NAD	C5A-C4A	2.38	1.47	1.40
2	B	1001	NAD	C5A-C4A	2.34	1.47	1.40
2	A	1001	NAD	C5A-C4A	2.26	1.46	1.40
2	F	1001	NAD	C5A-C4A	2.21	1.46	1.40
2	B	1001	NAD	O4D-C1D	2.18	1.44	1.41
2	F	1001	NAD	O4D-C1D	2.09	1.44	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	NAD	N3A-C2A-N1A	-4.04	122.37	128.68
2	E	1001	NAD	PN-O3-PA	-4.00	119.11	132.83
2	A	1001	NAD	N3A-C2A-N1A	-3.97	122.47	128.68
2	D	1001	NAD	N3A-C2A-N1A	-3.95	122.51	128.68
2	E	1001	NAD	N3A-C2A-N1A	-3.91	122.56	128.68
2	F	1001	NAD	N3A-C2A-N1A	-3.91	122.56	128.68
2	B	1001	NAD	N3A-C2A-N1A	-3.83	122.70	128.68
2	D	1001	NAD	PN-O3-PA	-3.58	120.53	132.83
2	B	1001	NAD	PN-O3-PA	-3.53	120.72	132.83
2	F	1001	NAD	C3D-C2D-C1D	3.50	106.25	100.98
2	C	1001	NAD	C3D-C2D-C1D	3.44	106.15	100.98
2	E	1001	NAD	C3D-C2D-C1D	3.27	105.91	100.98
2	F	1001	NAD	PN-O3-PA	-3.24	121.72	132.83
2	E	1001	NAD	C3N-C7N-N7N	3.22	121.62	117.75
2	A	1001	NAD	C3D-C2D-C1D	3.20	105.79	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	NAD	PN-O3-PA	-3.19	121.86	132.83
2	F	1001	NAD	C4A-C5A-N7A	-2.98	106.29	109.40
2	D	1001	NAD	C3D-C2D-C1D	2.96	105.44	100.98
2	B	1001	NAD	C3D-C2D-C1D	2.86	105.28	100.98
2	C	1001	NAD	C4A-C5A-N7A	-2.85	106.43	109.40
2	D	1001	NAD	C4A-C5A-N7A	-2.77	106.51	109.40
2	A	1001	NAD	PN-O3-PA	-2.70	123.55	132.83
2	E	1001	NAD	C4A-C5A-N7A	-2.66	106.62	109.40
2	D	1001	NAD	C3B-C2B-C1B	2.58	104.86	100.98
2	A	1001	NAD	C4A-C5A-N7A	-2.47	106.82	109.40
2	E	1001	NAD	C2A-N1A-C6A	2.35	122.77	118.75
2	B	1001	NAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	B	1001	NAD	O4B-C1B-C2B	-2.29	103.58	106.93
2	A	1001	NAD	C1B-N9A-C4A	-2.27	122.64	126.64
2	A	1001	NAD	C3N-C7N-N7N	2.22	120.41	117.75
2	C	1001	NAD	C2A-N1A-C6A	2.17	122.47	118.75
2	F	1001	NAD	O4B-C1B-C2B	-2.16	103.77	106.93
2	C	1001	NAD	C6N-N1N-C2N	-2.15	120.01	121.97
2	E	1001	NAD	C1B-N9A-C4A	-2.04	123.06	126.64
2	C	1001	NAD	C1B-N9A-C4A	-2.00	123.12	126.64
2	A	1001	NAD	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	NAD	C5D-O5D-PN-O2N
2	C	1001	NAD	C5D-O5D-PN-O2N
2	D	1001	NAD	C5D-O5D-PN-O3
2	E	1001	NAD	C5D-O5D-PN-O2N
2	F	1001	NAD	C5D-O5D-PN-O2N
2	C	1001	NAD	C2N-C3N-C7N-O7N
2	C	1001	NAD	C2N-C3N-C7N-N7N
2	F	1001	NAD	C2N-C3N-C7N-O7N
2	C	1001	NAD	C4N-C3N-C7N-O7N
2	C	1001	NAD	C4N-C3N-C7N-N7N
2	F	1001	NAD	C4N-C3N-C7N-O7N
2	F	1001	NAD	C4N-C3N-C7N-N7N
2	F	1001	NAD	C2N-C3N-C7N-N7N
2	B	1001	NAD	C5D-O5D-PN-O3
2	C	1001	NAD	C5D-O5D-PN-O3
2	E	1001	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	F	1001	NAD	C5D-O5D-PN-O3
2	B	1001	NAD	C5D-O5D-PN-O1N
2	D	1001	NAD	C5D-O5D-PN-O1N
2	F	1001	NAD	C5D-O5D-PN-O1N
2	D	1001	NAD	C4N-C3N-C7N-N7N
2	E	1001	NAD	O4B-C4B-C5B-O5B
2	D	1001	NAD	C4N-C3N-C7N-O7N
2	A	1001	NAD	O4B-C4B-C5B-O5B
2	B	1001	NAD	O4B-C4B-C5B-O5B
2	C	1001	NAD	O4B-C4B-C5B-O5B
2	D	1001	NAD	O4B-C4B-C5B-O5B
2	C	1001	NAD	C5D-O5D-PN-O1N
2	E	1001	NAD	C5D-O5D-PN-O1N
2	A	1001	NAD	O4D-C4D-C5D-O5D
2	F	1001	NAD	O4B-C4B-C5B-O5B

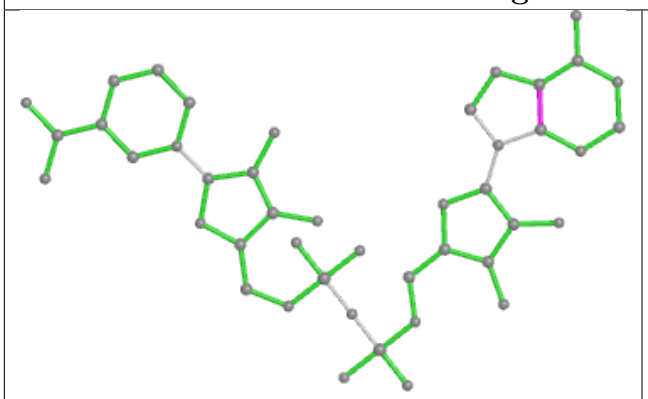
There are no ring outliers.

4 monomers are involved in 7 short contacts:

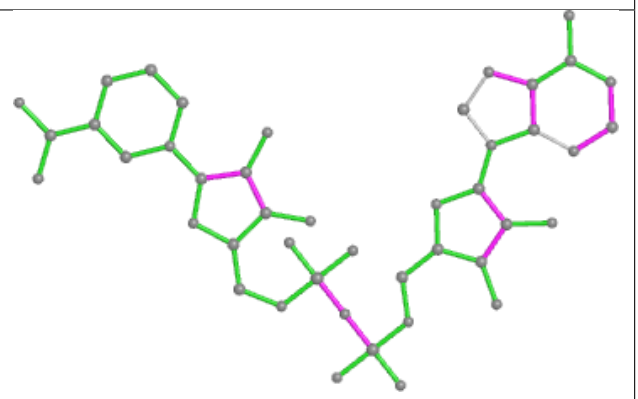
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAD	3	0
2	C	1001	NAD	1	0
2	F	1001	NAD	1	0
2	B	1001	NAD	2	0

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.

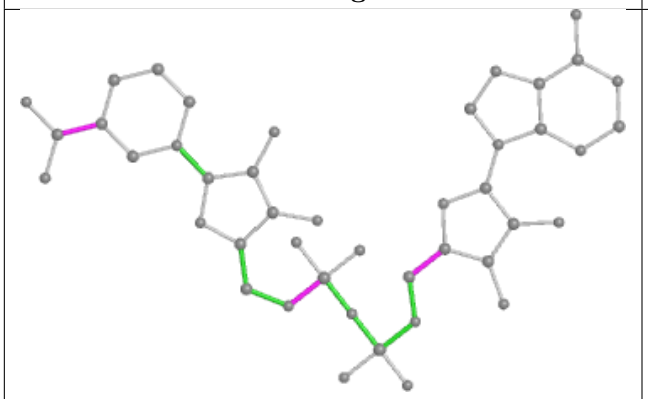
Ligand NAD D 1001



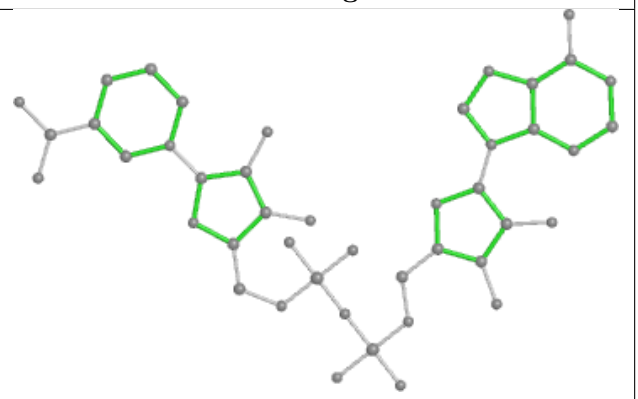
Bond lengths



Bond angles

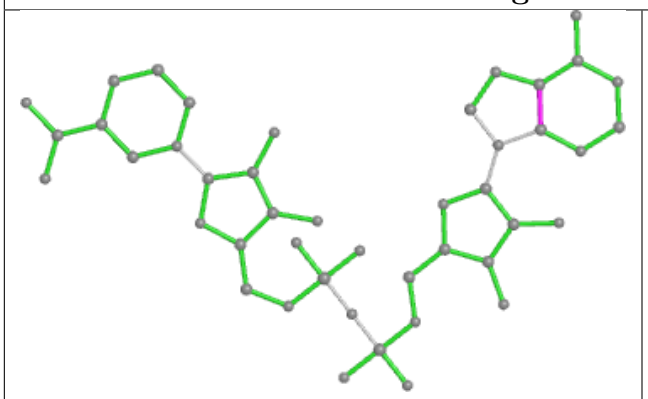


Torsions

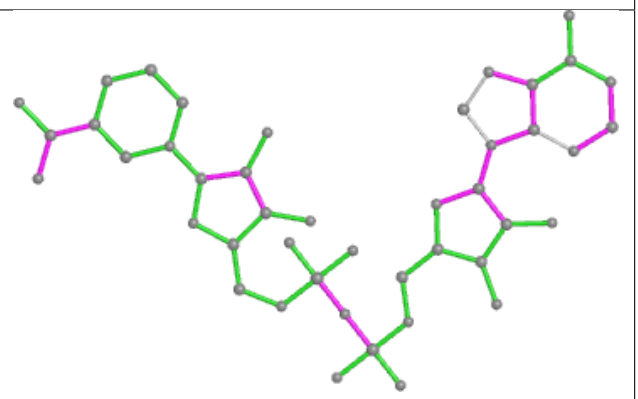


Rings

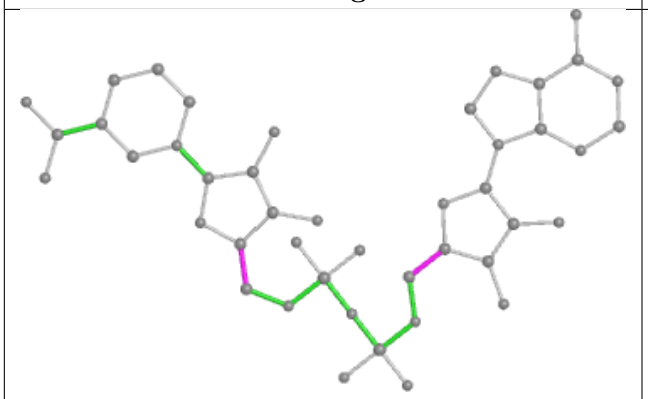
Ligand NAD A 1001



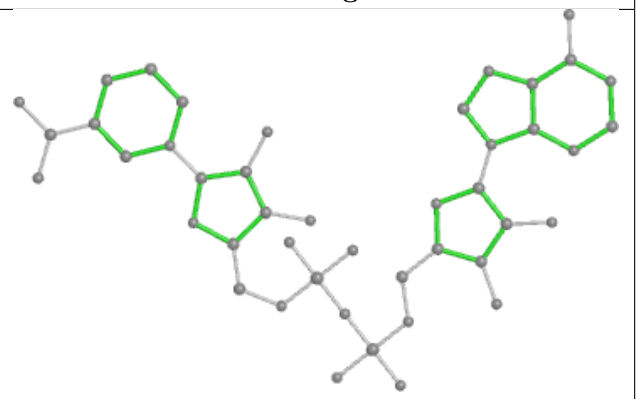
Bond lengths



Bond angles

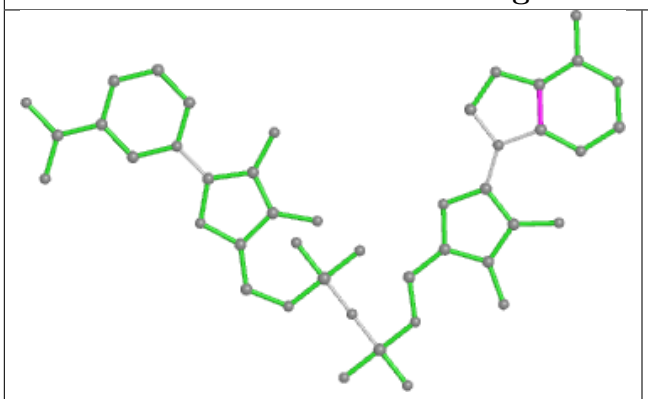


Torsions

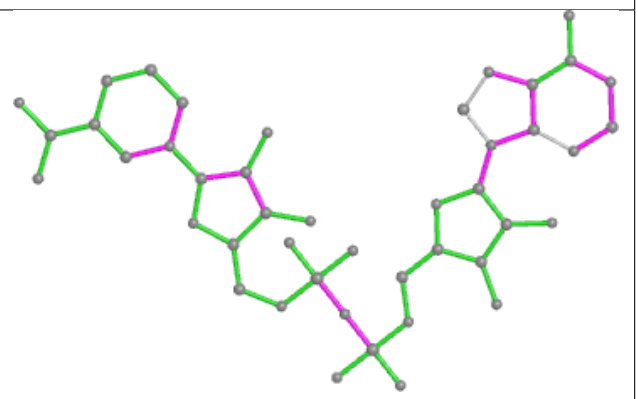


Rings

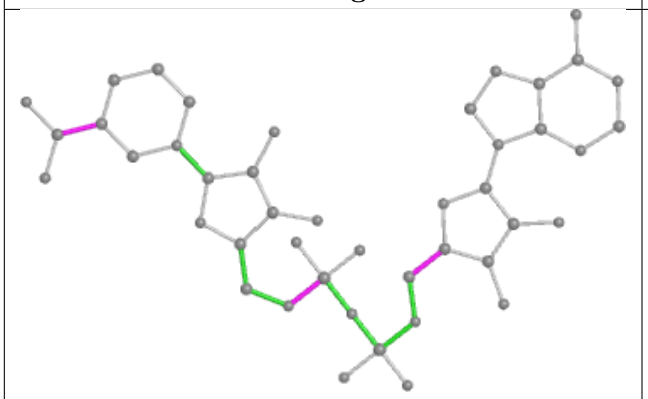
Ligand NAD C 1001



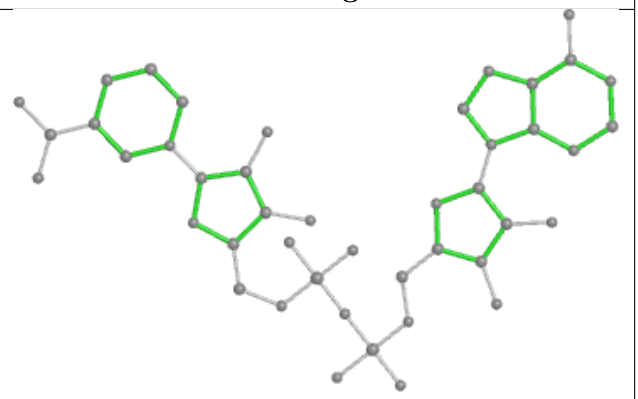
Bond lengths



Bond angles

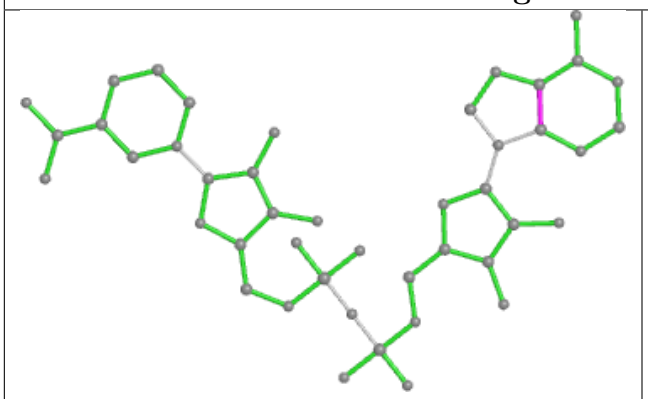


Torsions

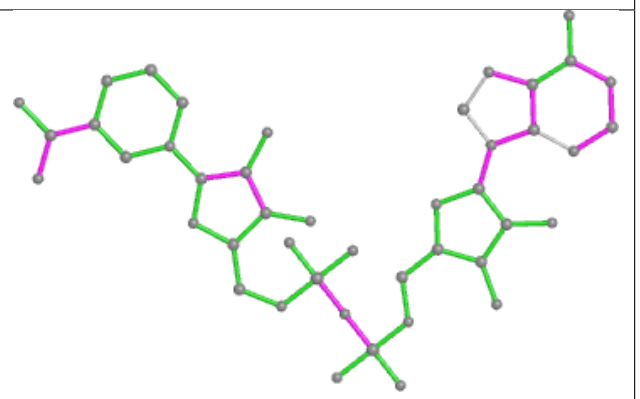


Rings

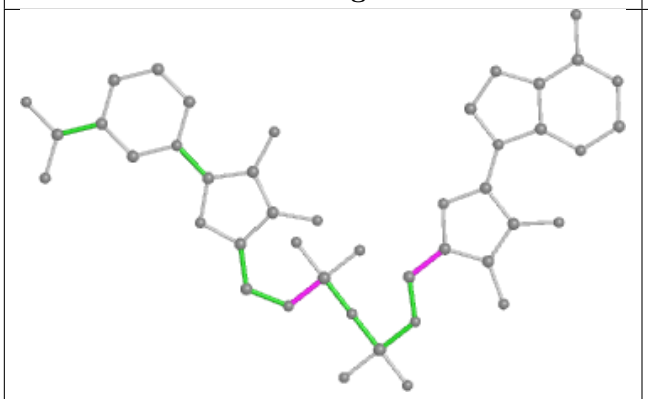
Ligand NAD E 1001



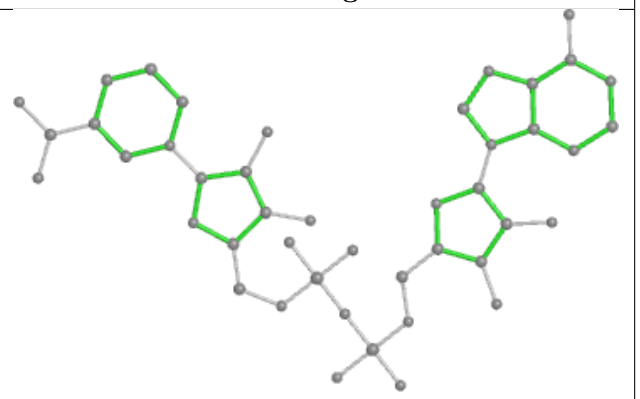
Bond lengths



Bond angles

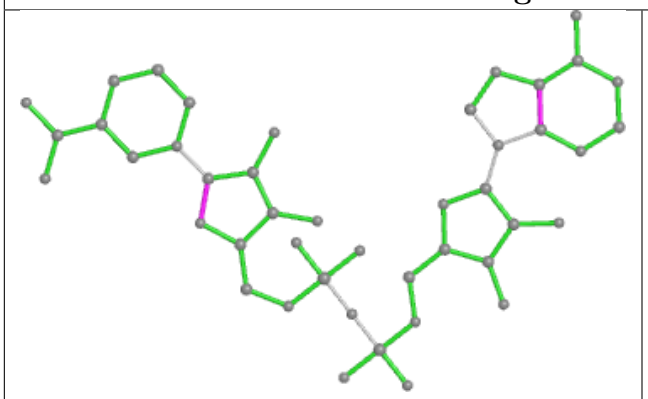


Torsions

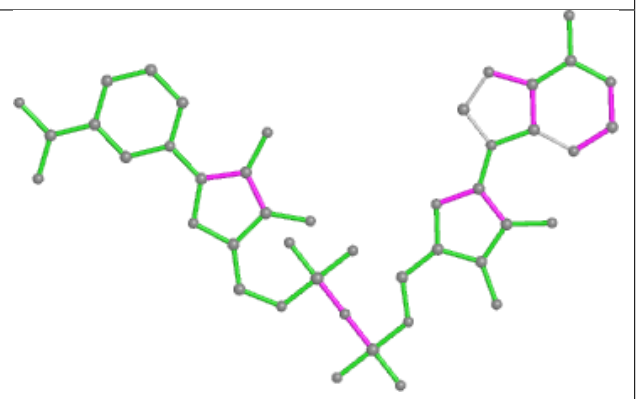


Rings

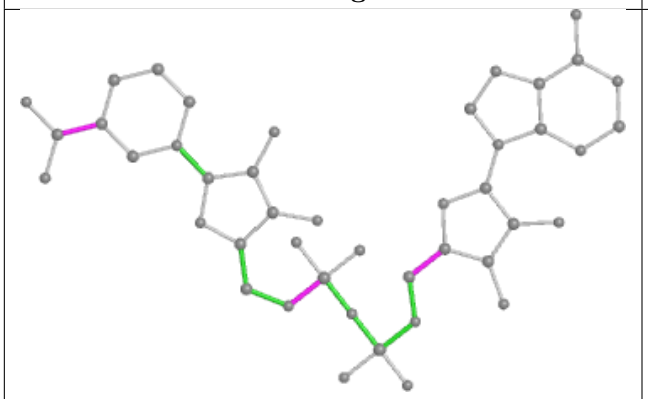
Ligand NAD F 1001



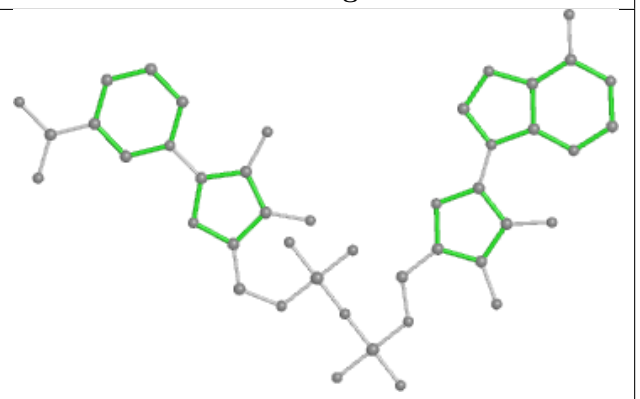
Bond lengths



Bond angles

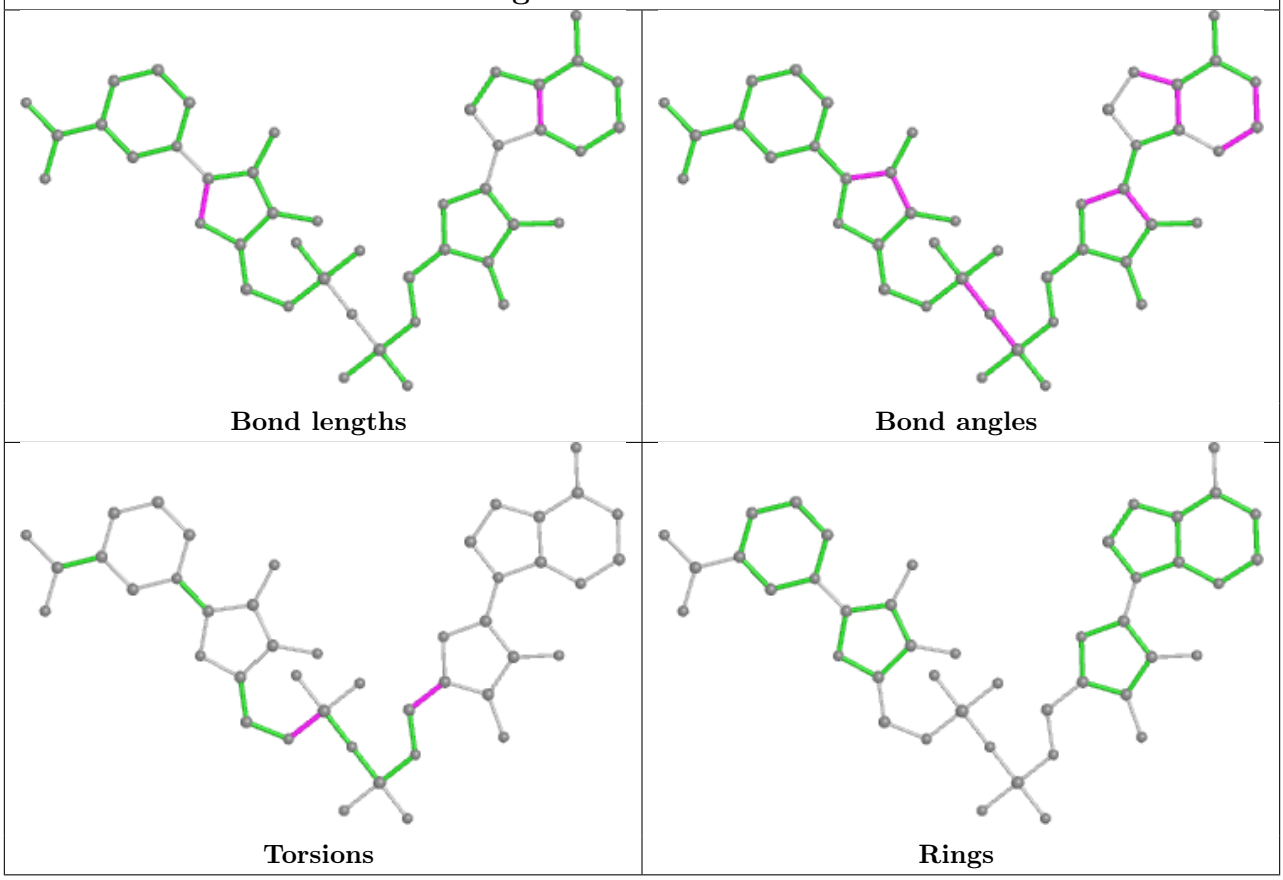


Torsions



Rings

Ligand NAD B 1001



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	206/329 (62%)	0.18	16 (7%)	13	12	55, 83, 118, 142	0
1	B	215/329 (65%)	0.07	5 (2%)	60	58	51, 73, 105, 133	0
1	C	249/329 (75%)	0.11	15 (6%)	21	21	43, 69, 128, 148	0
1	D	232/329 (70%)	0.05	11 (4%)	31	28	47, 71, 125, 146	0
1	E	223/329 (67%)	0.01	7 (3%)	49	47	45, 69, 101, 140	0
1	F	208/329 (63%)	0.13	11 (5%)	26	24	46, 70, 128, 169	0
All	All	1333/1974 (67%)	0.09	65 (4%)	29	27	43, 72, 121, 169	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	310	HIS	4.9
1	C	303	LEU	4.6
1	D	303	LEU	4.6
1	E	362	PHE	4.5
1	F	352	LEU	4.4
1	E	363	HIS	4.3
1	F	358	THR	4.1
1	D	362	PHE	3.6
1	C	263	LEU	3.6
1	A	355	LEU	3.6
1	C	229	ASP	3.4
1	E	263	LEU	3.4
1	C	355	LEU	3.3
1	F	360	LEU	3.3
1	B	355	LEU	3.3
1	E	359	MET	3.3
1	D	260	GLY	3.2
1	F	355	LEU	3.2
1	D	359	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	THR	3.1
1	F	356	VAL	3.1
1	F	357	ALA	3.1
1	A	356	VAL	2.8
1	F	353	PRO	2.8
1	B	358	THR	2.8
1	F	359	MET	2.7
1	C	227	SER	2.7
1	D	307	LEU	2.7
1	C	333	MET	2.7
1	C	304	ALA	2.7
1	F	225	ILE	2.7
1	A	133	SER	2.6
1	A	287	SER	2.5
1	B	357	ALA	2.5
1	A	351	ASP	2.5
1	A	66	GLN	2.5
1	B	133	SER	2.5
1	E	361	ASN	2.5
1	E	360	LEU	2.5
1	C	359	MET	2.5
1	C	356	VAL	2.4
1	A	132	LEU	2.4
1	D	356	VAL	2.4
1	A	291	TYR	2.3
1	E	358	THR	2.3
1	F	348	HIS	2.3
1	A	353	PRO	2.3
1	C	173	ALA	2.3
1	A	211	TYR	2.3
1	A	350	PHE	2.3
1	C	172	GLY	2.2
1	B	293	ILE	2.2
1	C	334	ILE	2.2
1	D	300	PRO	2.1
1	C	301	GLU	2.1
1	D	360	LEU	2.1
1	F	294	SER	2.1
1	D	304	ALA	2.1
1	D	261	THR	2.1
1	A	267	TYR	2.1
1	D	213	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	133	SER	2.0
1	A	282	PRO	2.0
1	A	217	PHE	2.0
1	A	283	ALA	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)

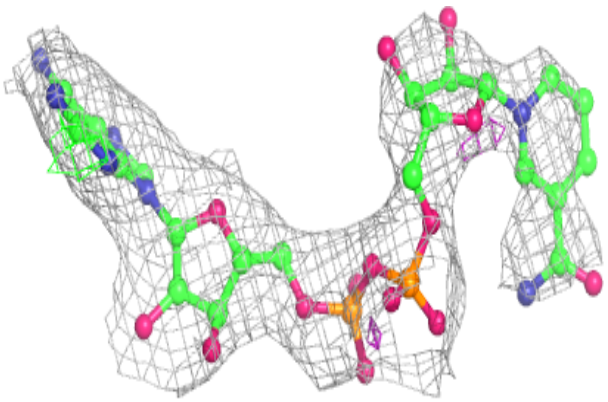
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

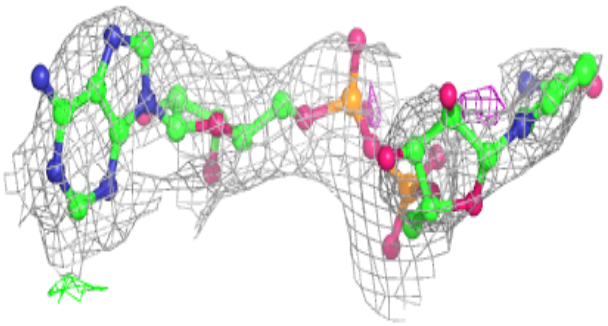
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	1001	44/44	0.87	0.33	87,121,134,143	0
2	NAD	B	1001	44/44	0.92	0.25	72,100,110,118	0
2	NAD	D	1001	44/44	0.93	0.23	66,95,107,109	0
2	NAD	F	1001	44/44	0.94	0.26	71,100,126,128	0
2	NAD	E	1001	44/44	0.95	0.25	66,80,99,103	0
2	NAD	C	1001	44/44	0.95	0.23	64,77,98,108	0

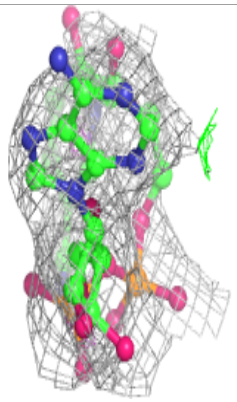
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 1001:

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

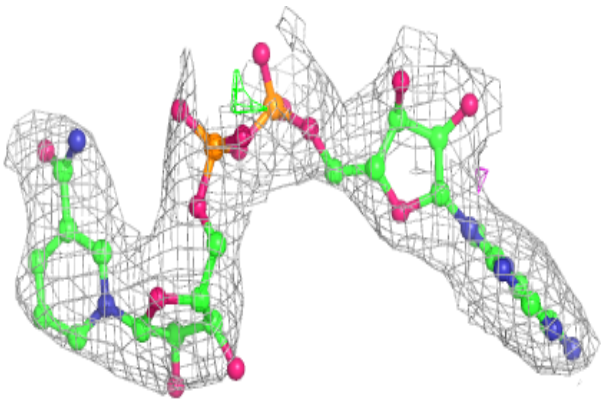


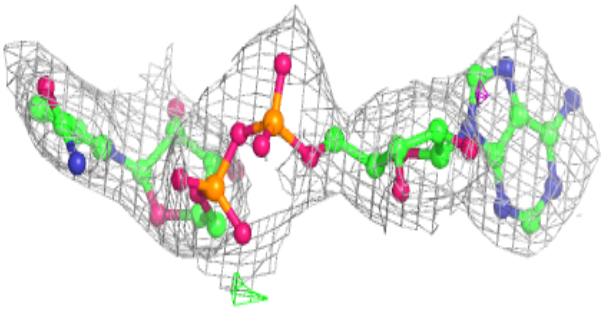


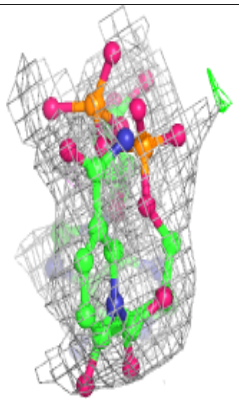


Electron density around NAD B 1001:

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

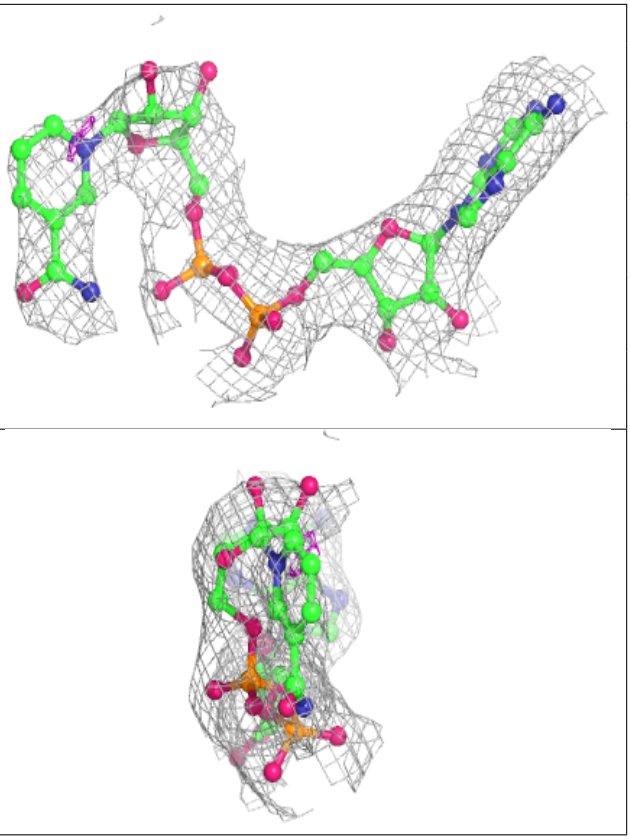


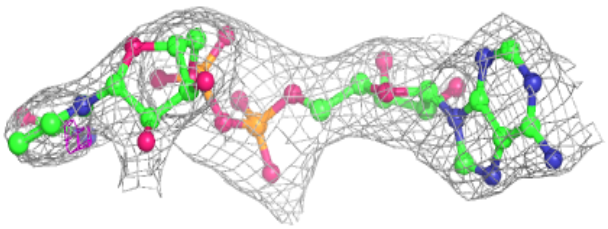




Electron density around NAD D 1001:

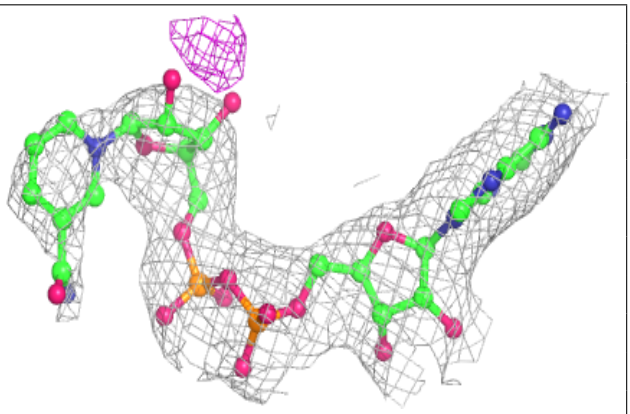
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

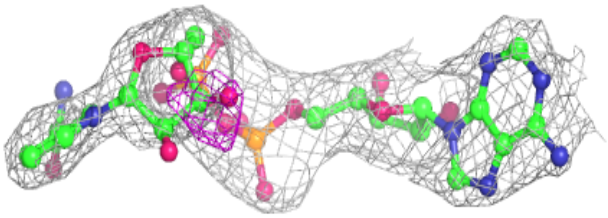


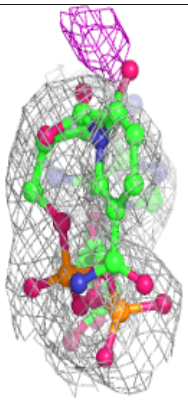


Electron density around NAD F 1001:

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

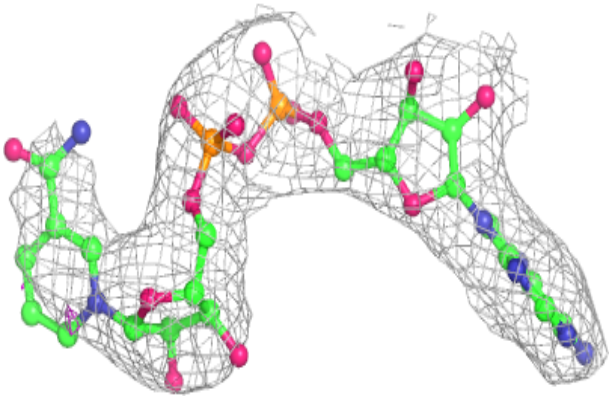


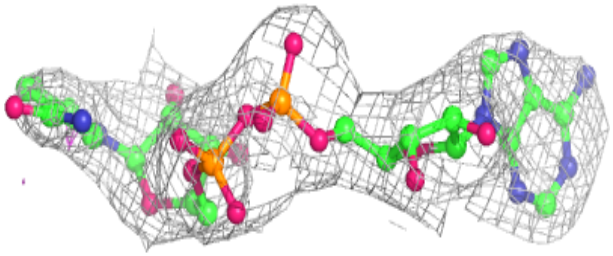


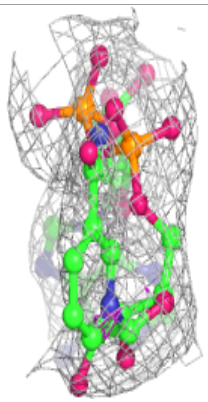


Electron density around NAD E 1001:

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

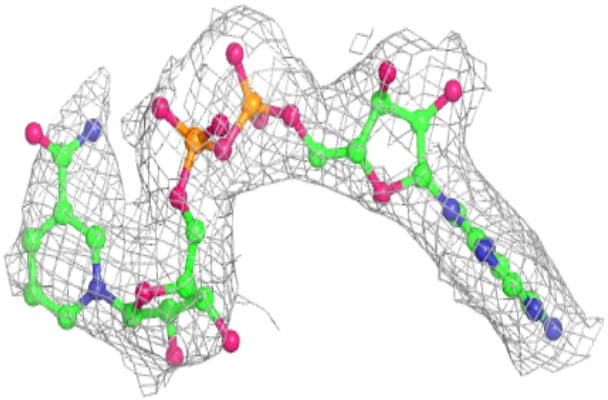


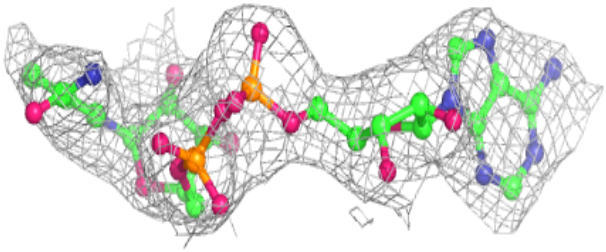


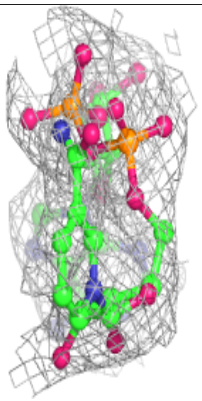


Electron density around NAD C 1001:

$2mF_o$-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.