



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:30 am BST

PDB ID : 1KQN
Title : Crystal structure of NMN/NaMN adenylyltransferase complexed with NAD
Authors : Zhou, T.; Kurnasov, O.; Tomchick, D.R.; Binns, D.D.; Grishin, N.V.; Marquez, V.E.; Osterman, A.L.; Zhang, H.
Deposited on : 2002-01-07
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

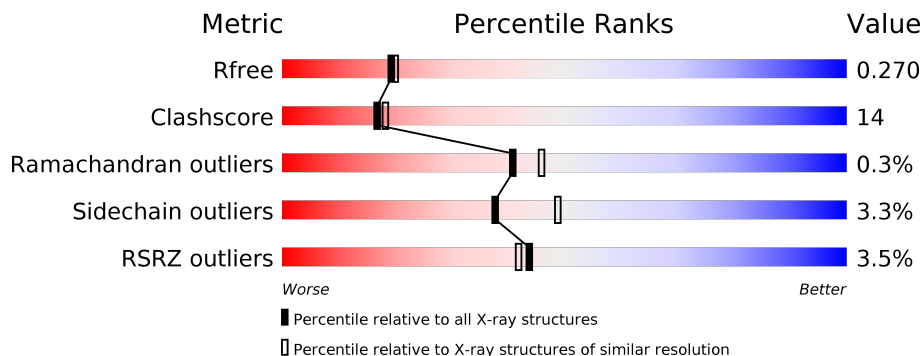
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	279	<p>0% 66% 15% 17%</p>
1	B	279	<p>3% 64% 16% 17%</p>
1	C	279	<p>0% 67% 15% 17%</p>
1	D	279	<p>3% 66% 16% 17%</p>
1	E	279	<p>4% 57% 25% 17%</p>
1	F	279	<p>5% 54% 26% 17%</p>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XE	A	749	-	-	X	-
3	XE	B	755	-	-	X	-
3	XE	D	761	-	-	X	-
3	XE	D	762	-	-	X	-
3	XE	E	757	-	-	X	-

2 Entry composition [i](#)

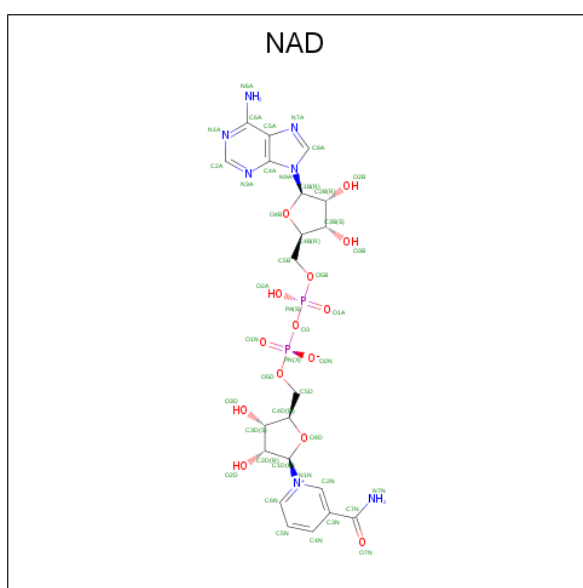
There are 4 unique types of molecules in this entry. The entry contains 12082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	Total 1866	C 1190	N 330	O 340	S 6	0	0	0
1	B	231	Total 1861	C 1187	N 329	O 339	S 6	0	0	0
1	C	231	Total 1861	C 1187	N 329	O 339	S 6	0	0	0
1	D	231	Total 1861	C 1187	N 329	O 339	S 6	0	0	0
1	E	232	Total 1866	C 1190	N 330	O 340	S 6	0	0	0
1	F	231	Total 1861	C 1187	N 329	O 339	S 6	0	0	0

- 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		

- Molecule 3 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Xe	0	0
			2	2		
3	E	2	Total	Xe	0	0
			2	2		
3	B	4	Total	Xe	0	0
			4	4		
3	C	3	Total	Xe	0	0
			3	3		
3	A	3	Total	Xe	0	0
			3	3		
3	F	1	Total	Xe	0	0
			1	1		

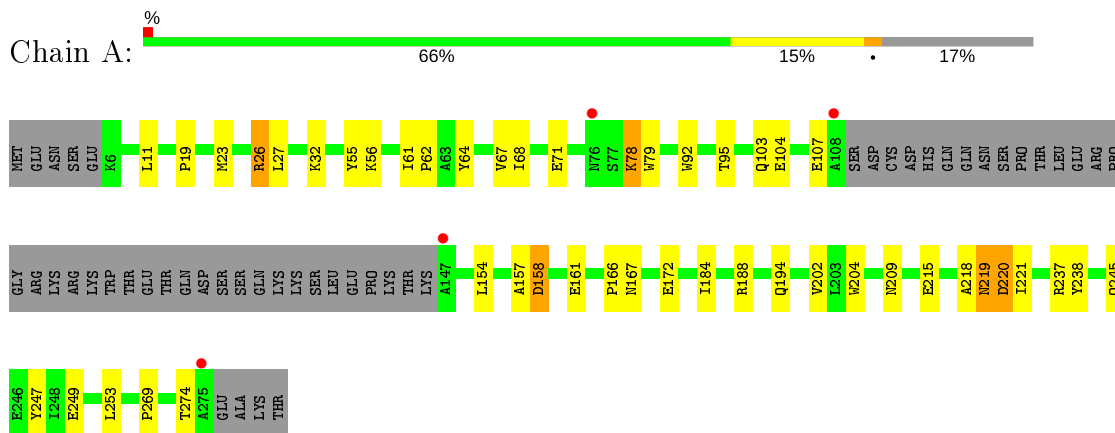
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	112	Total	O	0	0
			112	112		
4	C	144	Total	O	0	0
			144	144		
4	D	98	Total	O	0	0
			98	98		
4	E	81	Total	O	0	0
			81	81		
4	F	68	Total	O	0	0
			68	68		

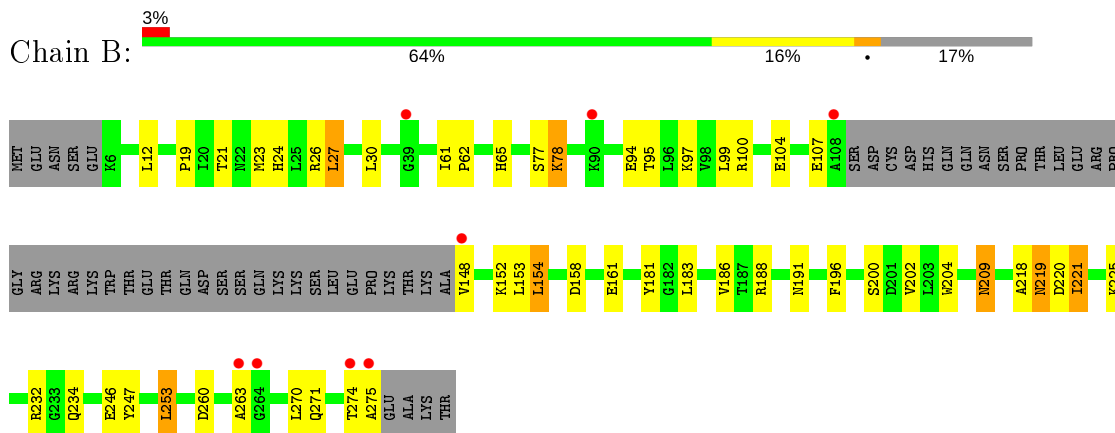
3 Residue-property plots [i](#)

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.

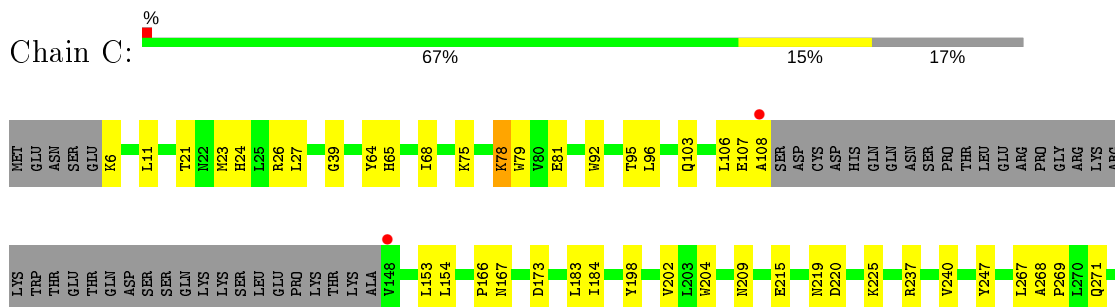
- Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE



- Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

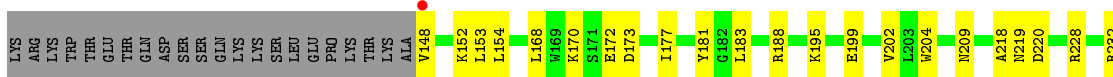


- Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

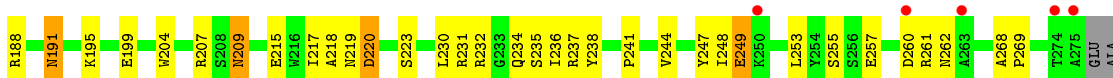
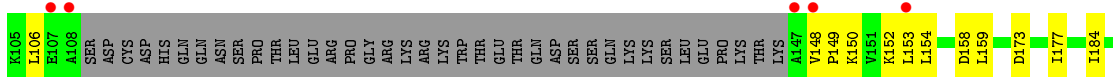




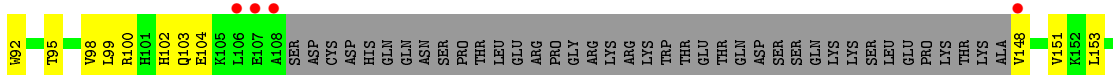
● Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE



● Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE



● Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE



2275
GLU
ALA
LYS
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.82Å 90.88Å 136.59Å 90.00° 116.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-2.20) 80.8 (20.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.19Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.250 0.237 , 0.270	Depositor DCC
R_{free} test set	6351 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.432	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.096 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, XE

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	0.71	1/1903 (0.1%)	0.80	1/2576 (0.0%)
1	B	0.67	0/1898	0.78	1/2569 (0.0%)
1	C	0.70	1/1898 (0.1%)	0.77	0/2569
1	D	0.67	0/1898	0.76	1/2569 (0.0%)
1	E	0.59	0/1903	0.75	0/2576
1	F	0.57	0/1898	0.77	2/2569 (0.1%)
All	All	0.65	2/11398 (0.0%)	0.77	5/15428 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	GLU	CG-CD	5.11	1.59	1.51
1	C	215	GLU	CG-CD	5.06	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	26	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	F	184	ILE	N-CA-C	-5.30	96.69	111.00
1	B	253	LEU	N-CA-C	5.26	125.22	111.00
1	A	26	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	26	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	1866	0	1897	46	0
1	B	1861	0	1892	64	0
1	C	1861	0	1892	40	0
1	D	1861	0	1892	49	0
1	E	1866	0	1897	73	0
1	F	1861	0	1892	76	0
2	A	44	0	26	1	0
2	B	44	0	26	5	0
2	C	44	0	26	3	0
2	D	44	0	26	4	0
2	E	44	0	26	3	0
2	F	44	0	26	2	0
3	A	3	0	0	3	0
3	B	4	0	0	3	0
3	C	3	0	0	1	0
3	D	2	0	0	5	0
3	E	2	0	0	6	0
3	F	1	0	0	1	0
4	A	124	0	0	8	0
4	B	112	0	0	10	0
4	C	144	0	0	8	0
4	D	98	0	0	7	0
4	E	81	0	0	6	0
4	F	68	0	0	6	0
All	All	12082	0	11518	324	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 14.

All (324) 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:23:MET:HG2	3:D:762:XE:XE	2.32	1.06
1:A:78:LYS:H	1:A:78:LYS:HD2	1.22	1.03
1:D:219:ASN:HB3	4:D:785:HOH:O	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LYS:HD2	1:C:78:LYS:H	1.26	1.01
1:B:21:THR:H	1:B:24:HIS:HD2	1.11	0.99
1:F:78:LYS:H	1:F:78:LYS:HD2	1.30	0.94
1:B:95:THR:H	2:B:778:NAD:H71N	1.17	0.91
1:D:27:LEU:HD22	3:D:761:XE:XE	2.49	0.91
1:B:12:LEU:HD23	1:B:99:LEU:HD23	1.53	0.88
1:C:21:THR:H	1:C:24:HIS:HD2	1.21	0.86
1:A:78:LYS:CD	1:A:78:LYS:H	1.85	0.86
1:B:219:ASN:HB3	4:B:871:HOH:O	1.76	0.86
1:B:27:LEU:HD22	3:B:760:XE:XE	2.55	0.84
1:C:78:LYS:N	1:C:78:LYS:HD2	1.91	0.83
1:C:95:THR:H	2:C:779:NAD:H71N	1.27	0.83
1:E:78:LYS:HD2	1:E:78:LYS:H	1.45	0.82
1:D:21:THR:H	1:D:24:HIS:HD2	1.24	0.82
1:F:78:LYS:H	1:F:78:LYS:CD	1.86	0.82
1:C:78:LYS:CD	1:C:78:LYS:H	1.82	0.82
1:A:78:LYS:N	1:A:78:LYS:HD2	1.95	0.81
1:E:21:THR:H	1:E:24:HIS:HD2	1.24	0.81
1:C:202:VAL:HG23	4:C:867:HOH:O	1.79	0.80
1:A:95:THR:H	2:A:777:NAD:H71N	1.29	0.80
1:F:188:ARG:HD2	1:F:218:ALA:HA	1.62	0.80
1:A:32:LYS:HE2	4:A:820:HOH:O	1.81	0.80
1:F:95:THR:H	2:F:782:NAD:H71N	1.30	0.80
1:B:78:LYS:CD	1:B:78:LYS:H	1.96	0.78
1:E:188:ARG:HH22	1:F:188:ARG:HH22	1.29	0.77
1:E:95:THR:H	2:E:781:NAD:H71N	1.33	0.76
1:E:65:HIS:HD2	1:E:247:TYR:OH	1.67	0.76
1:B:21:THR:H	1:B:24:HIS:CD2	2.02	0.76
1:D:234:GLN:HG2	4:D:797:HOH:O	1.84	0.76
1:C:65:HIS:HE1	4:C:877:HOH:O	1.68	0.76
1:A:245:GLN:O	1:A:249:GLU:HG2	1.86	0.76
1:E:78:LYS:HD2	1:E:78:LYS:N	2.01	0.76
1:F:65:HIS:HD2	1:F:247:TYR:OH	1.69	0.75
1:E:27:LEU:HD23	3:E:757:XE:XE	2.64	0.75
1:D:27:LEU:CD2	3:D:761:XE:XE	3.13	0.74
1:D:95:THR:H	2:D:780:NAD:H71N	1.35	0.74
1:F:27:LEU:HD23	4:F:783:HOH:O	1.86	0.74
1:E:27:LEU:CD2	3:E:757:XE:XE	3.14	0.73
1:F:268:ALA:HB3	1:F:269:PRO:HD3	1.71	0.73
1:F:64:TYR:O	1:F:68:ILE:HG12	1.89	0.72
1:B:234:GLN:HG2	4:B:821:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:LEU:HD23	1:D:99:LEU:HD23	1.72	0.72
1:A:202:VAL:HG23	4:A:856:HOH:O	1.89	0.72
1:B:220:ASP:CB	4:B:869:HOH:O	2.38	0.71
1:D:78:LYS:H	1:D:78:LYS:CD	2.03	0.71
1:F:92:TRP:CH2	1:F:269:PRO:HG3	2.24	0.71
1:F:189:ALA:O	1:F:192:ASP:OD1	2.09	0.71
1:B:21:THR:N	1:B:24:HIS:HD2	1.88	0.70
1:F:78:LYS:N	1:F:78:LYS:HD2	2.03	0.70
1:B:274:THR:HG22	1:B:275:ALA:N	2.07	0.69
1:D:270:LEU:O	1:D:274:THR:HB	1.92	0.69
1:B:220:ASP:C	4:B:869:HOH:O	2.31	0.68
1:F:67:VAL:O	1:F:71:GLU:HG3	1.93	0.68
1:C:65:HIS:HD2	1:C:247:TYR:OH	1.77	0.68
1:D:21:THR:N	1:D:24:HIS:HD2	1.92	0.68
1:F:92:TRP:CZ2	1:F:269:PRO:HG3	2.29	0.67
1:E:158:ASP:OD1	2:E:781:NAD:O2B	2.13	0.66
1:E:219:ASN:HB3	4:E:813:HOH:O	1.96	0.66
1:E:92:TRP:CH2	1:E:269:PRO:HG3	2.30	0.66
1:A:27:LEU:HD23	4:A:778:HOH:O	1.95	0.65
1:D:274:THR:HG22	1:D:275:ALA:N	2.10	0.65
1:C:21:THR:H	1:C:24:HIS:CD2	2.11	0.65
1:F:192:ASP:OD1	1:F:193:ALA:N	2.29	0.65
1:F:21:THR:H	1:F:24:HIS:HD2	1.43	0.65
1:E:21:THR:N	1:E:24:HIS:HD2	1.93	0.65
1:B:221:ILE:N	4:B:869:HOH:O	2.29	0.64
1:F:65:HIS:CD2	1:F:247:TYR:OH	2.50	0.63
1:D:148:VAL:N	4:D:809:HOH:O	2.31	0.63
1:D:172:GLU:H	1:D:172:GLU:CD	2.02	0.63
1:E:92:TRP:CZ2	1:E:269:PRO:HG3	2.34	0.63
1:C:153:LEU:HD23	1:C:183:LEU:HD22	1.80	0.62
1:F:23:MET:HG2	3:F:756:XE:XE	2.77	0.62
1:B:107:GLU:HG2	1:B:148:VAL:HG11	1.80	0.62
1:B:152:LYS:NZ	1:B:209:ASN:HD21	1.97	0.62
1:A:92:TRP:CH2	1:A:269:PRO:HG3	2.34	0.62
1:E:53:ASP:OD1	1:E:63:ALA:N	2.30	0.62
1:D:204:TRP:CD1	1:E:232:ARG:HD3	2.35	0.62
1:B:161:GLU:HG2	1:B:196:PHE:CD1	2.35	0.61
1:E:16:SER:HA	1:E:51:VAL:HG12	1.83	0.61
1:A:158:ASP:HB2	4:A:857:HOH:O	2.00	0.61
1:B:65:HIS:HD2	1:B:247:TYR:OH	1.83	0.61
1:A:194:GLN:NE2	4:A:854:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HG2	4:B:870:HOH:O	2.00	0.61
1:B:186:VAL:O	2:B:778:NAD:H2A	2.00	0.61
1:E:27:LEU:HB3	3:E:757:XE:XE	2.79	0.61
1:D:103:GLN:O	1:D:107:GLU:HG3	2.00	0.61
1:D:228:ARG:HD2	1:D:232:ARG:NH2	2.17	0.60
1:F:188:ARG:HD2	1:F:218:ALA:CA	2.31	0.60
1:F:220:ASP:HB2	4:F:837:HOH:O	2.02	0.60
1:B:148:VAL:N	4:B:843:HOH:O	2.34	0.60
1:E:218:ALA:O	1:F:220:ASP:HB3	2.02	0.60
1:F:245:GLN:O	1:F:249:GLU:HG2	2.01	0.60
1:F:22:ASN:O	1:F:26:ARG:HB2	2.02	0.59
1:B:220:ASP:HB3	4:B:869:HOH:O	1.98	0.59
1:D:27:LEU:HD12	3:D:762:XE:XE	2.80	0.59
1:D:78:LYS:HD2	1:D:78:LYS:H	1.64	0.59
1:E:204:TRP:O	1:E:207:ARG:HB3	2.02	0.59
1:F:228:ARG:HD2	1:F:232:ARG:NH2	2.18	0.59
1:B:220:ASP:CG	4:B:869:HOH:O	2.41	0.59
1:F:45:LYS:HD2	4:F:845:HOH:O	2.02	0.59
1:F:21:THR:HA	1:F:240:VAL:HG12	1.85	0.58
1:A:204:TRP:CD1	1:D:232:ARG:HD3	2.37	0.58
1:A:188:ARG:CZ	1:A:218:ALA:HB1	2.33	0.58
1:E:219:ASN:OD1	1:F:219:ASN:HA	2.03	0.58
1:E:268:ALA:HB3	1:E:269:PRO:HD3	1.85	0.58
1:F:153:LEU:HD23	1:F:183:LEU:CD2	2.33	0.58
1:F:47:ILE:HD11	4:F:845:HOH:O	2.02	0.58
1:E:158:ASP:OD1	1:E:159:LEU:N	2.35	0.57
1:E:78:LYS:CD	1:E:78:LYS:H	2.06	0.57
1:B:204:TRP:CD1	1:F:232:ARG:HD3	2.40	0.57
1:A:103:GLN:O	1:A:107:GLU:HG3	2.04	0.56
1:F:63:ALA:O	1:F:67:VAL:HG23	2.05	0.56
1:E:21:THR:H	1:E:24:HIS:CD2	2.15	0.56
1:C:219:ASN:HB3	4:C:806:HOH:O	2.04	0.56
1:A:11:LEU:HD22	1:A:184:ILE:HD12	1.88	0.56
1:A:64:TYR:CE2	1:A:68:ILE:HD11	2.41	0.55
1:D:168:LEU:O	2:D:780:NAD:H4N	2.06	0.55
1:C:27:LEU:HD23	4:C:780:HOH:O	2.05	0.55
1:D:188:ARG:CZ	1:D:218:ALA:HB1	2.36	0.55
1:A:157:ALA:O	1:A:161:GLU:HG3	2.05	0.55
1:A:92:TRP:CZ2	1:A:269:PRO:HG3	2.42	0.55
1:F:173:ASP:O	1:F:177:ILE:HG13	2.07	0.55
1:F:21:THR:N	1:F:24:HIS:HD2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LEU:HD22	3:E:757:XE:XE	2.85	0.55
1:E:23:MET:HG2	3:E:758:XE:XE	2.84	0.55
1:A:188:ARG:HD2	4:A:853:HOH:O	2.06	0.55
1:F:61:ILE:HB	1:F:62:PRO:CD	2.37	0.55
1:B:78:LYS:HD2	1:B:78:LYS:H	1.70	0.54
1:B:191:ASN:ND2	1:E:191:ASN:H	2.05	0.54
1:E:217:ILE:O	1:E:217:ILE:HG22	2.05	0.54
1:A:188:ARG:NH2	1:B:188:ARG:HH12	2.06	0.54
1:F:60:LEU:HD11	1:F:66:ARG:CZ	2.38	0.54
1:F:16:SER:HA	1:F:51:VAL:HG12	1.89	0.54
1:A:67:VAL:O	1:A:71:GLU:HG3	2.08	0.54
1:F:23:MET:CG	1:F:219:ASN:HD22	2.20	0.54
1:F:60:LEU:O	1:F:261:ARG:HD3	2.08	0.54
1:E:65:HIS:CD2	1:E:247:TYR:OH	2.55	0.53
1:A:219:ASN:ND2	1:A:221:ILE:HG13	2.22	0.53
1:D:170:LYS:HB3	1:D:172:GLU:OE1	2.09	0.53
1:D:152:LYS:HD3	1:D:181:TYR:O	2.08	0.53
1:C:78:LYS:HE3	1:D:237:ARG:HH12	1.74	0.53
1:B:152:LYS:HZ1	1:B:209:ASN:HD21	1.56	0.53
1:D:195:LYS:O	1:D:199:GLU:HG3	2.08	0.53
1:C:103:GLN:O	1:C:107:GLU:HG3	2.09	0.53
1:B:77:SER:HA	1:B:78:LYS:HE3	1.92	0.52
1:A:172:GLU:CD	1:A:172:GLU:H	2.12	0.52
1:C:219:ASN:CB	4:C:806:HOH:O	2.56	0.52
1:C:21:THR:N	1:C:24:HIS:HD2	2.00	0.52
1:E:230:LEU:HD21	1:E:236:ILE:HD13	1.91	0.52
1:B:191:ASN:HD21	1:E:191:ASN:H	1.57	0.52
1:B:27:LEU:HD11	2:B:778:NAD:N3A	2.23	0.52
1:E:11:LEU:HD22	1:E:184:ILE:HD12	1.91	0.52
1:E:78:LYS:NZ	4:E:814:HOH:O	2.40	0.52
1:D:202:VAL:HG23	4:D:851:HOH:O	2.09	0.52
1:F:103:GLN:OE1	1:F:151:VAL:HG12	2.10	0.52
1:E:152:LYS:NZ	1:E:209:ASN:HD21	2.07	0.52
1:F:244:VAL:O	1:F:248:ILE:HG13	2.09	0.52
1:A:237:ARG:O	1:A:238:TYR:HB2	2.10	0.51
1:B:271:GLN:O	1:B:275:ALA:HB2	2.10	0.51
1:F:217:ILE:O	1:F:217:ILE:HG22	2.10	0.51
1:B:78:LYS:CE	1:B:78:LYS:H	2.22	0.51
1:B:100:ARG:O	1:B:104:GLU:HG3	2.11	0.51
1:D:173:ASP:O	1:D:177:ILE:HG13	2.11	0.51
1:A:274:THR:HG22	1:A:274:THR:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD12	3:A:749:XE:XE	2.88	0.51
1:E:25:LEU:HD11	1:E:73:ALA:HB1	1.92	0.51
1:C:95:THR:OG1	2:C:779:NAD:H2N	2.11	0.51
1:E:10:VAL:HG21	1:E:106:LEU:HD11	1.93	0.51
1:E:27:LEU:CB	3:E:757:XE:XE	3.37	0.51
1:B:78:LYS:HE3	1:B:78:LYS:H	1.76	0.50
1:B:232:ARG:HD3	1:C:204:TRP:CD1	2.47	0.50
1:E:188:ARG:HD2	1:E:218:ALA:CB	2.41	0.50
1:F:202:VAL:HG23	4:F:823:HOH:O	2.10	0.50
1:F:65:HIS:O	1:F:69:MET:HG3	2.12	0.50
1:C:11:LEU:CD2	1:C:184:ILE:HD12	2.42	0.50
1:E:247:TYR:CE2	1:E:253:LEU:HD11	2.47	0.50
1:C:78:LYS:HD3	1:C:79:TRP:HD1	1.77	0.50
1:D:21:THR:H	1:D:24:HIS:CD2	2.15	0.50
1:D:170:LYS:O	1:D:173:ASP:HB2	2.12	0.49
1:C:64:TYR:CE2	1:C:68:ILE:HD11	2.47	0.49
1:A:237:ARG:HG2	1:A:238:TYR:CE1	2.47	0.49
1:F:247:TYR:CE2	1:F:253:LEU:HD11	2.47	0.49
1:E:83:ASP:OD1	1:E:102:HIS:HE1	1.94	0.48
1:B:152:LYS:HD3	1:B:181:TYR:O	2.12	0.48
1:E:173:ASP:O	1:E:177:ILE:HG13	2.13	0.48
1:B:27:LEU:HD23	1:B:154:LEU:CD2	2.43	0.48
1:C:271:GLN:NE2	4:C:921:HOH:O	2.46	0.48
1:E:69:MET:HB3	1:E:244:VAL:HG13	1.95	0.48
1:A:219:ASN:HA	1:B:219:ASN:ND2	2.29	0.48
1:D:12:LEU:HD23	1:D:99:LEU:CD2	2.42	0.48
1:E:30:LEU:HD11	1:E:215:GLU:CD	2.33	0.48
1:F:40:ARG:NH1	1:F:40:ARG:HG2	2.29	0.48
1:B:23:MET:HG2	3:B:755:XE:XE	2.92	0.48
1:B:270:LEU:O	1:B:274:THR:HB	2.14	0.48
1:F:32:LYS:HA	1:F:43:VAL:HG21	1.95	0.48
1:E:104:GLU:HG2	4:E:856:HOH:O	2.13	0.48
1:E:53:ASP:CG	1:E:63:ALA:H	2.18	0.48
1:F:21:THR:H	1:F:24:HIS:CD2	2.29	0.48
1:B:161:GLU:HA	1:B:196:PHE:CZ	2.49	0.47
1:F:26:ARG:HD2	1:F:26:ARG:HA	1.64	0.47
1:D:83:ASP:CG	1:D:102:HIS:HE1	2.17	0.47
1:D:27:LEU:HD11	2:D:780:NAD:C2A	2.43	0.47
1:E:11:LEU:CD2	1:E:184:ILE:HD12	2.44	0.47
1:C:75:LYS:HB3	4:C:917:HOH:O	2.14	0.47
1:D:220:ASP:O	1:D:220:ASP:CG	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:CD2	1:A:184:ILE:HD12	2.44	0.47
1:D:274:THR:CG2	1:D:275:ALA:N	2.78	0.47
1:B:27:LEU:HD12	3:B:755:XE:XE	2.93	0.47
1:F:40:ARG:HH11	1:F:40:ARG:HG2	1.80	0.47
1:E:261:ARG:O	1:E:262:ASN:HB2	2.15	0.46
1:E:219:ASN:ND2	1:F:221:ILE:HD11	2.29	0.46
1:F:148:VAL:HB	4:F:849:HOH:O	2.14	0.46
1:B:153:LEU:HD23	1:B:183:LEU:HD21	1.98	0.46
1:F:217:ILE:O	1:F:219:ASN:N	2.49	0.46
1:B:26:ARG:HA	1:B:26:ARG:HD2	1.77	0.46
1:A:220:ASP:CG	1:A:220:ASP:O	2.53	0.46
1:E:78:LYS:HD3	1:E:79:TRP:HD1	1.81	0.46
1:F:215:GLU:O	1:F:215:GLU:CG	2.64	0.46
1:F:168:LEU:HD11	2:F:782:NAD:H5N	1.98	0.46
1:D:78:LYS:HD2	1:D:79:TRP:HD1	1.80	0.46
1:A:247:TYR:CE2	1:A:253:LEU:HD11	2.51	0.46
1:A:32:LYS:HD3	4:A:886:HOH:O	2.15	0.46
1:C:106:LEU:C	1:C:108:ALA:H	2.20	0.45
1:F:188:ARG:CZ	1:F:218:ALA:HB1	2.46	0.45
1:F:237:ARG:O	1:F:238:TYR:HB2	2.16	0.45
1:A:188:ARG:NH2	1:B:188:ARG:NH1	2.64	0.45
1:B:12:LEU:HD23	1:B:99:LEU:CD2	2.37	0.45
1:E:209:ASN:HA	1:E:209:ASN:HD22	1.61	0.45
1:F:100:ARG:O	1:F:104:GLU:HG3	2.16	0.45
1:D:27:LEU:HD23	3:D:761:XE:XE	2.93	0.45
1:A:27:LEU:CD1	3:A:749:XE:XE	3.43	0.45
1:B:188:ARG:CZ	1:B:218:ALA:HB1	2.45	0.45
1:D:106:LEU:C	1:D:108:ALA:H	2.19	0.45
1:E:188:ARG:HD2	1:E:218:ALA:HB1	1.99	0.45
1:C:166:PRO:O	1:C:167:ASN:HB2	2.16	0.45
1:C:92:TRP:CH2	1:C:269:PRO:HG3	2.51	0.45
1:E:248:ILE:HG23	1:E:253:LEU:HB2	1.98	0.45
1:B:61:ILE:HB	1:B:62:PRO:CD	2.47	0.45
1:E:148:VAL:HA	1:E:149:PRO:HD3	1.87	0.45
1:E:81:GLU:OE2	4:E:860:HOH:O	2.21	0.45
1:A:55:TYR:O	1:A:56:LYS:HB2	2.18	0.44
1:C:78:LYS:HE3	1:D:237:ARG:NH1	2.32	0.44
1:C:96:LEU:HD22	1:C:173:ASP:HA	1.98	0.44
1:E:12:LEU:O	1:E:153:LEU:HD12	2.17	0.44
1:F:11:LEU:HD22	1:F:184:ILE:HD12	1.98	0.44
1:A:166:PRO:O	1:A:167:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ARG:HH11	1:D:78:LYS:NZ	2.15	0.44
1:B:274:THR:HG22	1:B:275:ALA:H	1.79	0.44
1:B:191:ASN:HD22	1:E:191:ASN:HB2	1.82	0.44
1:E:219:ASN:HD22	1:F:221:ILE:HD11	1.83	0.44
1:E:237:ARG:O	1:E:238:TYR:HB2	2.18	0.44
1:E:32:LYS:HA	1:E:43:VAL:HG21	1.99	0.44
1:F:151:VAL:HG13	1:F:151:VAL:O	2.17	0.44
1:F:170:LYS:O	1:F:173:ASP:HB2	2.17	0.44
1:D:78:LYS:NZ	4:D:855:HOH:O	2.50	0.44
1:E:191:ASN:HB3	4:E:810:HOH:O	2.18	0.44
1:F:153:LEU:HB3	1:F:183:LEU:HD23	1.99	0.44
1:E:9:VAL:HG23	1:E:150:LYS:O	2.18	0.44
1:A:188:ARG:HH22	1:B:188:ARG:NH1	2.16	0.43
1:A:26:ARG:HA	1:A:26:ARG:HD2	1.73	0.43
1:D:228:ARG:HD3	4:D:790:HOH:O	2.18	0.43
1:E:231:ARG:HG2	1:E:255:SER:HA	2.00	0.43
1:A:219:ASN:HD21	1:A:221:ILE:HG13	1.83	0.43
1:A:23:MET:HG2	3:A:749:XE:XE	2.96	0.43
1:C:21:THR:HA	1:C:240:VAL:HG12	2.01	0.43
1:E:95:THR:OG1	2:E:781:NAD:H1D	2.19	0.43
1:D:26:ARG:HD2	1:D:26:ARG:HA	1.85	0.43
1:C:268:ALA:HB3	1:C:269:PRO:HD3	1.99	0.43
1:E:220:ASP:O	1:E:220:ASP:CG	2.57	0.43
1:F:153:LEU:HD23	1:F:183:LEU:HD21	1.98	0.43
1:F:251:HIS:O	1:F:252:ASN:C	2.57	0.43
1:F:260:ASP:O	1:F:263:ALA:HB2	2.19	0.43
1:C:267:LEU:HG	1:C:269:PRO:HD2	2.01	0.43
1:B:27:LEU:HD23	1:B:154:LEU:HD22	2.01	0.42
1:E:9:VAL:HG21	1:E:152:LYS:HG3	2.01	0.42
1:D:65:HIS:HD2	1:D:247:TYR:OH	2.02	0.42
1:D:23:MET:HE1	2:D:780:NAD:N7A	2.34	0.42
1:F:65:HIS:HD2	1:F:247:TYR:CZ	2.38	0.42
1:A:104:GLU:HA	1:A:107:GLU:HG3	2.01	0.42
1:B:260:ASP:O	1:B:263:ALA:HB2	2.19	0.42
1:B:271:GLN:HE21	1:B:275:ALA:HB2	1.84	0.42
1:C:65:HIS:CD2	1:C:247:TYR:OH	2.65	0.42
1:F:64:TYR:C	1:F:64:TYR:CD2	2.93	0.42
1:D:153:LEU:HD23	1:D:183:LEU:HD21	2.01	0.42
1:A:103:GLN:O	1:A:107:GLU:CG	2.66	0.42
1:B:191:ASN:H	1:E:191:ASN:ND2	2.18	0.42
1:E:234:GLN:HA	1:F:33:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:HA	1:C:26:ARG:HD2	1.84	0.42
1:F:60:LEU:HD11	1:F:66:ARG:NE	2.35	0.42
1:C:6:LYS:HE2	1:C:39:GLY:O	2.19	0.42
1:E:195:LYS:HE2	1:E:199:GLU:OE2	2.20	0.42
1:D:16:SER:O	1:D:17:PHE:C	2.58	0.41
1:E:223:SER:HB2	4:E:854:HOH:O	2.19	0.41
1:E:241:PRO:HD2	1:E:244:VAL:CG2	2.50	0.41
1:C:95:THR:N	2:C:779:NAD:H71N	2.07	0.41
1:E:36:ASN:OD1	1:E:43:VAL:HG23	2.20	0.41
1:F:12:LEU:HD23	1:F:99:LEU:HD23	2.02	0.41
1:B:225:LYS:HG2	1:C:198:TYR:OH	2.19	0.41
1:C:220:ASP:OD2	1:C:225:LYS:NZ	2.53	0.41
1:E:247:TYR:HE2	1:E:253:LEU:HD11	1.85	0.41
1:F:49:SER:OG	1:F:86:GLU:OE2	2.37	0.41
1:B:220:ASP:O	1:B:221:ILE:C	2.58	0.41
4:C:909:HOH:O	1:D:218:ALA:CB	2.69	0.41
1:A:32:LYS:HD2	1:A:79:TRP:CZ2	2.56	0.41
1:A:188:ARG:HH22	1:B:188:ARG:CZ	2.33	0.41
1:B:188:ARG:NE	1:B:218:ALA:HB1	2.35	0.41
1:F:98:VAL:O	1:F:102:HIS:HD2	2.03	0.41
1:B:253:LEU:HA	1:B:253:LEU:HD23	1.85	0.41
1:A:61:ILE:HB	1:A:62:PRO:CD	2.51	0.41
1:B:30:LEU:HD11	4:B:782:HOH:O	2.21	0.41
1:B:94:GLU:OE1	1:B:97:LYS:HD2	2.20	0.41
1:B:95:THR:N	2:B:778:NAD:N7N	2.65	0.40
1:A:27:LEU:CD2	4:A:778:HOH:O	2.61	0.40
1:B:27:LEU:HD11	2:B:778:NAD:C2A	2.51	0.40
1:E:25:LEU:HD13	1:F:238:TYR:CE2	2.55	0.40
1:F:221:ILE:HG22	1:F:221:ILE:O	2.20	0.40
1:F:55:TYR:O	1:F:56:LYS:HB2	2.22	0.40
1:C:23:MET:HG2	3:C:753:XE:XE	3.00	0.40
1:D:219:ASN:ND2	4:D:860:HOH:O	2.54	0.40
1:C:153:LEU:HD23	1:C:183:LEU:CD2	2.48	0.40
1:F:45:LYS:HB2	1:F:45:LYS:HE3	1.94	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	228/279 (82%)	221 (97%)	7 (3%)	0	100	100
1	B	227/279 (81%)	214 (94%)	12 (5%)	1 (0%)	34	37
1	C	227/279 (81%)	222 (98%)	5 (2%)	0	100	100
1	D	227/279 (81%)	215 (95%)	12 (5%)	0	100	100
1	E	228/279 (82%)	217 (95%)	10 (4%)	1 (0%)	34	37
1	F	227/279 (81%)	215 (95%)	10 (4%)	2 (1%)	17	16
All	All	1364/1674 (82%)	1304 (96%)	56 (4%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	221	ILE
1	F	218	ALA
1	E	249	GLU
1	F	221	ILE

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	203/248 (82%)	196 (97%)	7 (3%)	37	47
1	B	203/248 (82%)	193 (95%)	10 (5%)	25	31
1	C	203/248 (82%)	199 (98%)	4 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	203/248 (82%)	197 (97%)	6 (3%)	41	53
1	E	203/248 (82%)	194 (96%)	9 (4%)	28	35
1	F	203/248 (82%)	199 (98%)	4 (2%)	55	69
All	All	1218/1488 (82%)	1178 (97%)	40 (3%)	38	49

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	A	78	LYS
1	A	154	LEU
1	A	158	ASP
1	A	209	ASN
1	A	219	ASN
1	A	220	ASP
1	B	19	PRO
1	B	27	LEU
1	B	78	LYS
1	B	154	LEU
1	B	158	ASP
1	B	200	SER
1	B	202	VAL
1	B	209	ASN
1	B	219	ASN
1	B	246	GLU
1	C	78	LYS
1	C	81	GLU
1	C	154	LEU
1	C	209	ASN
1	D	9	VAL
1	D	27	LEU
1	D	78	LYS
1	D	154	LEU
1	D	209	ASN
1	D	274	THR
1	E	78	LYS
1	E	154	LEU
1	E	191	ASN
1	E	209	ASN
1	E	220	ASP
1	E	235	SER

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Mol	Chain	Res	Type
1	E	249	GLU
1	E	257	GLU
1	E	260	ASP
1	F	78	LYS
1	F	209	ASN
1	F	219	ASN
1	F	260	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	209	ASN
1	A	219	ASN
1	B	24	HIS
1	B	65	HIS
1	B	191	ASN
1	B	209	ASN
1	B	214	ASN
1	B	219	ASN
1	B	271	GLN
1	C	24	HIS
1	C	65	HIS
1	C	89	GLN
1	C	101	HIS
1	C	102	HIS
1	C	206	HIS
1	C	251	HIS
1	D	24	HIS
1	D	65	HIS
1	D	76	ASN
1	D	102	HIS
1	D	209	ASN
1	D	219	ASN
1	E	24	HIS
1	E	65	HIS
1	E	101	HIS
1	E	102	HIS
1	E	191	ASN
1	E	209	ASN
1	E	245	GLN
1	E	273	ASN

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Mol	Chain	Res	Type
1	F	24	HIS
1	F	65	HIS
1	F	101	HIS
1	F	102	HIS
1	F	206	HIS
1	F	209	ASN
1	F	219	ASN
1	F	245	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	F	782	-	42,48,48	1.91	7 (16%)	50,73,73	1.68	8 (16%)
2	NAD	C	779	-	42,48,48	2.09	9 (21%)	50,73,73	1.78	7 (14%)
2	NAD	D	780	-	42,48,48	2.02	7 (16%)	50,73,73	1.63	7 (14%)
2	NAD	A	777	-	42,48,48	1.94	7 (16%)	50,73,73	1.71	9 (18%)
2	NAD	B	778	-	42,48,48	2.07	7 (16%)	50,73,73	1.82	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	E	781	-	42,48,48	1.92	8 (19%)	50,73,73	1.75	9 (18%)

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	F	782	-	-	4/26/62/62	0/5/5/5
2	NAD	C	779	-	-	4/26/62/62	0/5/5/5
2	NAD	D	780	-	-	5/26/62/62	0/5/5/5
2	NAD	A	777	-	-	3/26/62/62	0/5/5/5
2	NAD	B	778	-	-	3/26/62/62	0/5/5/5
2	NAD	E	781	-	-	3/26/62/62	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	780	NAD	C5N-C4N	6.80	1.53	1.38
2	F	782	NAD	C5N-C4N	6.46	1.52	1.38
2	B	778	NAD	C5N-C4N	6.39	1.52	1.38
2	D	780	NAD	C4N-C3N	6.19	1.49	1.39
2	E	781	NAD	C5N-C4N	6.17	1.51	1.38
2	C	779	NAD	C5N-C4N	6.12	1.51	1.38
2	A	777	NAD	C5N-C4N	6.05	1.51	1.38
2	B	778	NAD	C4N-C3N	6.04	1.49	1.39
2	F	782	NAD	C4N-C3N	5.75	1.49	1.39
2	A	777	NAD	C4N-C3N	5.64	1.49	1.39
2	E	781	NAD	C4N-C3N	5.49	1.48	1.39
2	C	779	NAD	C2N-N1N	5.20	1.41	1.35
2	B	778	NAD	C2N-C3N	5.06	1.46	1.39
2	C	779	NAD	C4N-C3N	4.95	1.47	1.39
2	C	779	NAD	C2N-C3N	4.77	1.46	1.39
2	A	777	NAD	C2N-N1N	4.35	1.40	1.35
2	D	780	NAD	C2N-N1N	4.31	1.40	1.35
2	B	778	NAD	C2N-N1N	4.29	1.40	1.35
2	F	782	NAD	C2N-C3N	4.03	1.45	1.39
2	D	780	NAD	C6N-N1N	3.99	1.45	1.35
2	E	781	NAD	O4B-C1B	-3.75	1.35	1.41
2	D	780	NAD	C2N-C3N	3.74	1.44	1.39
2	E	781	NAD	C6N-N1N	3.66	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	780	NAD	O4B-C1B	-3.65	1.36	1.41
2	B	778	NAD	C6N-N1N	3.65	1.44	1.35
2	E	781	NAD	C2N-C3N	3.64	1.44	1.39
2	F	782	NAD	C6N-N1N	3.62	1.44	1.35
2	A	777	NAD	C2N-C3N	3.60	1.44	1.39
2	C	779	NAD	O4B-C1B	-3.57	1.36	1.41
2	F	782	NAD	C2N-N1N	3.28	1.39	1.35
2	A	777	NAD	C6N-N1N	3.22	1.43	1.35
2	C	779	NAD	C6N-N1N	3.00	1.42	1.35
2	B	778	NAD	O4B-C1B	-2.96	1.36	1.41
2	E	781	NAD	C2N-N1N	2.92	1.38	1.35
2	A	777	NAD	O4B-C1B	-2.76	1.37	1.41
2	F	782	NAD	C7N-N7N	2.52	1.37	1.33
2	F	782	NAD	O4B-C1B	-2.48	1.37	1.41
2	D	780	NAD	C6N-C5N	-2.41	1.33	1.38
2	B	778	NAD	C2A-N1A	2.39	1.38	1.33
2	C	779	NAD	C6N-C5N	-2.37	1.33	1.38
2	E	781	NAD	C2A-N1A	2.37	1.38	1.33
2	C	779	NAD	C2A-N1A	2.31	1.38	1.33
2	A	777	NAD	C7N-N7N	2.29	1.37	1.33
2	E	781	NAD	C7N-N7N	2.22	1.37	1.33
2	C	779	NAD	C2D-C3D	-2.08	1.47	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	779	NAD	C3N-C7N-N7N	6.17	125.16	117.75
2	C	779	NAD	O7N-C7N-C3N	-6.10	112.34	119.63
2	B	778	NAD	C3N-C7N-N7N	5.74	124.64	117.75
2	B	778	NAD	O7N-C7N-C3N	-5.50	113.05	119.63
2	E	781	NAD	O7N-C7N-C3N	-5.42	113.14	119.63
2	A	777	NAD	O7N-C7N-C3N	-5.30	113.29	119.63
2	D	780	NAD	C3N-C7N-N7N	5.17	123.95	117.75
2	E	781	NAD	C3N-C7N-N7N	5.05	123.82	117.75
2	F	782	NAD	O7N-C7N-C3N	-4.96	113.69	119.63
2	A	777	NAD	C3N-C7N-N7N	4.74	123.44	117.75
2	D	780	NAD	O7N-C7N-C3N	-4.72	113.98	119.63
2	F	782	NAD	C5N-C4N-C3N	-4.50	115.02	120.34
2	E	781	NAD	O4B-C1B-C2B	-4.23	100.75	106.93
2	B	778	NAD	O4B-C1B-C2B	-4.17	100.83	106.93
2	A	777	NAD	O4B-C1B-C2B	-4.15	100.86	106.93
2	E	781	NAD	C5N-C4N-C3N	-4.13	115.45	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	779	NAD	O4B-C1B-C2B	-4.13	100.89	106.93
2	B	778	NAD	C5N-C4N-C3N	-3.91	115.72	120.34
2	F	782	NAD	C3N-C7N-N7N	3.82	122.34	117.75
2	E	781	NAD	C6N-N1N-C2N	-3.72	118.58	121.97
2	F	782	NAD	C6N-N1N-C2N	-3.72	118.58	121.97
2	D	780	NAD	O4B-C1B-C2B	-3.72	101.50	106.93
2	A	777	NAD	C5N-C4N-C3N	-3.63	116.05	120.34
2	D	780	NAD	C6N-N1N-C2N	-3.57	118.72	121.97
2	F	782	NAD	O4B-C1B-C2B	-3.47	101.86	106.93
2	F	782	NAD	C5A-C6A-N6A	3.47	125.62	120.35
2	B	778	NAD	C6N-N1N-C2N	-3.46	118.82	121.97
2	D	780	NAD	C5N-C4N-C3N	-3.44	116.27	120.34
2	B	778	NAD	C5A-C6A-N6A	3.29	125.36	120.35
2	C	779	NAD	C5A-C6A-N6A	3.27	125.32	120.35
2	A	777	NAD	C6N-N1N-C2N	-3.16	119.09	121.97
2	A	777	NAD	C5A-C6A-N6A	3.06	125.00	120.35
2	D	780	NAD	C5A-C6A-N6A	3.05	124.98	120.35
2	C	779	NAD	C5N-C4N-C3N	-3.04	116.74	120.34
2	B	778	NAD	C5N-C6N-N1N	2.85	124.49	120.40
2	C	779	NAD	C6N-N1N-C2N	-2.82	119.40	121.97
2	E	781	NAD	C5A-C6A-N6A	2.77	124.56	120.35
2	D	780	NAD	C5N-C6N-N1N	2.75	124.35	120.40
2	C	779	NAD	C5N-C6N-N1N	2.70	124.27	120.40
2	E	781	NAD	C5N-C6N-N1N	2.60	124.12	120.40
2	F	782	NAD	C5N-C6N-N1N	2.51	124.00	120.40
2	A	777	NAD	C5N-C6N-N1N	2.44	123.91	120.40
2	A	777	NAD	C4A-C5A-N7A	2.33	111.83	109.40
2	B	778	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
2	F	782	NAD	O2N-PN-O5D	2.22	118.04	107.75
2	E	781	NAD	O2N-PN-O5D	2.04	117.21	107.75
2	A	777	NAD	O4D-C1D-C2D	-2.04	103.95	106.93
2	E	781	NAD	C4A-C5A-N7A	2.03	111.51	109.40

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	780	NAD	O4D-C4D-C5D-O5D
2	E	781	NAD	O4D-C4D-C5D-O5D
2	F	782	NAD	O4D-C4D-C5D-O5D
2	F	782	NAD	C3D-C4D-C5D-O5D
2	C	779	NAD	O4D-C4D-C5D-O5D

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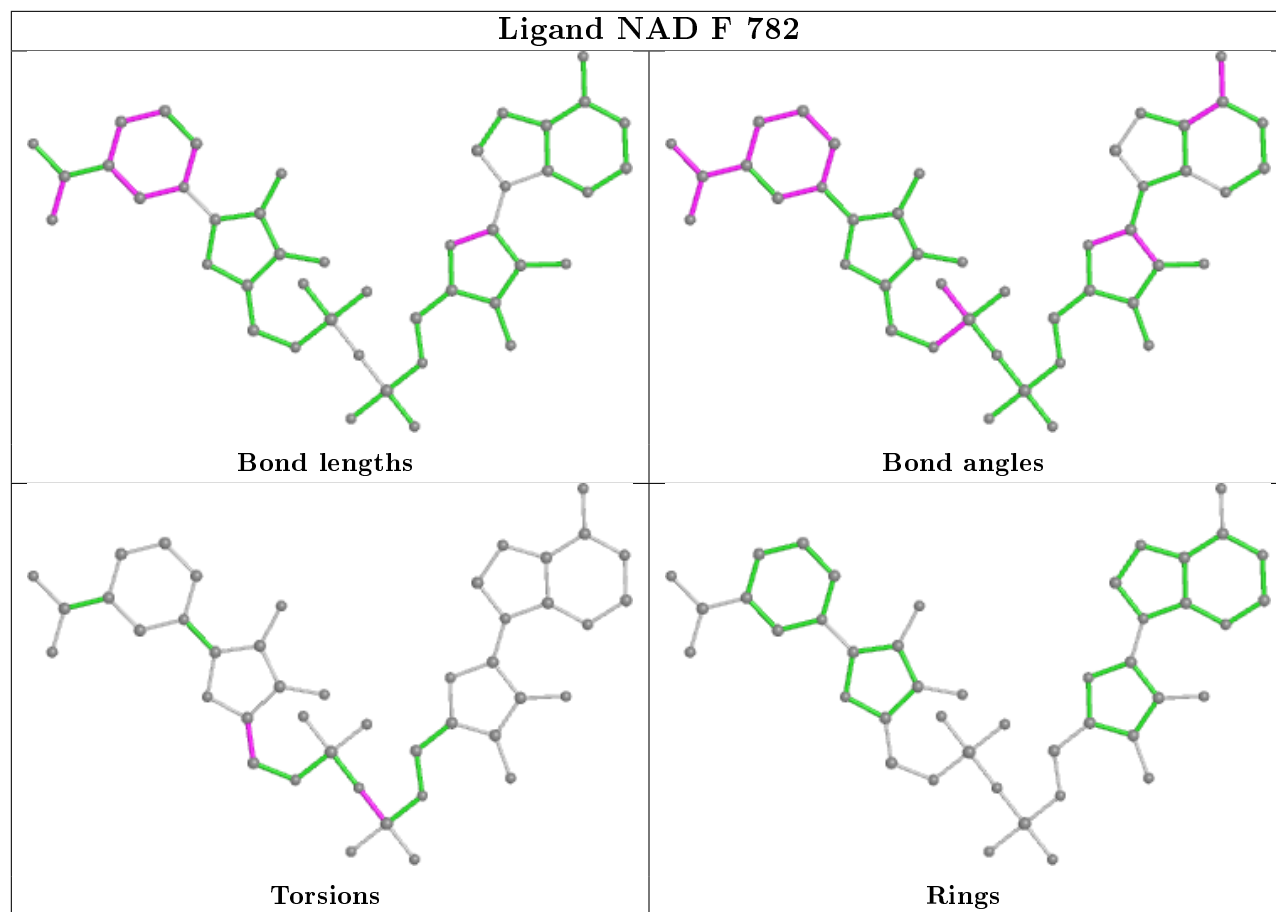
Mol	Chain	Res	Type	Atoms
2	C	779	NAD	C3D-C4D-C5D-O5D
2	A	777	NAD	O4D-C4D-C5D-O5D
2	A	777	NAD	C3D-C4D-C5D-O5D
2	B	778	NAD	O4D-C4D-C5D-O5D
2	B	778	NAD	C3D-C4D-C5D-O5D
2	E	781	NAD	C3D-C4D-C5D-O5D
2	D	780	NAD	C3D-C4D-C5D-O5D
2	F	782	NAD	PN-O3-PA-O1A
2	D	780	NAD	PN-O3-PA-O2A
2	C	779	NAD	PN-O3-PA-O2A
2	B	778	NAD	PN-O3-PA-O2A
2	E	781	NAD	PN-O3-PA-O1A
2	A	777	NAD	PN-O3-PA-O1A
2	F	782	NAD	PN-O3-PA-O2A
2	D	780	NAD	PN-O3-PA-O1A
2	C	779	NAD	C5B-O5B-PA-O1A
2	D	780	NAD	C5D-O5D-PN-O1N

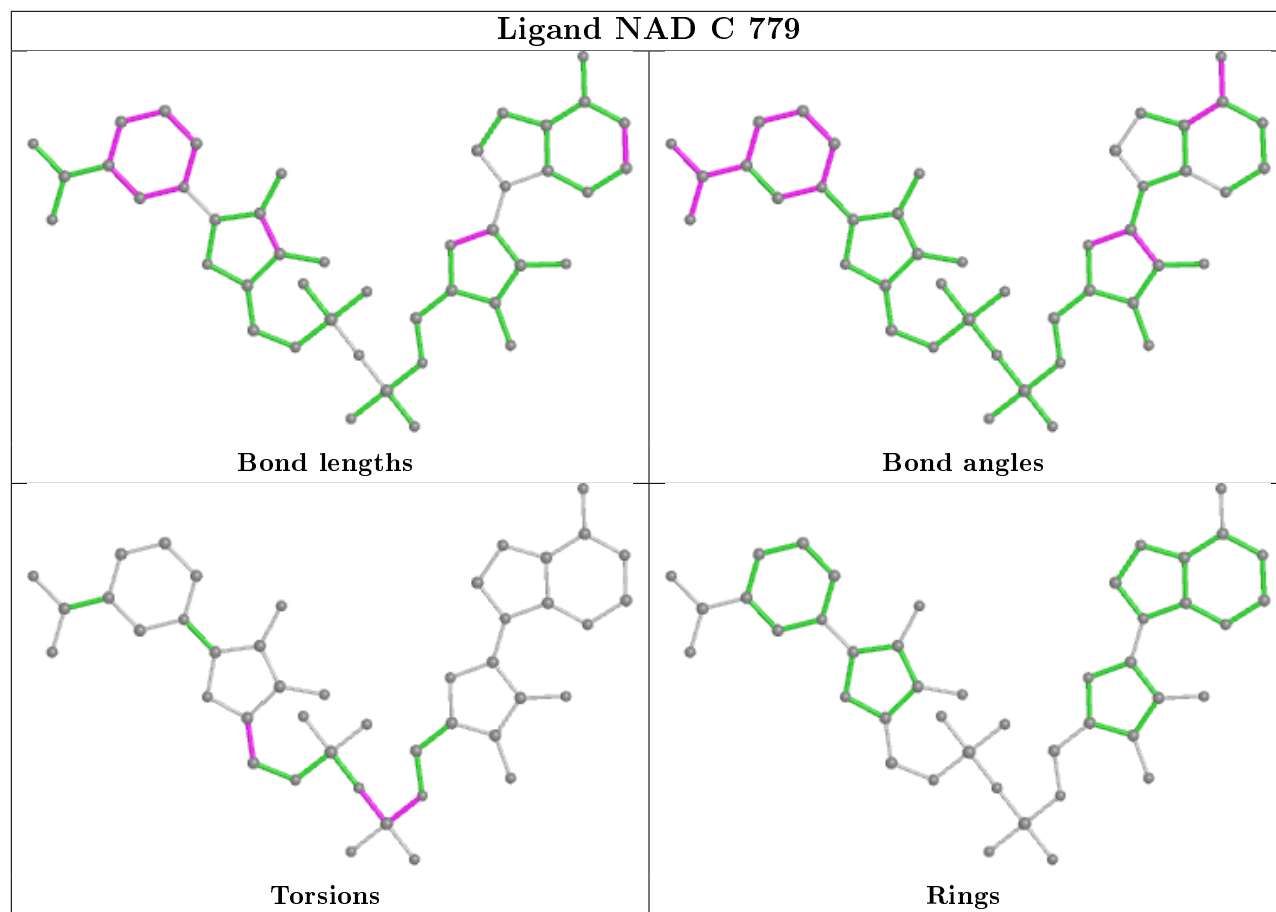
There are no ring outliers.

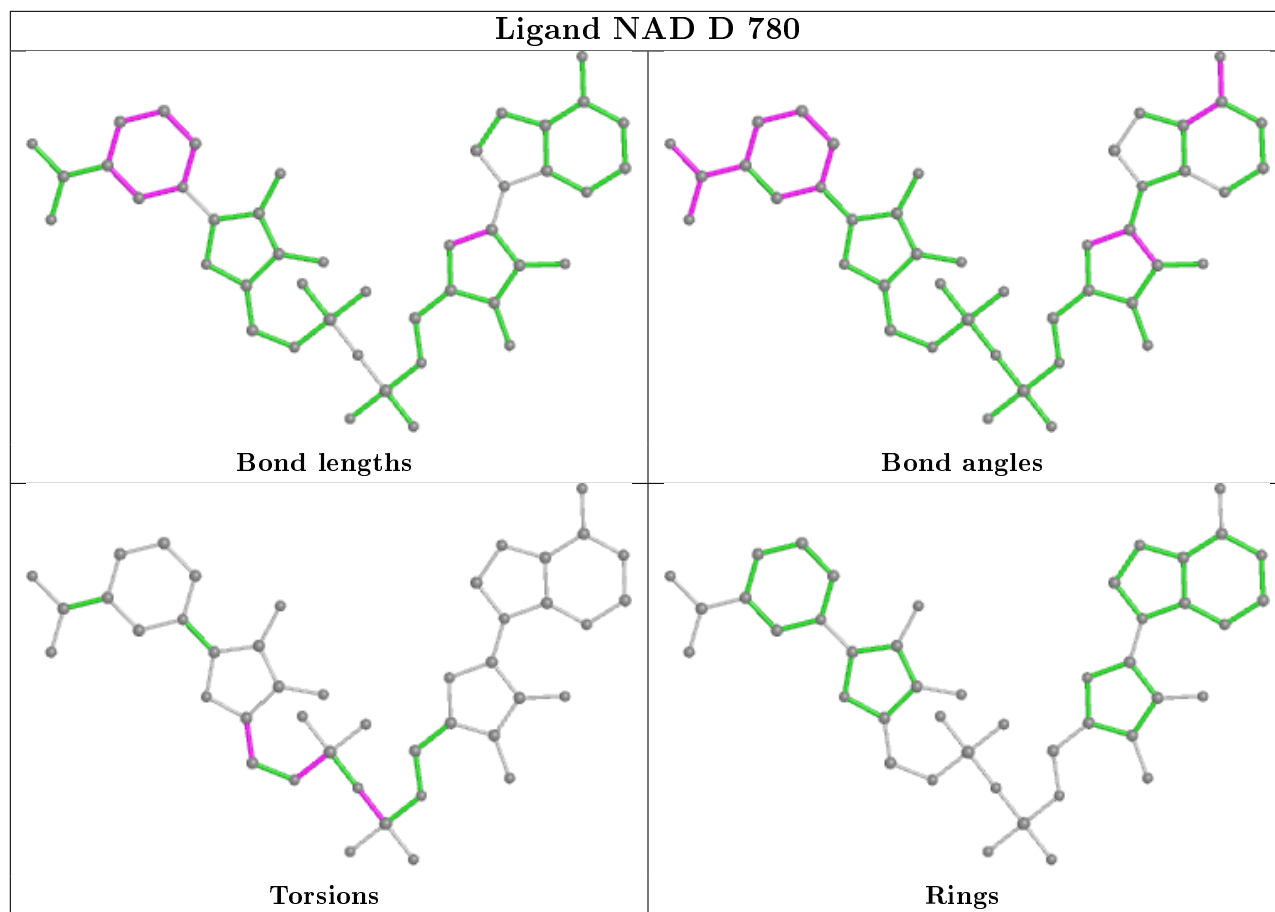
6 monomers are involved in 18 short contacts:

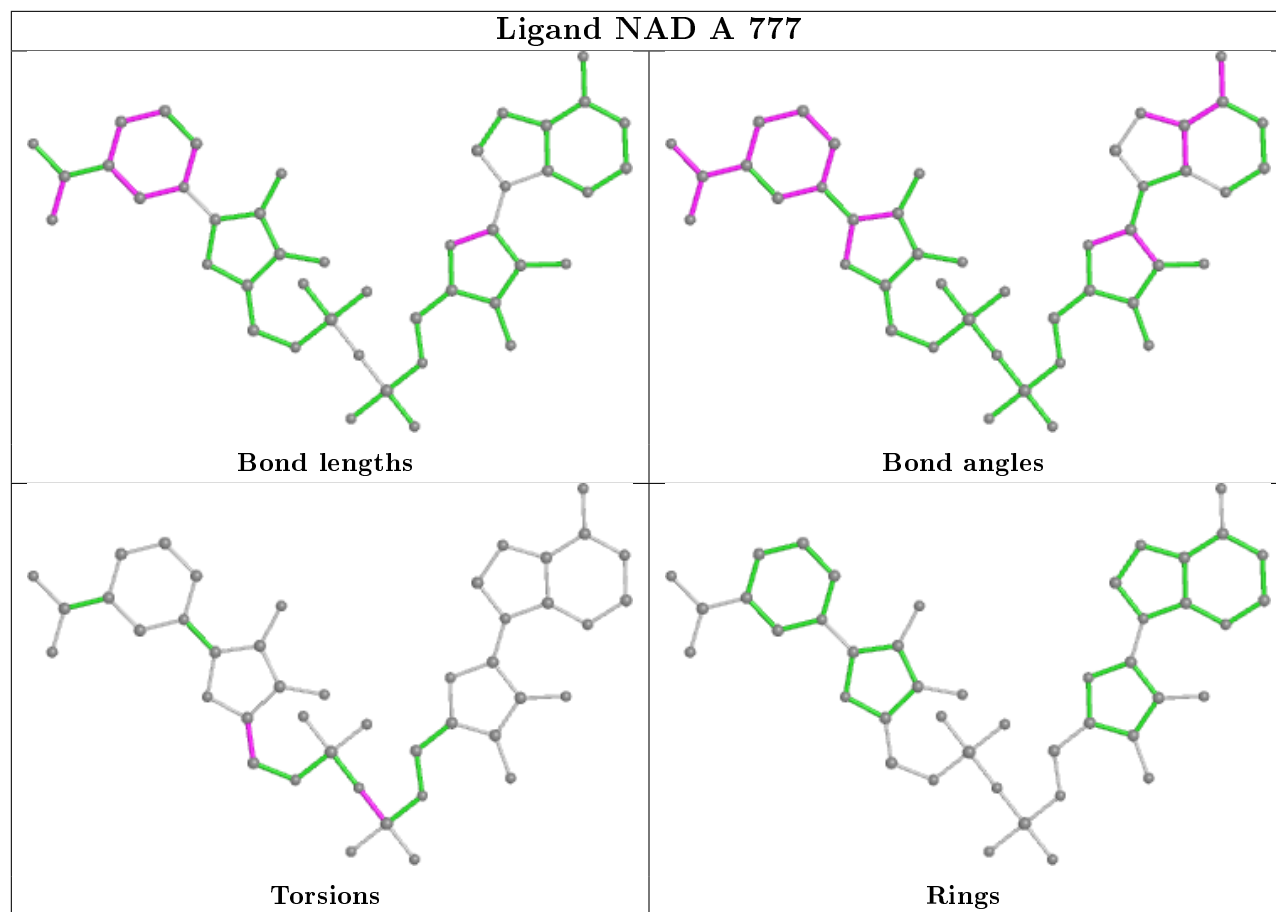
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	782	NAD	2	0
2	C	779	NAD	3	0
2	D	780	NAD	4	0
2	A	777	NAD	1	0
2	B	778	NAD	5	0
2	E	781	NAD	3	0

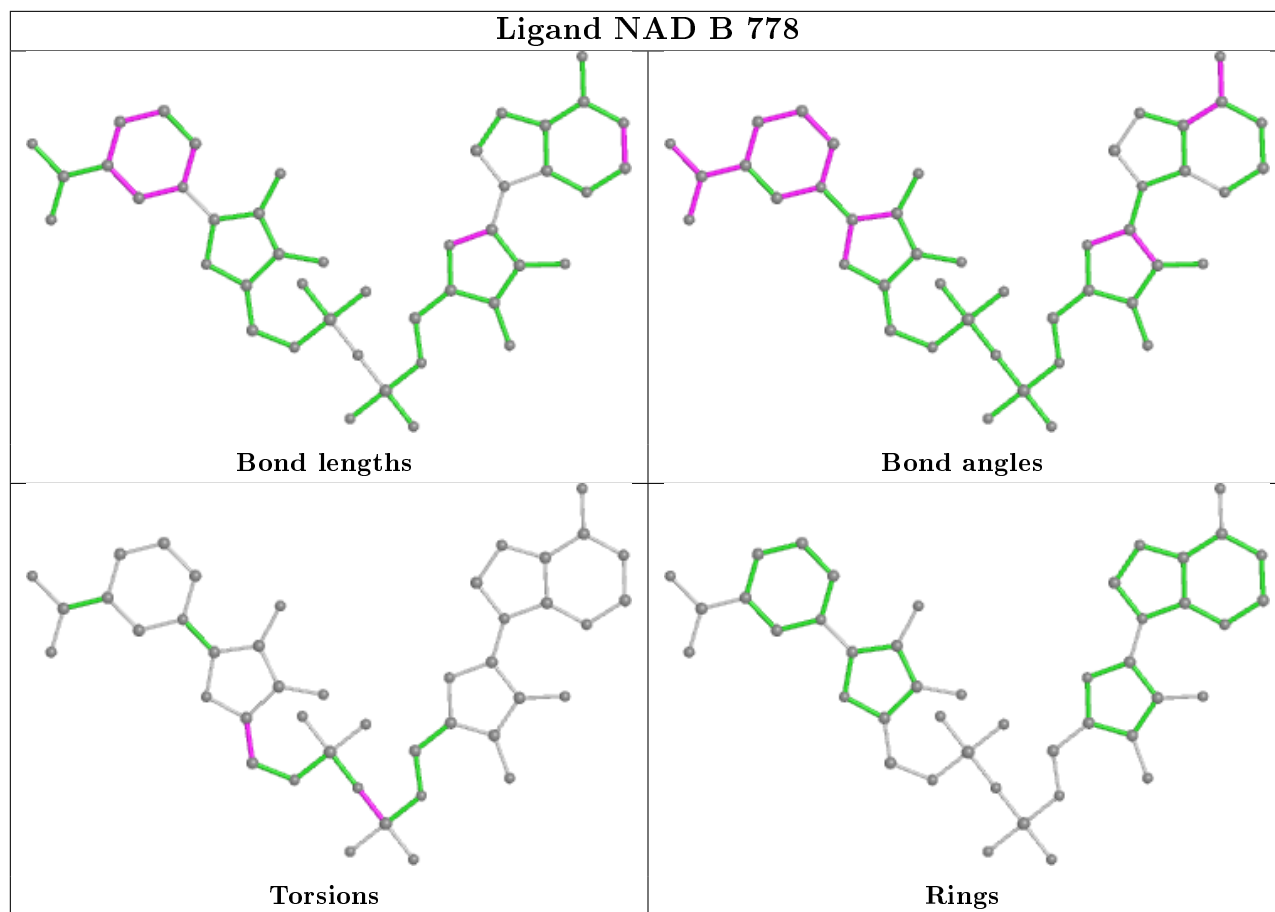
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

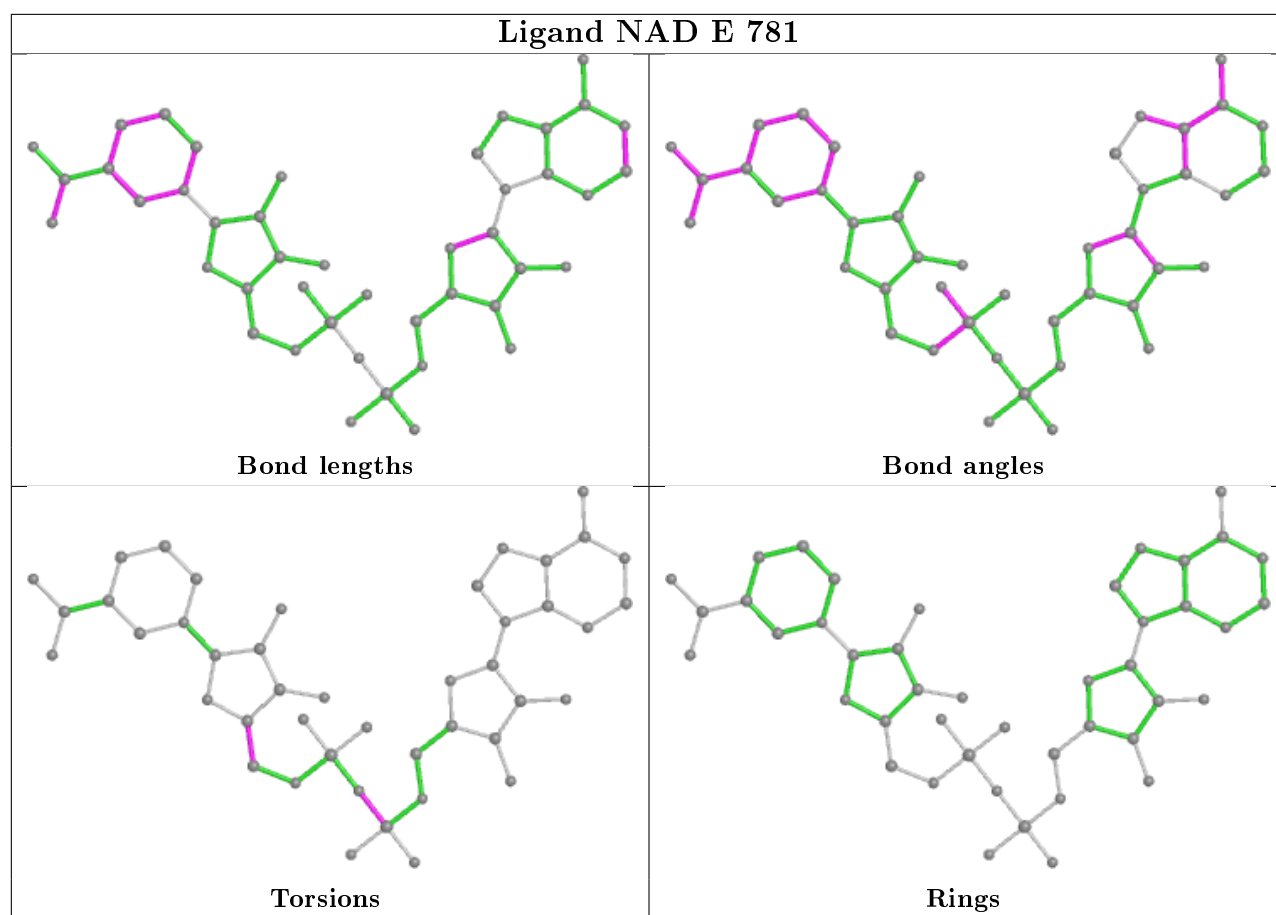












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/279 (83%)	-0.36	4 (1%) 70 68	16, 30, 49, 68	0
1	B	231/279 (82%)	-0.22	8 (3%) 44 42	19, 35, 56, 84	0
1	C	231/279 (82%)	-0.36	3 (1%) 77 75	19, 30, 51, 70	0
1	D	231/279 (82%)	-0.17	8 (3%) 44 42	20, 35, 54, 80	0
1	E	232/279 (83%)	0.03	12 (5%) 27 26	26, 43, 63, 80	0
1	F	231/279 (82%)	0.11	13 (5%) 24 23	29, 46, 66, 84	0
All	All	1388/1674 (82%)	-0.16	48 (3%) 44 42	16, 37, 61, 84	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	ALA	5.9
1	F	108	ALA	5.2
1	A	275	ALA	5.0
1	F	275	ALA	4.9
1	D	108	ALA	4.8
1	D	275	ALA	4.6
1	E	147	ALA	4.5
1	A	108	ALA	4.3
1	C	275	ALA	4.2
1	F	107	GLU	3.9
1	E	275	ALA	3.8
1	B	263	ALA	3.6
1	A	147	ALA	3.6
1	E	108	ALA	3.6
1	C	108	ALA	3.4
1	E	263	ALA	3.3
1	C	148	VAL	3.3
1	D	274	THR	3.2
1	F	265	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	148	VAL	3.2
1	B	90	LYS	3.1
1	F	39	GLY	3.0
1	B	108	ALA	2.9
1	E	250	LYS	2.8
1	D	148	VAL	2.7
1	B	148	VAL	2.6
1	A	76	ASN	2.5
1	F	90	LYS	2.5
1	B	274	THR	2.5
1	D	264	GLY	2.5
1	E	148	VAL	2.4
1	F	76	ASN	2.4
1	B	264	GLY	2.4
1	F	77	SER	2.4
1	E	107	GLU	2.4
1	F	78	LYS	2.3
1	F	40	ARG	2.2
1	E	274	THR	2.2
1	F	271	GLN	2.2
1	E	39	GLY	2.1
1	E	153	LEU	2.1
1	D	90	LYS	2.1
1	B	39	GLY	2.1
1	D	39	GLY	2.1
1	E	76	ASN	2.1
1	E	260	ASP	2.0
1	F	106	LEU	2.0
1	D	263	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 carbohydrates in this entry.

6.4 Ligands [i](#)

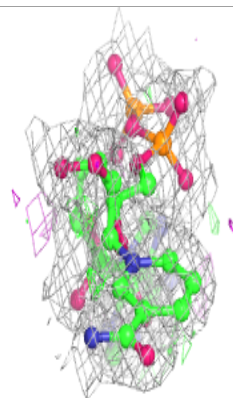
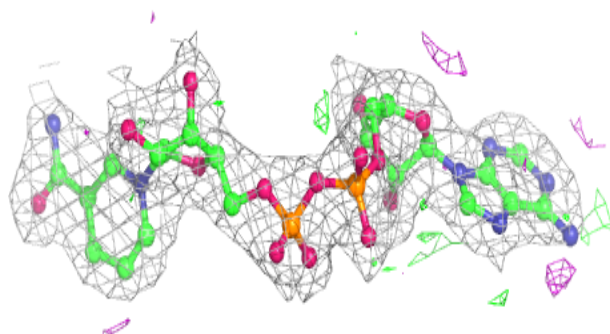
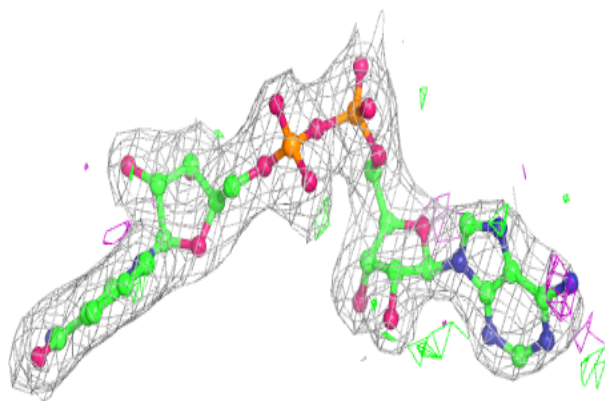
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XE	E	758	1/1	0.60	0.22	167,167,167,167	0
3	XE	E	757	1/1	0.68	0.20	153,153,153,153	0
3	XE	B	752	1/1	0.69	0.07	156,156,156,156	0
3	XE	C	754	1/1	0.76	0.11	142,142,142,142	0
3	XE	D	762	1/1	0.80	0.17	163,163,163,163	0
3	XE	A	750	1/1	0.80	0.13	136,136,136,136	0
3	XE	F	756	1/1	0.86	0.12	139,139,139,139	0
3	XE	A	748	1/1	0.88	0.10	88,88,88,88	0
2	NAD	B	778	44/44	0.93	0.12	35,42,50,52	0
2	NAD	D	780	44/44	0.94	0.12	30,44,50,50	0
3	XE	C	753	1/1	0.94	0.13	121,121,121,121	0
2	NAD	E	781	44/44	0.94	0.13	30,43,53,55	0
2	NAD	F	782	44/44	0.95	0.12	29,46,53,54	0
3	XE	B	755	1/1	0.95	0.15	130,130,130,130	0
3	XE	B	751	1/1	0.95	0.32	200,200,200,200	0
2	NAD	C	779	44/44	0.96	0.10	18,36,45,49	0
2	NAD	A	777	44/44	0.96	0.10	20,34,41,43	0
3	XE	B	760	1/1	0.97	0.08	96,96,96,96	0
3	XE	A	749	1/1	0.98	0.08	94,94,94,94	0
3	XE	D	761	1/1	0.99	0.07	97,97,97,97	0
3	XE	C	759	1/1	0.99	0.05	51,51,51,51	0

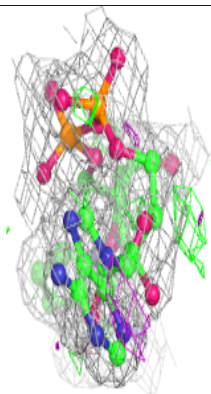
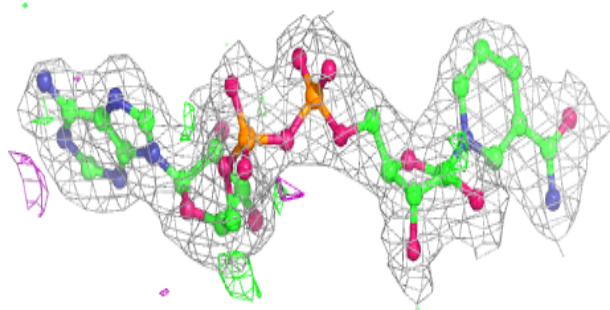
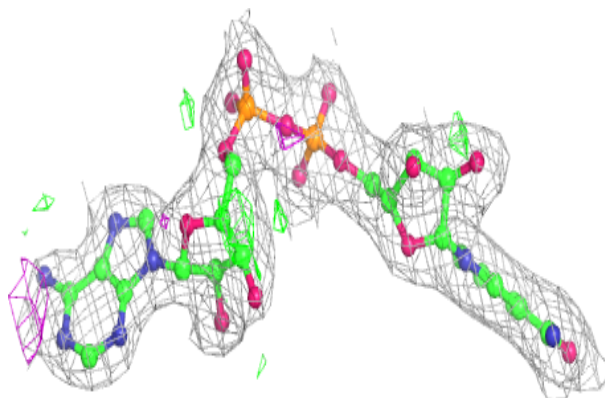
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 778:

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

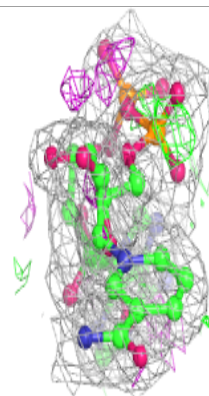
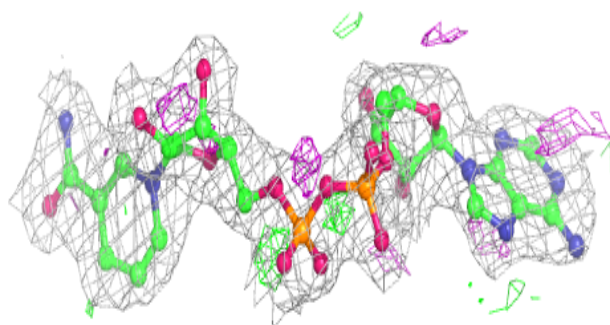
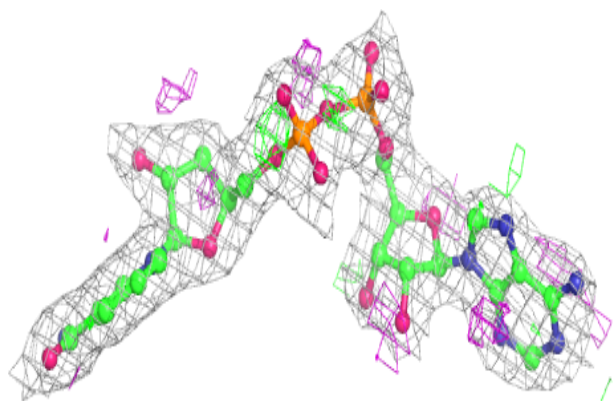
**Electron density around NAD D 780:**

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

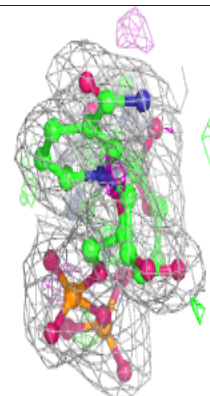
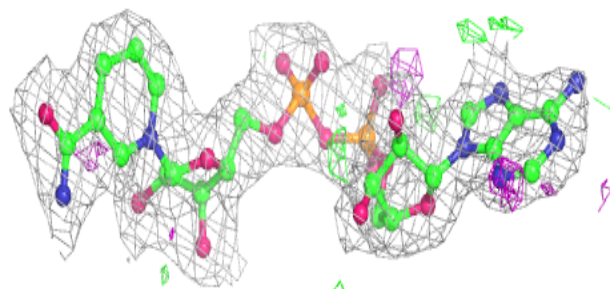
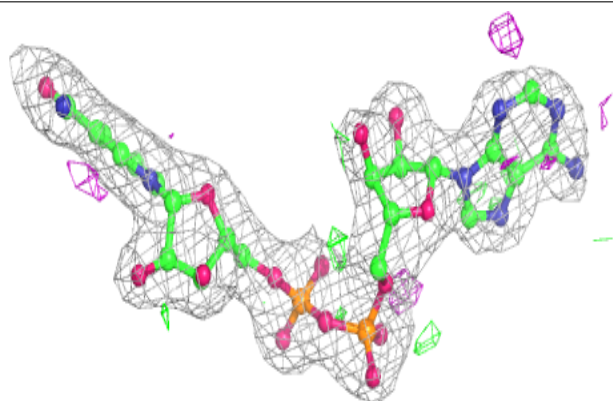


Electron density around NAD E 781:

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

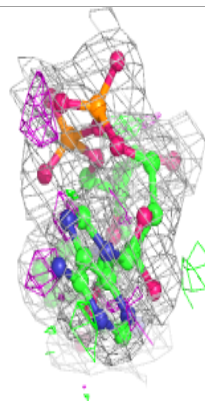
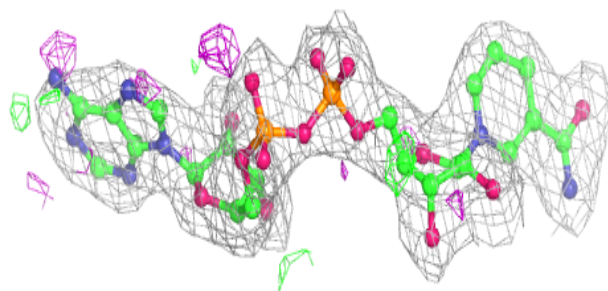
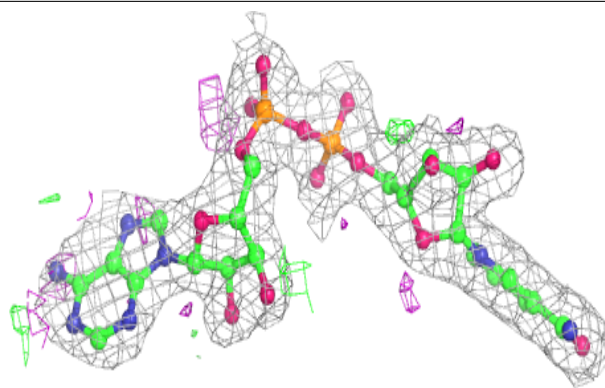
**Electron density around NAD F 782:**

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

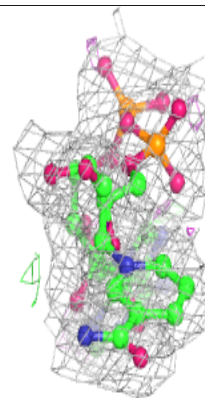
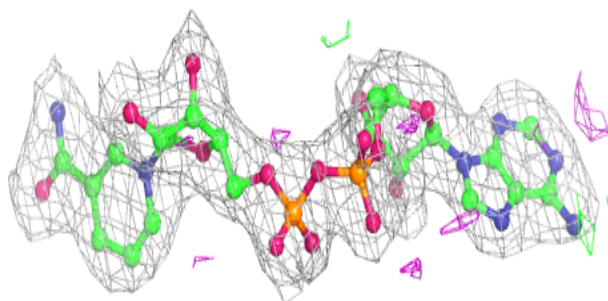
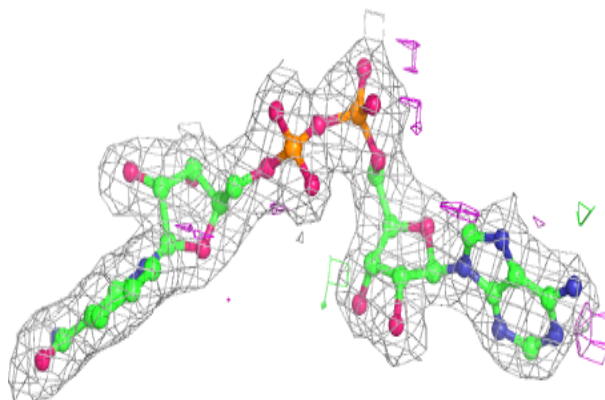


Electron density around NAD C 779:

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

**Electron density around NAD A 777:**

$2mF_o-DF_c$ (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.