



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 5TEN / pdb_00005ten
Title : Structure of 4-Hydroxy-tetrahydrodipicolinate Reductase from *Vibrio vulnificus* with 2,5 Furan Dicarboxylic and NADH with Intact Polyhistidine Tag
Authors : Mank, N.; Pote, S.; Arnette, K.; Klapper, V.; Chruszcz, M.
Deposited on : 2016-09-22
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

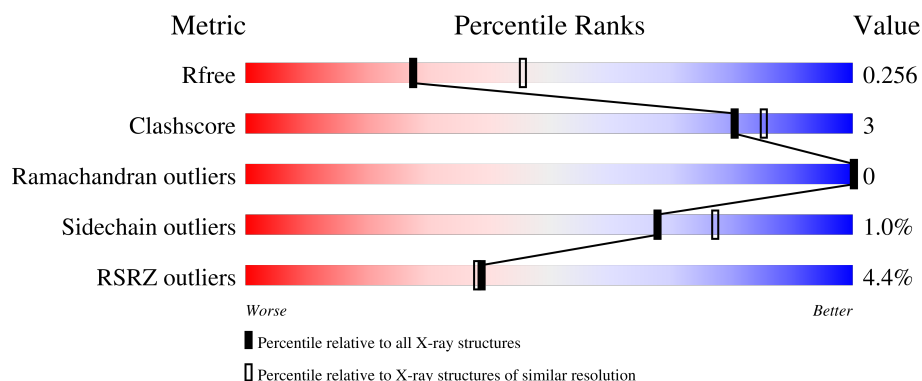
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	269	 2% 90% 10%
1	B	269	 % 93% 7%
1	C	269	 2% 91% 9%
1	D	269	 % 91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	269	6% 93% 6%
1	F	269	9% 91% 9%
1	G	269	5% 91% 8% .
1	H	269	9% 92% 6% ..

2 Entry composition

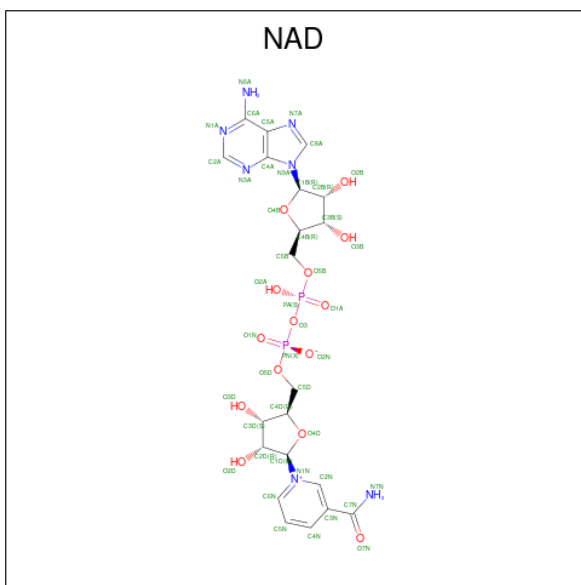
There are 5 unique types of molecules in this entry. The entry contains 16407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-hydroxy-tetrahydrodipicolinate reductase.

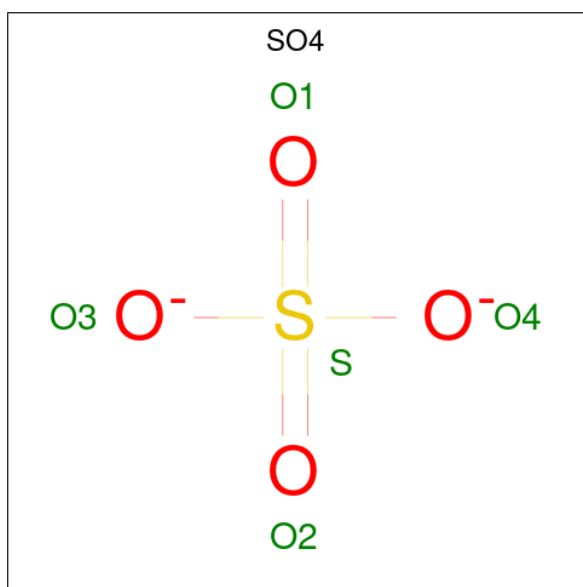
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1964	1232	341	378	13			
1	B	269	Total	C	N	O	S	0	0	0
			1961	1230	344	374	13			
1	C	269	Total	C	N	O	S	0	0	0
			1987	1247	348	379	13			
1	D	269	Total	C	N	O	S	0	0	0
			1988	1247	348	380	13			
1	E	269	Total	C	N	O	S	0	0	0
			1928	1212	335	368	13			
1	F	269	Total	C	N	O	S	0	0	0
			1940	1217	340	370	13			
1	G	269	Total	C	N	O	S	0	0	0
			1959	1232	344	370	13			
1	H	267	Total	C	N	O	S	0	0	0
			1927	1208	342	364	13			

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



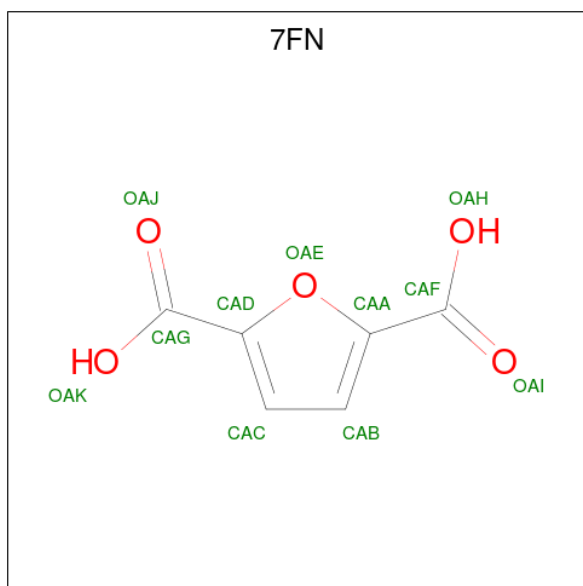
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	H	1	Total 5	O 4	S 1	0	0
3	H	1	Total 5	O 4	S 1	0	0
3	H	1	Total 5	O 4	S 1	0	0

- Molecule 4 is 2,5 Furan Dicarboxylic Acid (CCD ID: 7FN) (formula: $C_6H_4O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 11	C 6	O 5	0	0
4	C	1	Total 11	C 6	O 5	0	0
4	C	1	Total 11	C 6	O 5	0	0
4	D	1	Total 11	C 6	O 5	0	0
4	E	1	Total 11	C 6	O 5	0	0
4	F	1	Total 11	C 6	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			11	6	5		
4	H	1	Total	C	O	0	0
			11	6	5		

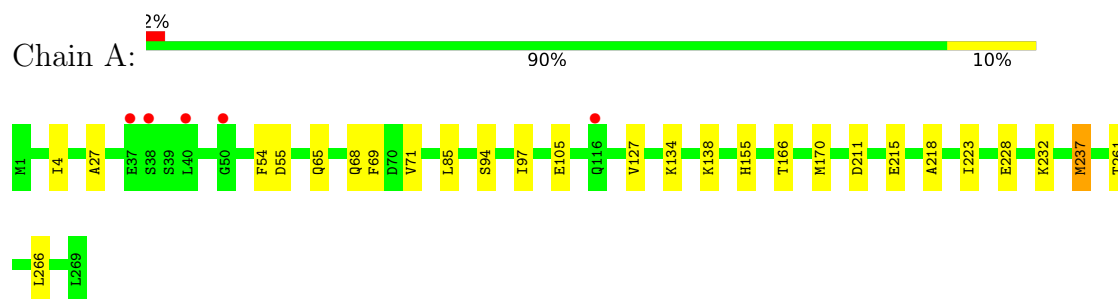
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	33	Total	O	0	0
			33	33		
5	C	24	Total	O	0	0
			24	24		
5	D	30	Total	O	0	0
			30	30		
5	E	10	Total	O	0	0
			10	10		
5	F	21	Total	O	0	0
			21	21		
5	G	32	Total	O	0	0
			32	32		
5	H	37	Total	O	0	0
			37	37		

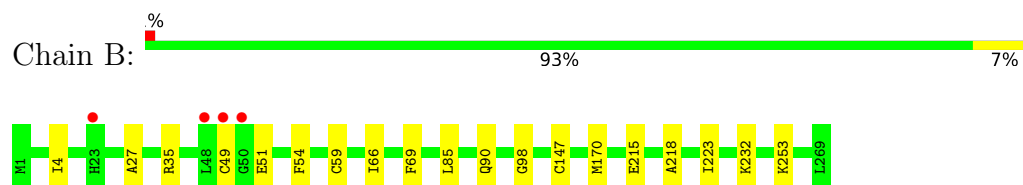
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

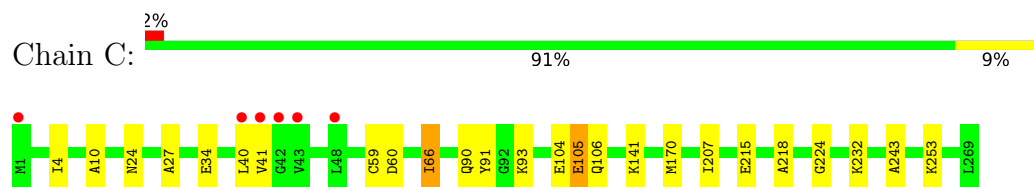
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



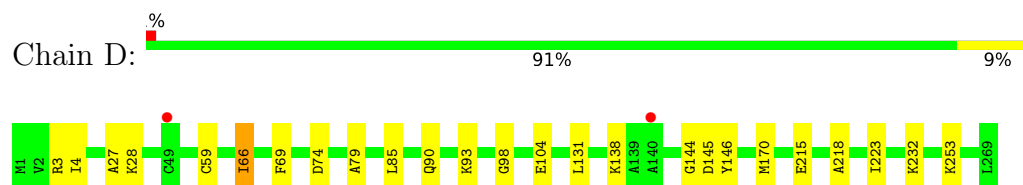
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

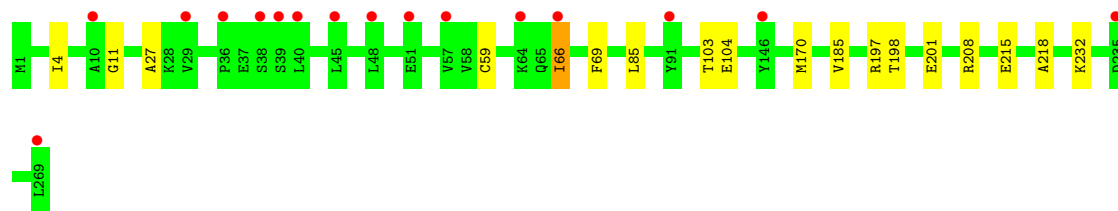


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

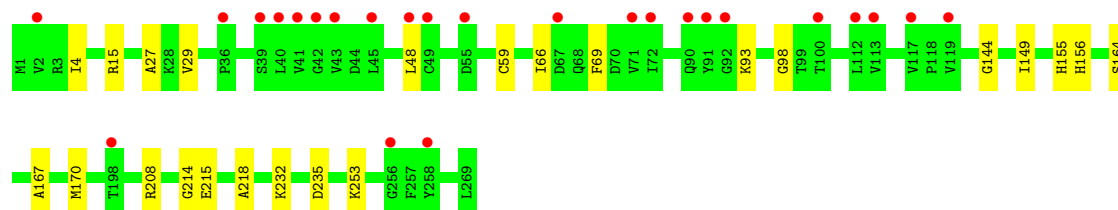
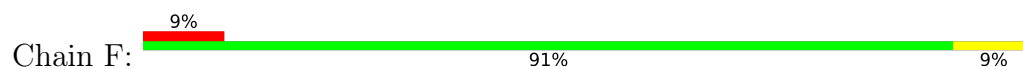


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

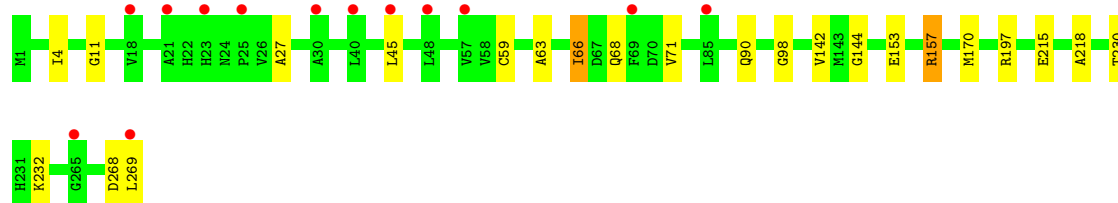




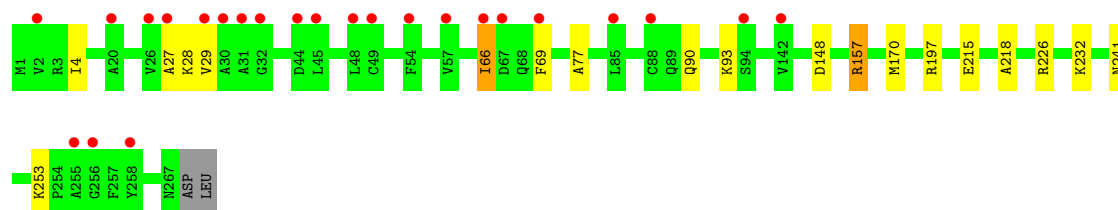
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.44Å 117.55Å 131.52Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 50.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-2.45) 96.9 (50.00-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.223 , 0.255 0.226 , 0.256	Depositor DCC
R_{free} test set	3726 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	1.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16407	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9733e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 7FN, 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	1.32	3/1994 (0.2%)	1.22	2/2706 (0.1%)
1	B	1.26	1/1991 (0.1%)	1.15	3/2702 (0.1%)
1	C	1.25	4/2017 (0.2%)	1.15	2/2732 (0.1%)
1	D	1.29	4/2018 (0.2%)	1.16	4/2732 (0.1%)
1	E	1.17	2/1958 (0.1%)	1.10	1/2663 (0.0%)
1	F	1.23	5/1970 (0.3%)	1.15	3/2677 (0.1%)
1	G	1.33	3/1989 (0.2%)	1.22	6/2699 (0.2%)
1	H	1.23	1/1956 (0.1%)	1.15	6/2658 (0.2%)
All	All	1.26	23/15893 (0.1%)	1.16	27/21569 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	230	THR	CA-C	6.62	1.60	1.52
1	C	24	ASN	CA-C	6.57	1.60	1.52
1	A	228	GLU	CA-C	5.77	1.59	1.52
1	E	185	VAL	C-O	-5.43	1.19	1.24
1	D	223	ILE	C-O	-5.42	1.18	1.24
1	C	243	ALA	CA-C	5.38	1.59	1.52
1	D	145	ASP	N-CA	5.34	1.52	1.46
1	D	74	ASP	CA-C	5.33	1.59	1.53
1	C	207	ILE	CA-C	5.29	1.58	1.52
1	B	223	ILE	C-O	-5.27	1.18	1.24
1	D	79	ALA	N-CA	5.21	1.52	1.46
1	H	77	ALA	CA-C	5.21	1.57	1.52
1	E	208	ARG	N-CA	5.20	1.52	1.46
1	A	223	ILE	CA-CB	5.16	1.60	1.53
1	F	164	SER	C-O	-5.15	1.17	1.23
1	A	166	THR	CA-C	5.13	1.59	1.52
1	F	167	ALA	N-CA	5.10	1.52	1.46
1	F	149	ILE	N-CA	5.09	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	156	HIS	N-CA	5.07	1.52	1.46
1	G	153	GLU	N-CA	5.06	1.52	1.46
1	F	235	ASP	N-CA	5.04	1.52	1.46
1	G	142	VAL	C-O	-5.04	1.18	1.24
1	C	141	LYS	C-O	-5.03	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	157	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	D	144	GLY	N-CA-C	6.45	120.47	112.73
1	H	157	ARG	N-CA-C	6.43	120.22	112.38
1	G	157	ARG	N-CA-C	6.41	120.20	112.38
1	E	66	ILE	N-CA-C	6.32	117.83	110.62
1	H	157	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	D	66	ILE	N-CA-C	6.26	117.01	110.62
1	G	71	VAL	N-CA-C	5.82	116.50	108.12
1	C	66	ILE	N-CA-C	5.71	117.14	110.62
1	F	253	LYS	N-CA-C	5.71	117.82	110.39
1	C	253	LYS	N-CA-C	5.69	117.86	110.40
1	G	66	ILE	N-CA-C	5.62	117.02	110.62
1	D	253	LYS	N-CA-C	5.55	118.34	110.24
1	H	66	ILE	N-CA-C	5.55	116.95	110.62
1	G	144	GLY	N-CA-C	5.53	119.36	112.73
1	F	29	VAL	CB-CA-C	-5.48	105.38	111.35
1	H	253	LYS	N-CA-C	5.47	118.23	110.24
1	D	131	LEU	N-CA-C	-5.34	105.35	111.07
1	F	144	GLY	N-CA-C	5.32	119.32	112.83
1	A	69	PHE	N-CA-C	5.30	117.87	109.50
1	G	90	GLN	N-CA-C	5.21	116.96	111.28
1	H	226	ARG	N-CA-C	5.16	116.91	109.07
1	B	147	CYS	N-CA-C	5.14	118.49	110.32
1	B	90	GLN	N-CA-C	5.12	116.86	111.28
1	B	253	LYS	N-CA-C	5.07	117.15	110.36
1	A	97	ILE	N-CA-C	5.05	115.36	107.99
1	G	45	LEU	N-CA-C	5.01	116.75	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1964	0	1925	13	0
1	B	1961	0	1922	10	0
1	C	1987	0	1976	12	0
1	D	1988	0	1976	10	0
1	E	1928	0	1867	9	0
1	F	1940	0	1879	12	0
1	G	1959	0	1933	11	0
1	H	1927	0	1885	11	0
2	A	44	0	26	0	0
2	B	44	0	26	2	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	1	0
2	F	44	0	26	1	0
2	G	44	0	26	2	0
2	H	44	0	26	0	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	G	10	0	0	0	0
3	H	15	0	0	1	0
4	B	11	0	0	0	0
4	C	22	0	0	0	0
4	D	11	0	0	0	0
4	E	11	0	0	0	0
4	F	11	0	0	0	0
4	G	11	0	0	0	0
4	H	11	0	0	0	0
5	A	31	0	0	1	0
5	B	33	0	0	0	0
5	C	24	0	0	0	0
5	D	30	0	0	0	0
5	E	10	0	0	0	0
5	F	21	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	32	0	0	1	0
5	H	37	0	0	0	0
All	All	16407	0	15571	82	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 3.

All (82) 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:B:49:CYS:SG	1:B:51:GLU:HB2	2.08	0.93
1:B:215:GLU:HG2	1:B:232:LYS:HG2	1.78	0.65
1:H:215:GLU:HG2	1:H:232:LYS:HG2	1.79	0.64
1:F:15:ARG:HG2	1:F:48:LEU:CD2	2.30	0.61
1:A:215:GLU:HG2	1:A:232:LYS:HG2	1.83	0.60
1:E:215:GLU:HG2	1:E:232:LYS:HG2	1.82	0.60
1:G:215:GLU:HG2	1:G:232:LYS:HG2	1.81	0.60
1:A:127:VAL:HG11	1:D:146:TYR:OH	2.01	0.60
1:D:215:GLU:HG2	1:D:232:LYS:HG2	1.83	0.59
1:B:51:GLU:HG2	1:B:54:PHE:HZ	1.68	0.59
1:C:215:GLU:HG2	1:C:232:LYS:HG2	1.83	0.59
1:F:215:GLU:HG2	1:F:232:LYS:HG2	1.83	0.59
1:E:197:ARG:NH2	1:E:201:GLU:O	2.37	0.57
1:C:90:GLN:HG3	1:C:91:TYR:CD2	2.39	0.57
1:H:28:LYS:HD2	1:H:29:VAL:H	1.69	0.56
1:E:11:GLY:HA3	2:E:1001:NAD:H52A	1.88	0.55
1:G:68:GLN:NE2	5:G:1101:HOH:O	2.39	0.54
1:A:65:GLN:O	1:A:68:GLN:HG2	2.08	0.54
1:F:66:ILE:HD12	1:F:69:PHE:CZ	2.42	0.54
1:G:63:ALA:O	1:G:66:ILE:HG23	2.08	0.53
1:A:71:VAL:HG23	1:A:94:SER:C	2.33	0.53
1:D:104:GLU:H	1:D:104:GLU:CD	2.16	0.53
1:F:15:ARG:HG2	1:F:48:LEU:HD23	1.89	0.53
1:H:241:ASN:ND2	3:H:1005:SO4:O4	2.39	0.52
1:G:197:ARG:O	1:H:157:ARG:NH1	2.43	0.52
1:A:155:HIS:NE2	5:A:1101:HOH:O	2.34	0.52
1:H:66:ILE:HD12	1:H:69:PHE:CZ	2.45	0.52
1:A:54:PHE:O	1:A:55:ASP:HB2	2.08	0.51
1:G:268:ASP:O	1:G:269:LEU:HB2	2.09	0.51
1:B:66:ILE:HD12	1:B:69:PHE:CZ	2.45	0.51
1:E:197:ARG:HG2	1:E:198:THR:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:ARG:NH1	1:H:148:ASP:OD1	2.43	0.51
1:C:4:ILE:HD12	1:C:27:ALA:HB1	1.93	0.50
1:F:15:ARG:CG	1:F:48:LEU:HD21	2.42	0.50
1:E:66:ILE:HD12	1:E:69:PHE:CZ	2.46	0.50
1:B:49:CYS:SG	1:B:51:GLU:CB	2.94	0.50
1:F:98:GLY:O	2:F:1001:NAD:H2N	2.12	0.50
1:C:41:VAL:HG21	1:C:60:ASP:HB3	1.93	0.50
1:D:66:ILE:HD12	1:D:69:PHE:CZ	2.46	0.50
1:D:4:ILE:HD12	1:D:27:ALA:HB1	1.94	0.49
1:E:197:ARG:NH1	1:E:201:GLU:HG3	2.28	0.49
1:A:138:LYS:HG3	1:D:138:LYS:HE2	1.93	0.49
1:B:4:ILE:HD12	1:B:27:ALA:HB1	1.94	0.49
1:F:15:ARG:HG2	1:F:48:LEU:HD21	1.94	0.48
1:G:4:ILE:HD12	1:G:27:ALA:HB1	1.95	0.48
1:B:51:GLU:HG2	1:B:54:PHE:CZ	2.48	0.48
1:B:35:ARG:HG3	2:B:1001:NAD:C5A	2.44	0.48
1:C:105:GLU:HG2	1:C:106:GLN:N	2.29	0.48
1:G:98:GLY:O	2:G:1001:NAD:H2N	2.14	0.47
1:A:4:ILE:HD12	1:A:27:ALA:HB1	1.96	0.47
1:E:4:ILE:HD12	1:E:27:ALA:HB1	1.95	0.46
1:F:214:GLY:HA3	5:F:1104:HOH:O	2.14	0.46
1:D:3:ARG:HG2	1:D:28:LYS:HD3	1.98	0.46
1:F:4:ILE:HD12	1:F:27:ALA:HB1	1.98	0.46
1:A:261:THR:HG23	1:A:266:LEU:HB2	1.98	0.45
1:G:157:ARG:NH2	1:H:197:ARG:O	2.49	0.45
1:E:103:THR:HG22	1:E:104:GLU:N	2.33	0.44
1:A:134:LYS:HE3	1:A:138:LYS:HE2	1.99	0.44
1:G:170:MET:HE2	1:G:218:ALA:HB2	1.99	0.44
1:A:170:MET:HE2	1:A:218:ALA:HB2	2.00	0.43
1:D:66:ILE:HD11	1:D:93:LYS:HG3	2.01	0.43
1:D:170:MET:HE2	1:D:218:ALA:HB2	2.00	0.43
1:H:4:ILE:HD12	1:H:27:ALA:HB1	2.01	0.43
1:C:66:ILE:HG23	1:C:93:LYS:HE3	2.01	0.43
1:D:98:GLY:O	2:D:1001:NAD:H2N	2.18	0.43
1:E:170:MET:HE2	1:E:218:ALA:HB2	2.01	0.42
1:H:66:ILE:HD11	1:H:93:LYS:HG3	2.01	0.41
1:F:155:HIS:HB2	1:F:208:ARG:NH1	2.35	0.41
1:G:11:GLY:HA3	2:G:1001:NAD:H52A	2.02	0.41
1:A:237:MET:O	1:A:237:MET:HG2	2.21	0.41
1:B:98:GLY:O	2:B:1001:NAD:H2N	2.21	0.41
1:C:40:LEU:O	1:C:40:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:OD2	1:C:224:GLY:N	2.45	0.41
1:C:170:MET:HE2	1:C:218:ALA:HB2	2.03	0.41
1:H:170:MET:HE2	1:H:218:ALA:HB2	2.02	0.41
1:F:170:MET:HE2	1:F:218:ALA:HB2	2.02	0.41
1:C:104:GLU:HG2	1:C:105:GLU:N	2.36	0.40
1:F:66:ILE:CD1	1:F:93:LYS:HE3	2.52	0.40
1:H:66:ILE:CD1	1:H:93:LYS:HE3	2.52	0.40
1:C:10:ALA:HB2	1:C:40:LEU:HD22	2.03	0.40
1:B:170:MET:HE2	1:B:218:ALA:HB2	2.04	0.40
1:C:34:GLU:HG3	1:C:40:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
1	B	267/269 (99%)	260 (97%)	7 (3%)	0	100	100
1	C	267/269 (99%)	261 (98%)	6 (2%)	0	100	100
1	D	267/269 (99%)	260 (97%)	7 (3%)	0	100	100
1	E	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
1	F	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
1	G	267/269 (99%)	259 (97%)	8 (3%)	0	100	100
1	H	265/269 (98%)	258 (97%)	7 (3%)	0	100	100
All	All	2134/2152 (99%)	2075 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	197/207 (95%)	194 (98%)	3 (2%)	57	70
1	B	195/207 (94%)	193 (99%)	2 (1%)	68	77
1	C	202/207 (98%)	200 (99%)	2 (1%)	68	77
1	D	202/207 (98%)	199 (98%)	3 (2%)	57	70
1	E	188/207 (91%)	186 (99%)	2 (1%)	65	76
1	F	189/207 (91%)	188 (100%)	1 (0%)	81	87
1	G	195/207 (94%)	194 (100%)	1 (0%)	81	87
1	H	189/207 (91%)	188 (100%)	1 (0%)	81	87
All	All	1557/1656 (94%)	1542 (99%)	15 (1%)	68	77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	105	GLU
1	A	237	MET
1	B	59	CYS
1	B	85	LEU
1	C	59	CYS
1	C	105	GLU
1	D	59	CYS
1	D	85	LEU
1	D	90	GLN
1	E	59	CYS
1	E	85	LEU
1	F	59	CYS
1	G	59	CYS
1	H	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	B	23	HIS
1	C	90	GLN
1	D	23	HIS
1	E	23	HIS
1	E	251	HIS
1	F	109	GLN
1	H	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	C	1001	-	46,48,48	1.33	5 (10%)	64,73,73	1.92	19 (29%)
4	7FN	B	1002	-	11,11,11	3.18	5 (45%)	13,15,15	1.88	4 (30%)
3	SO4	F	1004	-	4,4,4	0.53	0	6,6,6	0.50	0
3	SO4	A	1004	-	4,4,4	0.41	0	6,6,6	0.30	0
4	7FN	D	1002	-	11,11,11	2.97	4 (36%)	13,15,15	1.64	4 (30%)
4	7FN	H	1002	-	11,11,11	3.20	5 (45%)	13,15,15	2.02	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	1003	-	4,4,4	0.38	0	6,6,6	0.59	0
3	SO4	H	1005	-	4,4,4	0.82	0	6,6,6	0.63	0
4	7FN	C	1002	-	11,11,11	3.06	4 (36%)	13,15,15	2.02	5 (38%)
2	NAD	E	1001	-	46,48,48	1.52	8 (17%)	64,73,73	1.89	17 (26%)
3	SO4	F	1003	-	4,4,4	0.50	0	6,6,6	0.33	0
3	SO4	F	1005	-	4,4,4	0.80	0	6,6,6	0.39	0
3	SO4	H	1003	-	4,4,4	0.49	0	6,6,6	0.15	0
2	NAD	G	1001	-	46,48,48	1.50	6 (13%)	64,73,73	1.95	19 (29%)
4	7FN	F	1002	-	11,11,11	4.31	5 (45%)	13,15,15	1.54	3 (23%)
3	SO4	A	1005	-	4,4,4	0.56	0	6,6,6	0.33	0
2	NAD	B	1001	-	46,48,48	1.45	6 (13%)	64,73,73	2.02	17 (26%)
3	SO4	C	1005	-	4,4,4	0.44	0	6,6,6	0.73	0
2	NAD	D	1001	-	46,48,48	1.23	3 (6%)	64,73,73	1.73	16 (25%)
3	SO4	A	1002	-	4,4,4	0.49	0	6,6,6	0.52	0
3	SO4	B	1003	-	4,4,4	0.45	0	6,6,6	0.67	0
4	7FN	E	1002	-	11,11,11	2.75	2 (18%)	13,15,15	1.83	2 (15%)
2	NAD	H	1001	-	46,48,48	1.29	6 (13%)	64,73,73	1.89	18 (28%)
4	7FN	G	1002	-	11,11,11	3.04	4 (36%)	13,15,15	1.74	3 (23%)
3	SO4	A	1003	-	4,4,4	0.46	0	6,6,6	0.57	0
3	SO4	G	1004	-	4,4,4	0.50	0	6,6,6	0.34	0
3	SO4	C	1003	-	4,4,4	0.47	0	6,6,6	0.56	0
3	SO4	C	1004	-	4,4,4	0.44	0	6,6,6	0.45	0
4	7FN	C	1006	-	11,11,11	2.83	4 (36%)	13,15,15	1.85	4 (30%)
2	NAD	F	1001	-	46,48,48	1.51	5 (10%)	64,73,73	1.81	15 (23%)
2	NAD	A	1001	-	46,48,48	1.39	7 (15%)	64,73,73	1.98	16 (25%)
3	SO4	H	1004	-	4,4,4	0.50	0	6,6,6	0.37	0
3	SO4	E	1003	-	4,4,4	0.47	0	6,6,6	0.39	0
3	SO4	E	1004	-	4,4,4	0.51	0	6,6,6	0.59	0
3	SO4	D	1003	-	4,4,4	0.53	0	6,6,6	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	1001	-	-	6/30/62/62	0/5/5/5
2	NAD	D	1001	-	-	5/30/62/62	0/5/5/5
4	7FN	C	1006	-	-	0/8/8/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7FN	E	1002	-	-	0/8/8/8	0/1/1/1
4	7FN	F	1002	-	-	0/8/8/8	0/1/1/1
4	7FN	C	1002	-	-	0/8/8/8	0/1/1/1
2	NAD	E	1001	-	-	8/30/62/62	0/5/5/5
2	NAD	F	1001	-	-	4/30/62/62	0/5/5/5
2	NAD	H	1001	-	-	3/30/62/62	0/5/5/5
4	7FN	D	1002	-	-	0/8/8/8	0/1/1/1
4	7FN	B	1002	-	-	0/8/8/8	0/1/1/1
4	7FN	G	1002	-	-	0/8/8/8	0/1/1/1
2	NAD	A	1001	-	-	8/30/62/62	0/5/5/5
2	NAD	G	1001	-	-	6/30/62/62	0/5/5/5
4	7FN	H	1002	-	-	1/8/8/8	0/1/1/1
2	NAD	B	1001	-	-	4/30/62/62	0/5/5/5

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1002	7FN	OAE-CAD	-8.48	1.24	1.38
4	G	1002	7FN	CAD-CAG	-6.90	1.33	1.48
4	F	1002	7FN	CAD-CAG	-6.57	1.34	1.48
4	B	1002	7FN	OAE-CAA	-6.25	1.28	1.38
4	E	1002	7FN	CAA-CAF	-6.19	1.34	1.48
4	H	1002	7FN	CAA-CAF	-6.16	1.35	1.48
4	C	1006	7FN	CAD-CAG	-6.06	1.35	1.48
4	F	1002	7FN	OAE-CAA	-6.02	1.28	1.38
4	D	1002	7FN	CAA-CAF	-5.93	1.35	1.48
4	E	1002	7FN	CAD-CAG	-5.74	1.35	1.48
4	F	1002	7FN	CAA-CAF	-5.72	1.36	1.48
4	C	1002	7FN	OAE-CAD	-5.58	1.29	1.38
4	G	1002	7FN	CAA-CAF	-5.58	1.36	1.48
2	F	1001	NAD	C5A-C4A	5.44	1.48	1.39
4	C	1006	7FN	CAA-CAF	-5.36	1.36	1.48
4	C	1002	7FN	CAD-CAG	-5.26	1.37	1.48
4	H	1002	7FN	OAE-CAA	-5.25	1.29	1.38
4	B	1002	7FN	CAD-CAG	-5.10	1.37	1.48
4	D	1002	7FN	OAE-CAA	-5.03	1.30	1.38
2	G	1001	NAD	PA-O3	4.98	1.64	1.59
2	E	1001	NAD	C5A-C4A	4.79	1.47	1.39
2	F	1001	NAD	PA-O3	4.70	1.64	1.59
2	A	1001	NAD	C5A-C4A	4.68	1.47	1.39
4	B	1002	7FN	CAA-CAF	-4.67	1.38	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1002	7FN	CAD-CAG	-4.67	1.38	1.48
4	C	1002	7FN	CAA-CAF	-4.66	1.38	1.48
2	G	1001	NAD	C5A-C4A	4.58	1.47	1.39
4	D	1002	7FN	CAD-CAG	-4.54	1.38	1.48
2	H	1001	NAD	C5A-C4A	4.54	1.47	1.39
2	D	1001	NAD	C5A-C4A	4.45	1.47	1.39
2	B	1001	NAD	C5A-C4A	4.44	1.47	1.39
2	B	1001	NAD	PA-O3	4.38	1.64	1.59
2	E	1001	NAD	PA-O3	4.32	1.64	1.59
2	C	1001	NAD	C5A-C4A	4.20	1.46	1.39
2	G	1001	NAD	PN-O3	4.05	1.63	1.59
2	E	1001	NAD	PN-O3	3.56	1.63	1.59
2	F	1001	NAD	C5A-C6A	3.53	1.50	1.41
2	A	1001	NAD	O4D-C1D	3.37	1.45	1.40
2	D	1001	NAD	C5A-N7A	-3.21	1.33	1.39
2	A	1001	NAD	PA-O3	3.19	1.62	1.59
2	C	1001	NAD	O4D-C1D	3.16	1.45	1.40
4	C	1002	7FN	OAI-CAF	3.11	1.30	1.22
2	A	1001	NAD	C5A-C6A	3.07	1.49	1.41
2	E	1001	NAD	C5A-C6A	3.06	1.49	1.41
4	H	1002	7FN	OAE-CAD	-3.04	1.33	1.38
2	C	1001	NAD	C4A-N9A	-3.03	1.31	1.37
4	C	1006	7FN	OAE-CAA	-2.99	1.33	1.38
4	F	1002	7FN	OAI-CAF	2.99	1.29	1.22
2	B	1001	NAD	C5A-N7A	-2.92	1.33	1.39
2	F	1001	NAD	PN-O3	2.86	1.62	1.59
4	B	1002	7FN	OAE-CAD	-2.85	1.33	1.38
2	E	1001	NAD	C8A-N7A	2.85	1.37	1.31
2	F	1001	NAD	C8A-N7A	2.83	1.37	1.31
4	B	1002	7FN	OAJ-CAG	2.76	1.29	1.22
4	G	1002	7FN	OAE-CAD	-2.75	1.34	1.38
2	G	1001	NAD	C5A-C6A	2.74	1.48	1.41
2	E	1001	NAD	C5A-N7A	-2.69	1.34	1.39
2	C	1001	NAD	C5A-C6A	2.65	1.48	1.41
2	B	1001	NAD	PN-O3	2.60	1.62	1.59
2	H	1001	NAD	C8A-N7A	2.59	1.36	1.31
2	H	1001	NAD	C5A-C6A	2.52	1.48	1.41
4	G	1002	7FN	OAE-CAA	-2.51	1.34	1.38
4	D	1002	7FN	OAJ-CAG	2.44	1.28	1.22
2	D	1001	NAD	C4A-N9A	-2.44	1.32	1.37
2	B	1001	NAD	C4A-N9A	-2.41	1.32	1.37
2	E	1001	NAD	C4A-N9A	-2.39	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1001	NAD	PA-O3	2.38	1.62	1.59
2	B	1001	NAD	C8A-N7A	2.35	1.36	1.31
2	G	1001	NAD	C4A-N9A	-2.34	1.32	1.37
2	A	1001	NAD	C5A-N7A	-2.25	1.35	1.39
4	C	1006	7FN	OAK-CAG	-2.21	1.24	1.30
2	H	1001	NAD	C4A-N9A	-2.15	1.33	1.37
2	E	1001	NAD	C8A-N9A	-2.14	1.33	1.37
2	H	1001	NAD	C3N-C7N	2.08	1.53	1.50
2	G	1001	NAD	C8A-N7A	2.07	1.35	1.31
4	H	1002	7FN	OAH-CAF	-2.06	1.25	1.30
2	A	1001	NAD	C8A-N7A	2.06	1.35	1.31
2	C	1001	NAD	C3N-C7N	2.04	1.53	1.50
2	A	1001	NAD	C4A-N9A	-2.01	1.33	1.37

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAD	O4B-C1B-N9A	5.88	119.38	108.09
2	G	1001	NAD	C5A-C4A-N3A	-5.78	118.75	126.72
2	A	1001	NAD	C5A-C4A-N3A	-5.54	119.09	126.72
2	F	1001	NAD	C5A-C4A-N3A	-5.51	119.13	126.72
2	G	1001	NAD	O4B-C1B-N9A	5.48	118.62	108.09
2	E	1001	NAD	C5A-C4A-N3A	-5.18	119.58	126.72
2	H	1001	NAD	C5A-C4A-N3A	-4.99	119.85	126.72
2	D	1001	NAD	C5A-C4A-N3A	-4.86	120.02	126.72
2	B	1001	NAD	C6N-N1N-C2N	-4.76	117.83	121.88
2	G	1001	NAD	N3A-C4A-N9A	4.66	135.09	127.17
2	H	1001	NAD	C3N-C7N-N7N	4.65	123.46	117.74
2	C	1001	NAD	O2N-PN-O3	4.60	119.72	107.27
2	B	1001	NAD	C3N-C7N-N7N	4.58	123.38	117.74
2	A	1001	NAD	N3A-C4A-N9A	4.47	134.78	127.17
2	D	1001	NAD	N3A-C4A-N9A	4.47	134.77	127.17
2	B	1001	NAD	C5A-C4A-N3A	-4.45	120.59	126.72
2	E	1001	NAD	C4A-C5A-N7A	-4.45	105.50	110.58
2	B	1001	NAD	C5N-C4N-C3N	-4.37	116.06	120.36
2	H	1001	NAD	N3A-C4A-N9A	4.28	134.44	127.17
2	C	1001	NAD	O4B-C1B-N9A	4.28	116.30	108.09
2	E	1001	NAD	N3A-C2A-N1A	-4.24	122.16	128.58
2	C	1001	NAD	N3A-C2A-N1A	-4.23	122.18	128.58
2	A	1001	NAD	N3A-C2A-N1A	-4.20	122.22	128.58
2	B	1001	NAD	N3A-C2A-N1A	-4.14	122.31	128.58
4	E	1002	7FN	OAH-CAF-CAA	4.09	123.32	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1001	NAD	C4A-C5A-N7A	-4.07	105.92	110.58
2	B	1001	NAD	N3A-C4A-N9A	4.05	134.05	127.17
2	C	1001	NAD	C4A-N9A-C8A	4.02	109.96	105.74
4	H	1002	7FN	OAK-CAG-CAD	4.02	123.16	114.06
2	A	1001	NAD	C4A-C5A-N7A	-3.99	106.02	110.58
2	F	1001	NAD	C2A-N3A-C4A	3.96	121.51	111.83
4	G	1002	7FN	OAH-CAF-CAA	3.94	122.98	114.06
2	F	1001	NAD	C4D-O4D-C1D	3.93	113.52	109.92
2	G	1001	NAD	C3N-C7N-N7N	3.93	122.58	117.74
2	F	1001	NAD	N3A-C4A-N9A	3.93	133.85	127.17
2	H	1001	NAD	O4B-C1B-N9A	3.93	115.63	108.09
2	A	1001	NAD	C2A-N3A-C4A	3.90	121.35	111.83
2	B	1001	NAD	O4B-C1B-N9A	3.87	115.52	108.09
2	H	1001	NAD	N3A-C2A-N1A	-3.81	122.82	128.58
2	G	1001	NAD	C2A-N3A-C4A	3.80	121.11	111.83
2	B	1001	NAD	O2N-PN-O3	3.78	117.50	107.27
2	H	1001	NAD	C6N-N1N-C2N	-3.77	118.67	121.88
2	F	1001	NAD	N3A-C2A-N1A	-3.77	122.88	128.58
2	E	1001	NAD	C2A-N3A-C4A	3.74	120.97	111.83
2	G	1001	NAD	N3A-C2A-N1A	-3.74	122.92	128.58
4	H	1002	7FN	OAK-CAG-OAJ	-3.70	115.09	123.90
2	F	1001	NAD	C6N-N1N-C2N	-3.69	118.74	121.88
2	C	1001	NAD	N3A-C4A-N9A	3.63	133.34	127.17
2	E	1001	NAD	N3A-C4A-N9A	3.63	133.34	127.17
4	B	1002	7FN	OAH-CAF-CAA	3.58	122.17	114.06
2	C	1001	NAD	C3N-C7N-N7N	3.55	122.11	117.74
2	H	1001	NAD	C4A-N9A-C8A	3.52	109.44	105.74
2	D	1001	NAD	C4A-N9A-C8A	3.50	109.41	105.74
4	C	1002	7FN	OAK-CAG-CAD	3.49	121.96	114.06
2	A	1001	NAD	C4A-N9A-C8A	3.42	109.33	105.74
2	H	1001	NAD	C2A-N3A-C4A	3.40	120.14	111.83
4	E	1002	7FN	OAK-CAG-CAD	3.39	121.74	114.06
2	D	1001	NAD	O2N-PN-O3	3.37	116.39	107.27
2	C	1001	NAD	C5A-C4A-N3A	-3.29	122.19	126.72
2	H	1001	NAD	O7N-C7N-N7N	-3.27	117.89	122.62
2	A	1001	NAD	C5A-N7A-C8A	3.26	108.58	103.45
4	C	1002	7FN	OAK-CAG-OAJ	-3.25	116.16	123.90
4	C	1006	7FN	OAH-CAF-CAA	3.23	121.38	114.06
4	C	1006	7FN	OAK-CAG-CAD	3.21	121.33	114.06
2	D	1001	NAD	O4B-C1B-N9A	3.19	114.22	108.09
2	E	1001	NAD	O4B-C1B-N9A	3.17	114.17	108.09
2	B	1001	NAD	C4A-N9A-C8A	3.16	109.06	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	NAD	C4A-N9A-C1B	-3.13	119.32	126.63
2	C	1001	NAD	C2A-N3A-C4A	3.10	119.41	111.83
2	A	1001	NAD	O7N-C7N-N7N	-3.10	118.14	122.62
2	B	1001	NAD	O7N-C7N-N7N	-3.09	118.15	122.62
2	E	1001	NAD	C6A-C5A-N7A	3.05	137.97	132.09
2	E	1001	NAD	C5A-N7A-C8A	3.04	108.22	103.45
2	D	1001	NAD	N3A-C2A-N1A	-2.96	124.10	128.58
2	E	1001	NAD	C4A-N9A-C8A	2.96	108.84	105.74
2	B	1001	NAD	C2A-N3A-C4A	2.95	119.05	111.83
2	G	1001	NAD	C6N-N1N-C2N	-2.95	119.37	121.88
2	D	1001	NAD	C6N-N1N-C1D	2.94	125.49	119.73
2	F	1001	NAD	C6A-C5A-N7A	2.93	137.73	132.09
2	C	1001	NAD	C6N-N1N-C1D	2.89	125.39	119.73
2	E	1001	NAD	C2A-N1A-C6A	2.88	123.47	118.73
2	D	1001	NAD	C2A-N3A-C4A	2.87	118.83	111.83
2	H	1001	NAD	C4A-C5A-N7A	-2.86	107.31	110.58
2	C	1001	NAD	C2A-N1A-C6A	2.84	123.40	118.73
4	F	1002	7FN	OAK-CAG-CAD	2.82	120.46	114.06
2	A	1001	NAD	N9A-C8A-N7A	-2.82	109.93	113.94
4	D	1002	7FN	OAK-CAG-CAD	2.81	120.44	114.06
2	C	1001	NAD	O2A-PA-O1A	2.81	125.50	112.44
4	B	1002	7FN	OAK-CAG-CAD	2.80	120.40	114.06
2	G	1001	NAD	O7N-C7N-N7N	-2.79	118.58	122.62
4	B	1002	7FN	OAH-CAF-OAI	-2.79	117.25	123.90
2	G	1001	NAD	C4A-C5A-N7A	-2.79	107.39	110.58
2	G	1001	NAD	O2A-PA-O5B	-2.78	94.97	107.57
4	C	1006	7FN	OAH-CAF-OAI	-2.76	117.32	123.90
2	C	1001	NAD	C2D-C3D-C4D	2.76	107.95	102.61
2	G	1001	NAD	O4B-C1B-C2B	-2.76	100.71	106.62
2	B	1001	NAD	O2A-PA-O1A	2.76	125.28	112.44
2	D	1001	NAD	C4A-C5A-N7A	-2.76	107.43	110.58
4	G	1002	7FN	OAH-CAF-OAI	-2.72	117.41	123.90
2	G	1001	NAD	C4B-O4B-C1B	-2.70	103.50	109.47
2	B	1001	NAD	C4A-N9A-C1B	-2.69	120.34	126.63
2	F	1001	NAD	C5A-N7A-C8A	2.68	107.67	103.45
2	A	1001	NAD	C4D-O4D-C1D	2.68	112.38	109.92
2	H	1001	NAD	C6N-N1N-C1D	2.67	124.96	119.73
2	E	1001	NAD	O2A-PA-O3	2.66	114.45	107.27
2	E	1001	NAD	O5B-PA-O1A	2.65	119.44	108.94
2	B	1001	NAD	C2A-N1A-C6A	2.65	123.08	118.73
2	A	1001	NAD	C6A-C5A-N7A	2.65	137.20	132.09
2	D	1001	NAD	O7N-C7N-N7N	-2.65	118.79	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1001	NAD	C2A-N1A-C6A	2.60	123.01	118.73
4	C	1006	7FN	OAK-CAG-OAJ	-2.58	117.76	123.90
2	C	1001	NAD	O7N-C7N-N7N	-2.57	118.90	122.62
2	D	1001	NAD	O2A-PA-O1A	2.57	124.41	112.44
2	A	1001	NAD	C2A-N1A-C6A	2.56	122.94	118.73
2	H	1001	NAD	C6A-C5A-N7A	2.54	136.99	132.09
2	D	1001	NAD	C5N-C4N-C3N	-2.53	117.87	120.36
2	E	1001	NAD	N9A-C8A-N7A	-2.53	110.35	113.94
2	E	1001	NAD	C4A-N9A-C1B	-2.53	120.72	126.63
2	A	1001	NAD	C6N-N1N-C2N	-2.52	119.74	121.88
4	D	1002	7FN	OAH-CAF-CAA	2.51	119.76	114.06
4	D	1002	7FN	OAK-CAG-OAJ	-2.51	117.92	123.90
2	E	1001	NAD	O2N-PN-O3	2.51	114.06	107.27
2	D	1001	NAD	C5A-N7A-C8A	2.50	107.38	103.45
2	A	1001	NAD	C3N-C7N-N7N	2.48	120.80	117.74
4	D	1002	7FN	OAE-CAD-CAC	-2.45	106.84	109.68
4	C	1002	7FN	OAE-CAA-CAB	-2.44	106.85	109.68
2	F	1001	NAD	C3N-C7N-N7N	2.44	120.75	117.74
2	E	1001	NAD	O2A-PA-O5B	-2.44	96.50	107.57
2	G	1001	NAD	C4A-N9A-C8A	2.43	108.29	105.74
2	G	1001	NAD	O2A-PA-O1A	2.41	123.67	112.44
2	F	1001	NAD	O7N-C7N-N7N	-2.41	119.13	122.62
2	F	1001	NAD	C4A-N9A-C8A	2.41	108.27	105.74
2	C	1001	NAD	C6A-C5A-N7A	2.39	136.70	132.09
2	C	1001	NAD	C2N-N1N-C1D	-2.39	113.86	119.13
2	D	1001	NAD	N9A-C8A-N7A	-2.37	110.58	113.94
4	B	1002	7FN	CAD-OAE-CAA	2.36	109.58	106.91
4	H	1002	7FN	OAE-CAD-CAC	-2.32	107.00	109.68
2	A	1001	NAD	O4B-C1B-C2B	-2.31	101.68	106.62
2	G	1001	NAD	C6A-C5A-N7A	2.28	136.49	132.09
2	F	1001	NAD	C2A-N1A-C6A	2.28	122.48	118.73
2	D	1001	NAD	C2N-N1N-C1D	-2.26	114.15	119.13
4	G	1002	7FN	CAC-CAB-CAA	2.26	108.96	106.94
4	C	1002	7FN	CAB-CAC-CAD	2.25	108.96	106.94
2	B	1001	NAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	C	1001	NAD	O4B-C4B-C3B	2.23	109.58	105.15
2	B	1001	NAD	C6N-N1N-C1D	2.22	124.08	119.73
2	C	1001	NAD	O3D-C3D-C4D	-2.21	104.72	111.08
2	E	1001	NAD	O4D-C4D-C5D	2.21	116.42	109.33
2	H	1001	NAD	O2A-PA-O1A	2.19	122.65	112.44
2	H	1001	NAD	N9A-C8A-N7A	-2.19	110.83	113.94
2	G	1001	NAD	C6N-N1N-C1D	2.16	123.97	119.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	NAD	C2A-N1A-C6A	2.15	122.27	118.73
4	C	1002	7FN	OAH-CAF-CAA	2.14	118.90	114.06
4	F	1002	7FN	CAD-OAE-CAA	2.12	109.30	106.91
2	H	1001	NAD	C4A-N9A-C1B	-2.11	121.70	126.63
2	C	1001	NAD	C6A-C5A-C4A	-2.09	114.33	117.18
2	D	1001	NAD	N6A-C6A-N1A	2.08	123.00	118.38
2	G	1001	NAD	O2N-PN-O3	2.07	112.87	107.27
2	H	1001	NAD	C5A-N7A-C8A	2.07	106.70	103.45
2	G	1001	NAD	O3-PA-O1A	-2.06	104.52	110.70
2	H	1001	NAD	C2D-C3D-C4D	2.05	106.58	102.61
2	F	1001	NAD	O3-PN-O1N	-2.04	104.55	110.70
4	F	1002	7FN	CAC-CAB-CAA	-2.04	105.12	106.94
2	B	1001	NAD	C4D-O4D-C1D	2.04	111.79	109.92
2	F	1001	NAD	O5D-C5D-C4D	2.02	115.89	108.99

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAD	C5B-O5B-PA-O1A
2	A	1001	NAD	O4D-C4D-C5D-O5D
2	B	1001	NAD	O4D-C1D-N1N-C2N
2	B	1001	NAD	O4D-C1D-N1N-C6N
2	B	1001	NAD	C2D-C1D-N1N-C2N
2	B	1001	NAD	C2D-C1D-N1N-C6N
2	C	1001	NAD	O4D-C1D-N1N-C2N
2	C	1001	NAD	O4D-C1D-N1N-C6N
2	C	1001	NAD	C2D-C1D-N1N-C2N
2	D	1001	NAD	O4D-C1D-N1N-C2N
2	D	1001	NAD	O4D-C1D-N1N-C6N
2	D	1001	NAD	C2D-C1D-N1N-C2N
2	D	1001	NAD	C2D-C1D-N1N-C6N
2	E	1001	NAD	O4D-C1D-N1N-C2N
2	E	1001	NAD	O4D-C1D-N1N-C6N
2	E	1001	NAD	C2D-C1D-N1N-C2N
2	F	1001	NAD	O4D-C1D-N1N-C2N
2	F	1001	NAD	O4D-C1D-N1N-C6N
2	F	1001	NAD	C2D-C1D-N1N-C2N
2	F	1001	NAD	C2D-C1D-N1N-C6N
2	G	1001	NAD	O4D-C1D-N1N-C2N
2	G	1001	NAD	O4D-C1D-N1N-C6N
2	G	1001	NAD	C2D-C1D-N1N-C2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	1001	NAD	C2D-C1D-N1N-C6N
2	H	1001	NAD	O4D-C1D-N1N-C2N
2	H	1001	NAD	O4D-C1D-N1N-C6N
2	H	1001	NAD	C2D-C1D-N1N-C2N
2	A	1001	NAD	C3D-C4D-C5D-O5D
2	G	1001	NAD	O4B-C4B-C5B-O5B
2	C	1001	NAD	O4B-C4B-C5B-O5B
2	G	1001	NAD	C3B-C4B-C5B-O5B
2	C	1001	NAD	C3B-C4B-C5B-O5B
2	A	1001	NAD	PA-O3-PN-O1N
2	E	1001	NAD	O4B-C4B-C5B-O5B
2	A	1001	NAD	C5B-O5B-PA-O2A
2	A	1001	NAD	C5B-O5B-PA-O3
2	E	1001	NAD	C5D-O5D-PN-O3
2	C	1001	NAD	C2D-C1D-N1N-C6N
2	E	1001	NAD	C2D-C1D-N1N-C6N
2	A	1001	NAD	O4D-C1D-N1N-C2N
2	E	1001	NAD	C3B-C4B-C5B-O5B
2	D	1001	NAD	O4B-C4B-C5B-O5B
4	H	1002	7FN	OAE-CAD-CAG-OAJ
2	A	1001	NAD	PA-O3-PN-O2N
2	E	1001	NAD	O4D-C4D-C5D-O5D

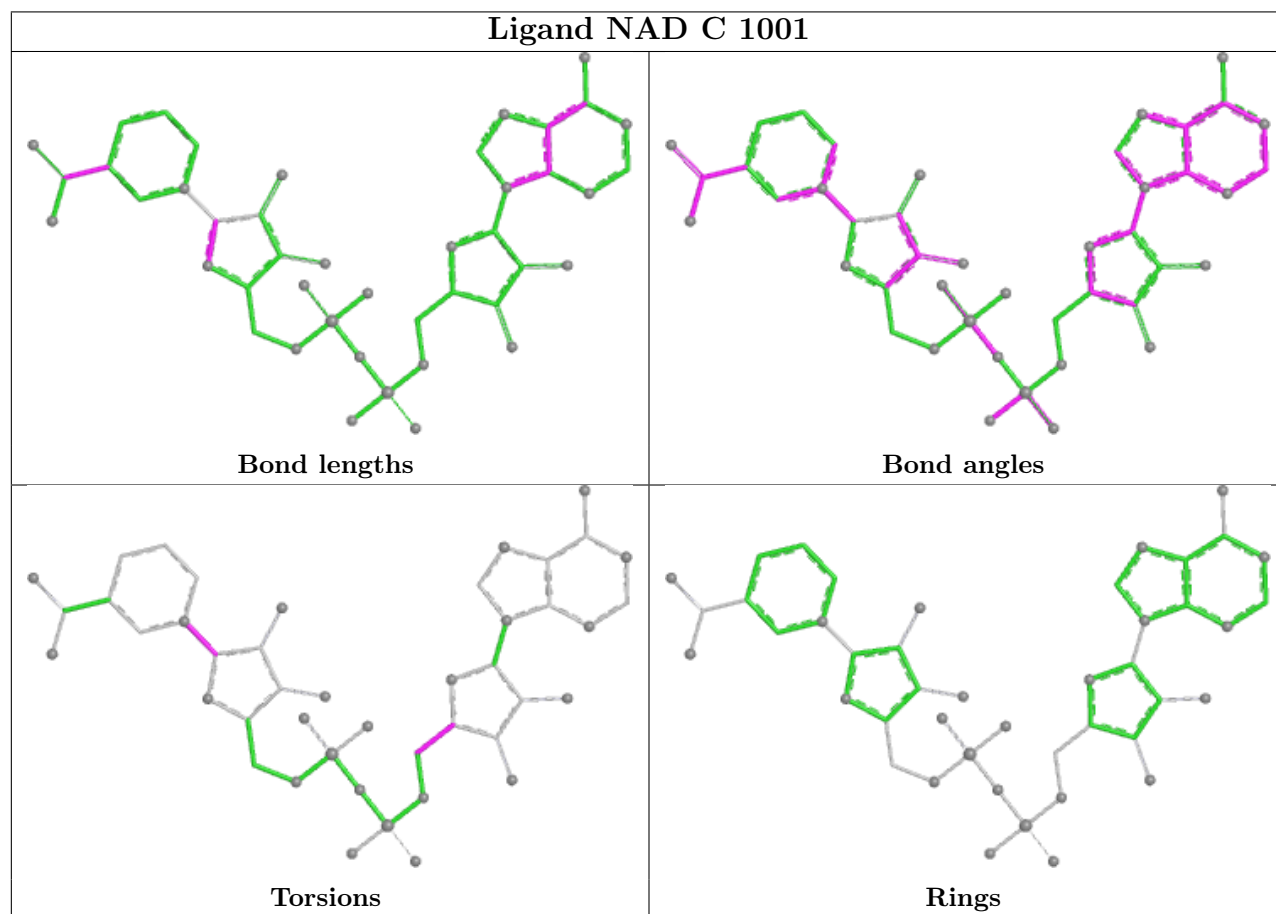
There are no ring outliers.

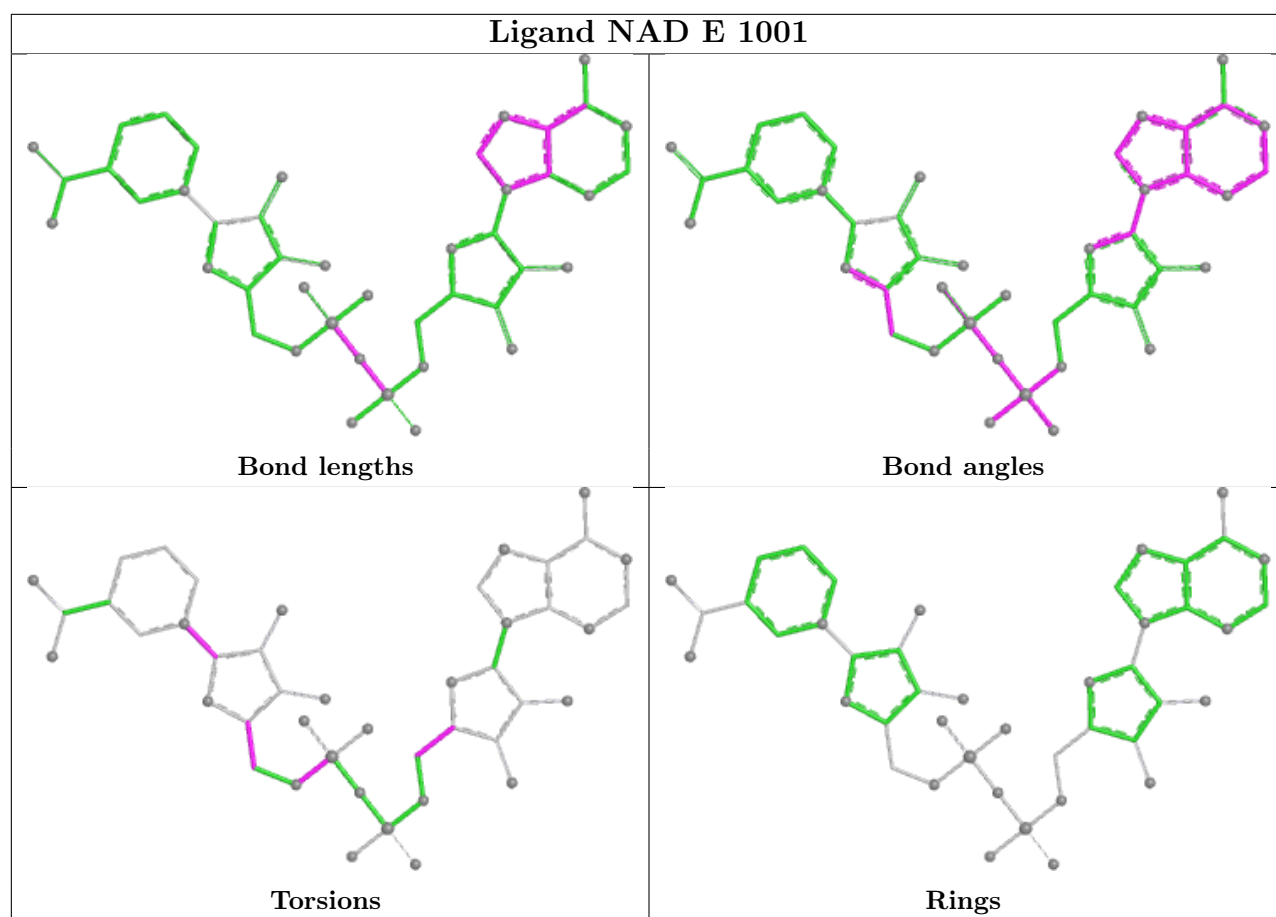
6 monomers are involved in 8 short contacts:

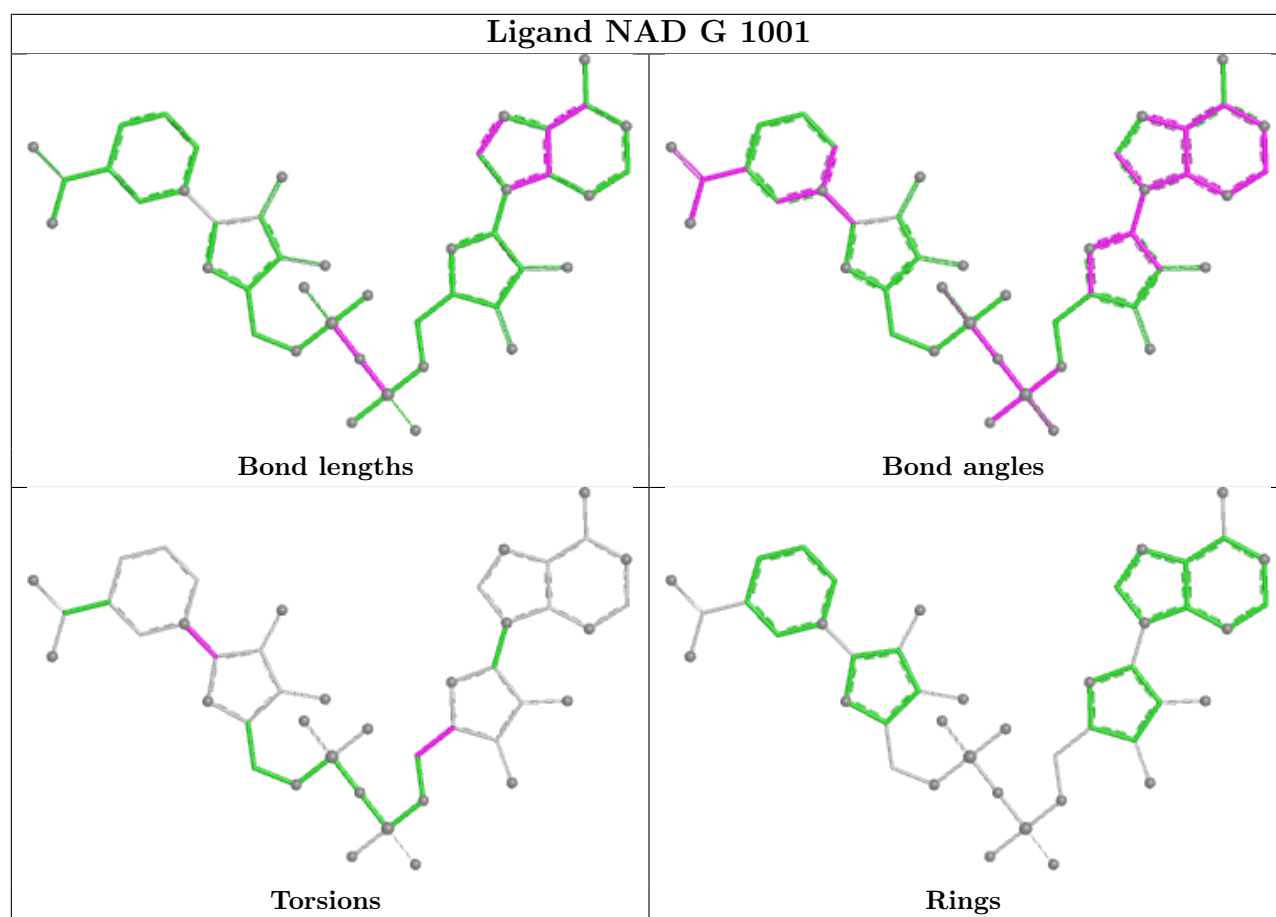
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1005	SO4	1	0
2	E	1001	NAD	1	0
2	G	1001	NAD	2	0
2	B	1001	NAD	2	0
2	D	1001	NAD	1	0
2	F	1001	NAD	1	0

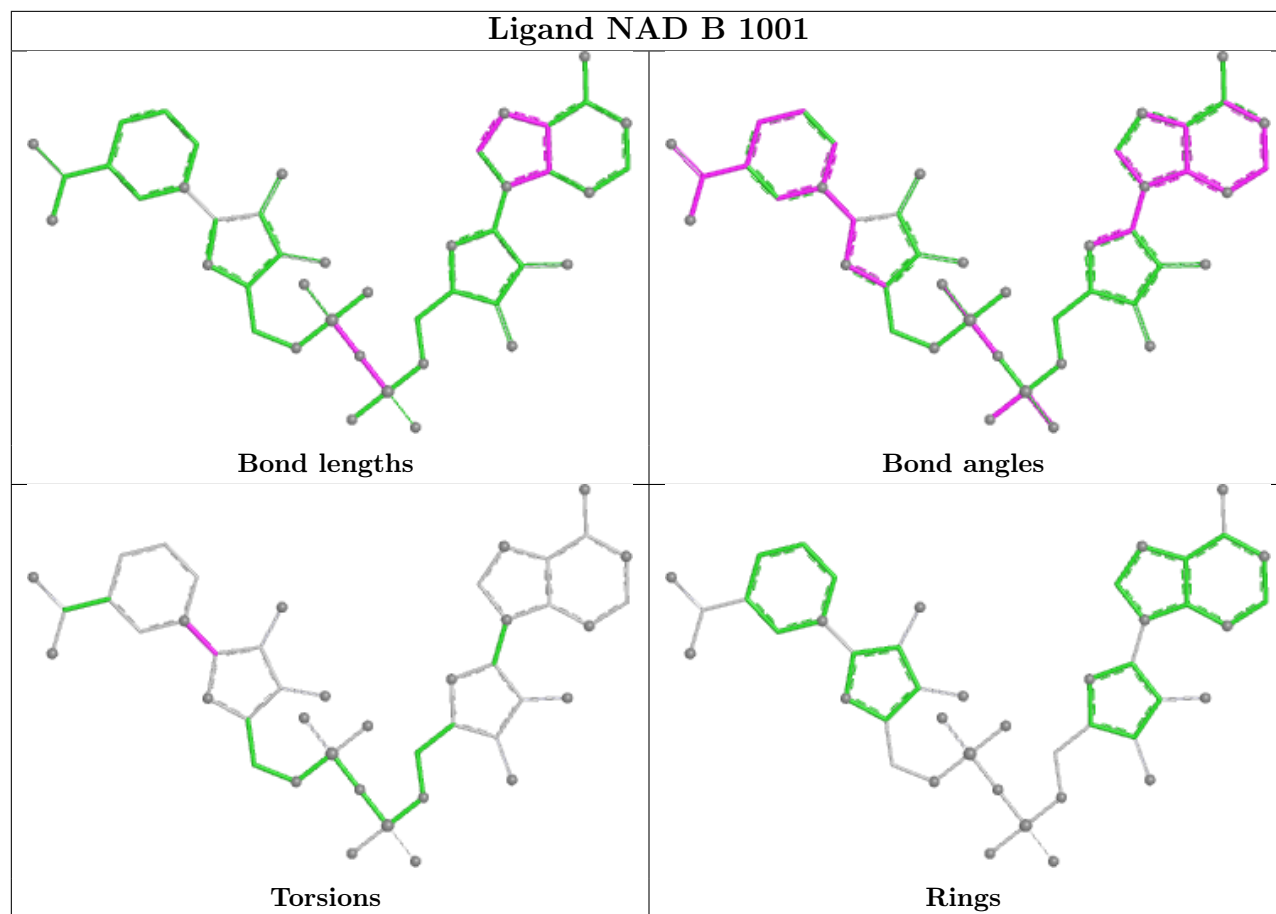
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

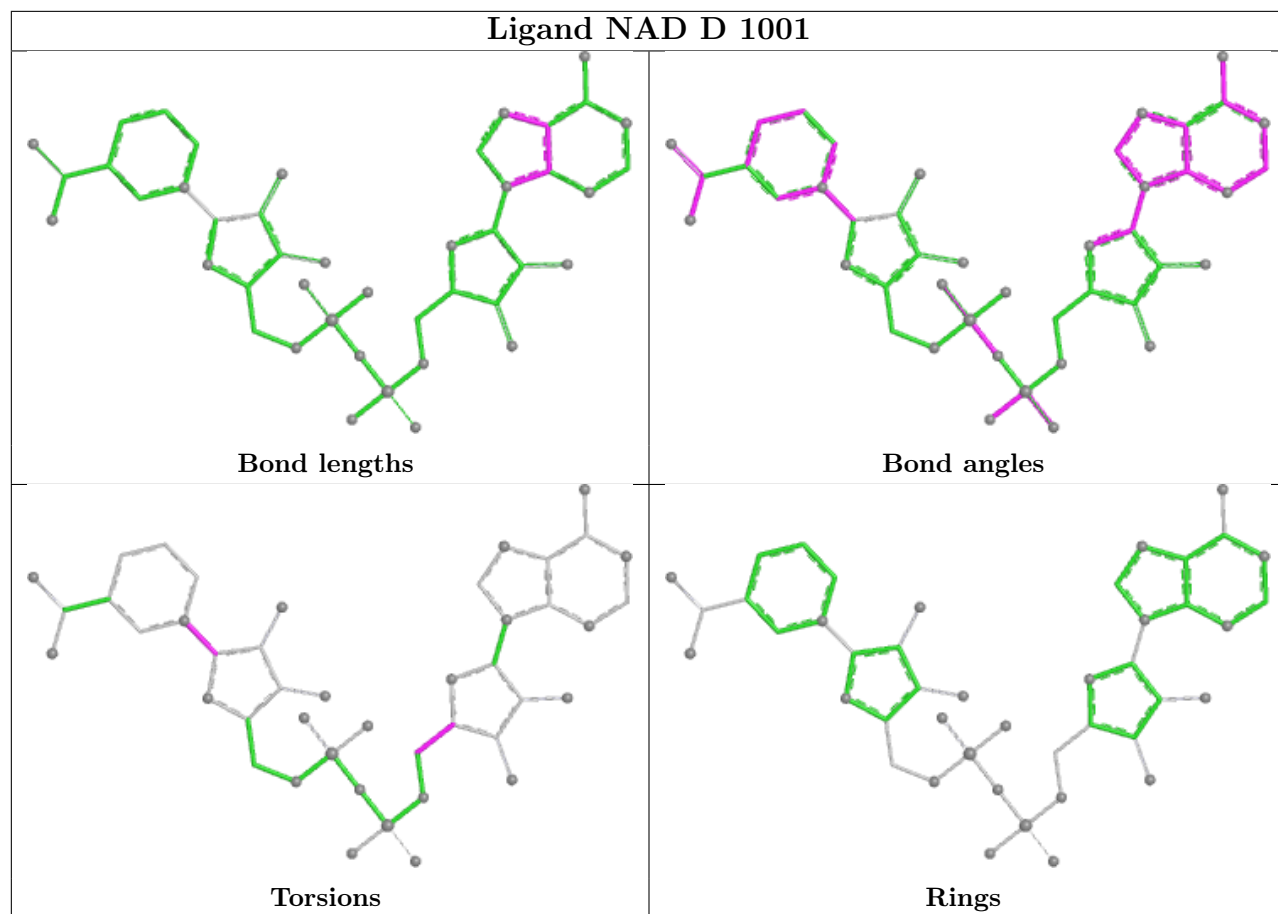
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

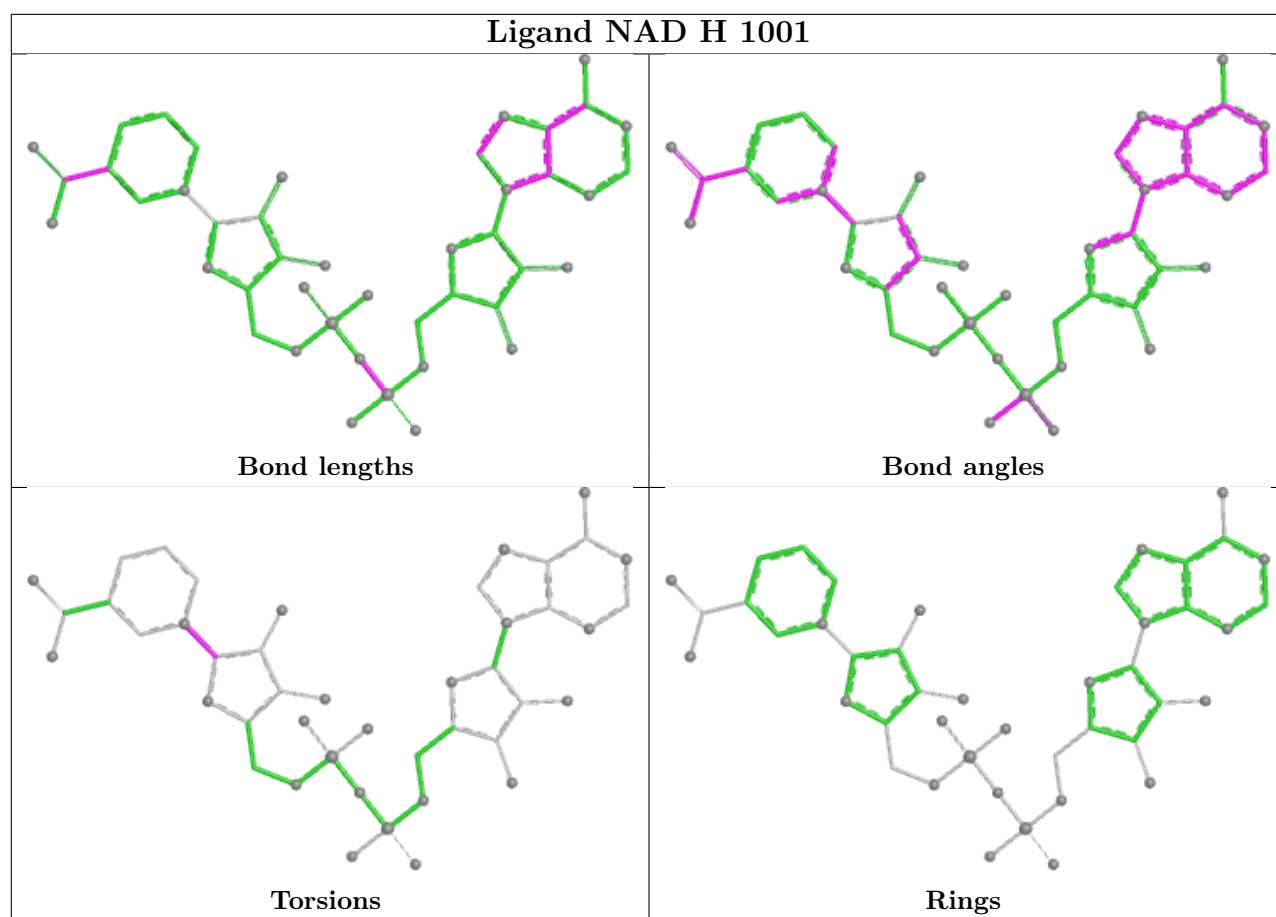


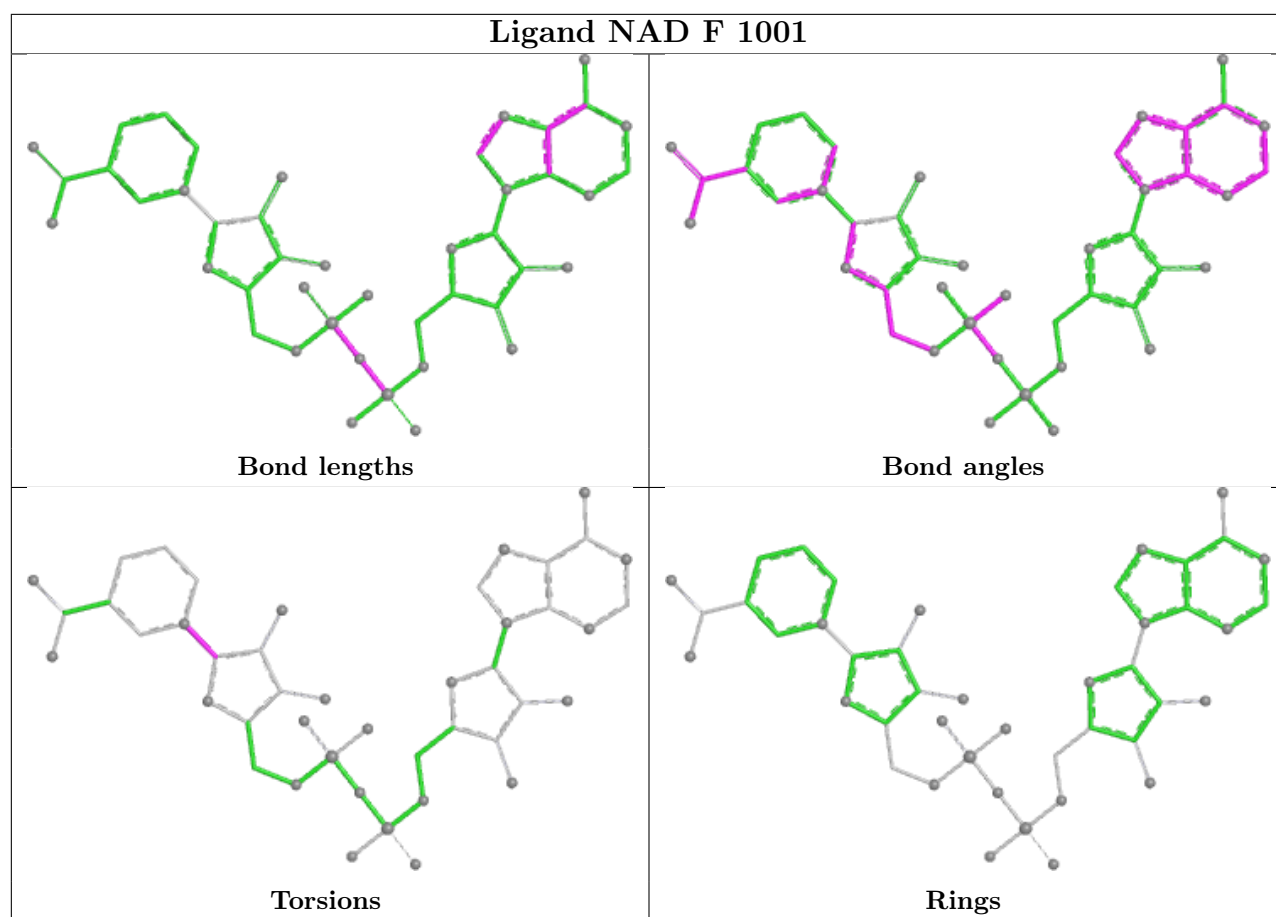


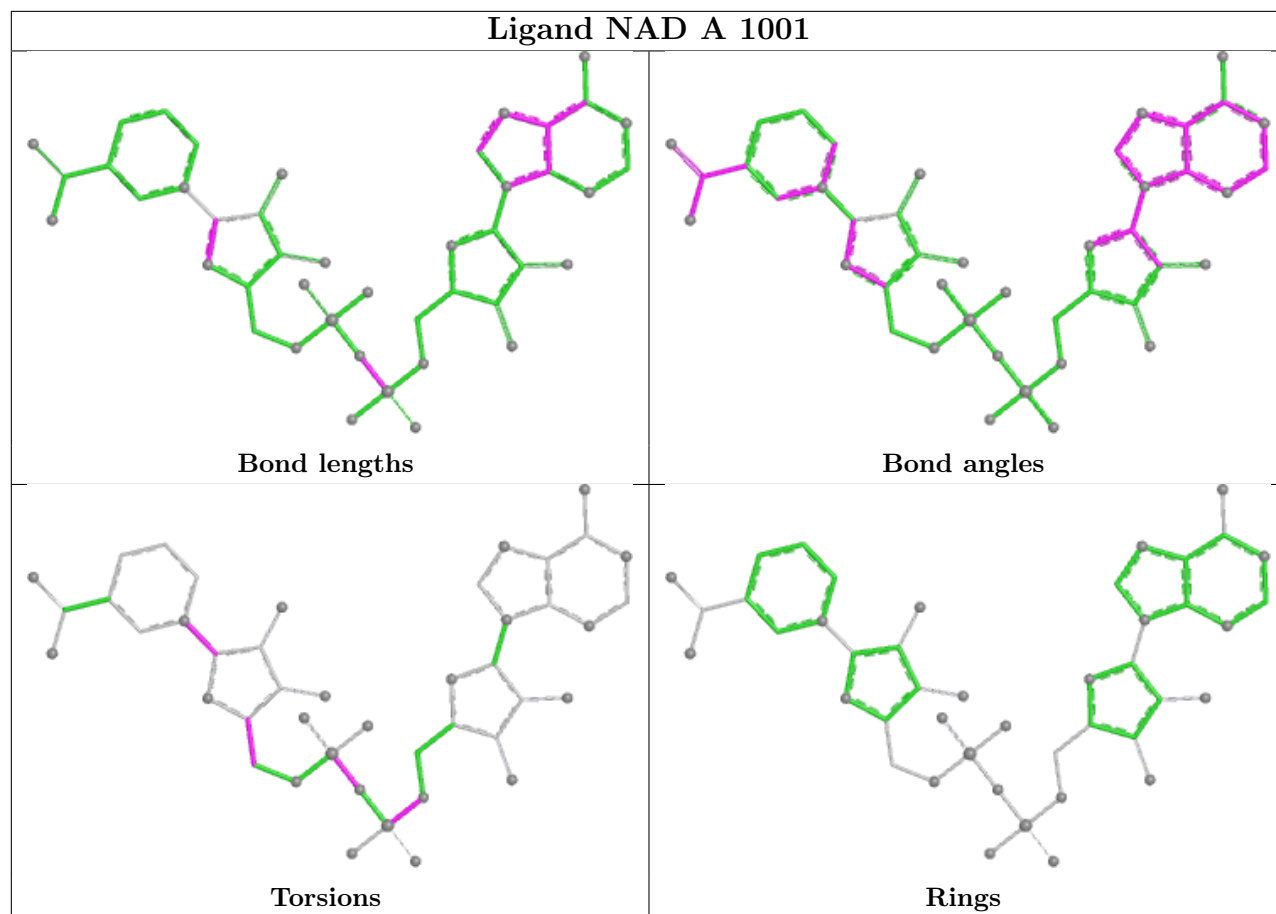












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/269 (100%)	0.34	5 (1%) 66 67	27, 44, 78, 99	0
1	B	269/269 (100%)	0.10	4 (1%) 72 74	28, 40, 73, 110	0
1	C	269/269 (100%)	0.29	6 (2%) 62 64	29, 42, 80, 105	0
1	D	269/269 (100%)	0.07	2 (0%) 84 86	27, 38, 71, 86	0
1	E	269/269 (100%)	0.62	16 (5%) 28 25	30, 55, 106, 128	0
1	F	269/269 (100%)	0.77	25 (9%) 14 12	33, 55, 96, 112	0
1	G	269/269 (100%)	0.51	13 (4%) 35 34	29, 47, 76, 105	0
1	H	267/269 (99%)	0.62	24 (8%) 15 13	26, 48, 95, 118	0
All	All	2150/2152 (99%)	0.41	95 (4%) 39 38	26, 46, 89, 128	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	39	SER	4.6
1	E	48	LEU	4.5
1	C	40	LEU	4.1
1	G	48	LEU	4.0
1	F	39	SER	3.6
1	E	40	LEU	3.5
1	H	45	LEU	3.5
1	H	20	ALA	3.5
1	F	43	VAL	3.3
1	B	49	CYS	3.3
1	H	48	LEU	3.3
1	E	29	VAL	3.3
1	G	25	PRO	3.2
1	G	57	VAL	3.2
1	F	55	ASP	3.2
1	F	40	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	198	THR	3.1
1	B	23	HIS	3.0
1	H	31	ALA	3.0
1	G	269	LEU	2.9
1	E	269	LEU	2.9
1	A	37	GLU	2.8
1	F	91	TYR	2.8
1	C	41	VAL	2.8
1	F	119	VAL	2.8
1	G	45	LEU	2.8
1	E	51	GLU	2.8
1	H	67	ASP	2.8
1	H	27	ALA	2.7
1	H	44	ASP	2.6
1	F	48	LEU	2.6
1	E	38	SER	2.6
1	F	256	GLY	2.6
1	E	57	VAL	2.6
1	H	85	LEU	2.6
1	B	50	GLY	2.5
1	B	48	LEU	2.5
1	G	40	LEU	2.5
1	F	67	ASP	2.5
1	A	40	LEU	2.5
1	H	30	ALA	2.5
1	H	88	CYS	2.4
1	H	29	VAL	2.4
1	G	69	PHE	2.4
1	G	18	VAL	2.4
1	G	30	ALA	2.4
1	F	42	GLY	2.4
1	H	26	VAL	2.4
1	E	45	LEU	2.3
1	G	23	HIS	2.3
1	H	57	VAL	2.3
1	E	66	ILE	2.3
1	H	66	ILE	2.3
1	E	235	ASP	2.3
1	C	1	MET	2.3
1	E	64	LYS	2.3
1	H	49	CYS	2.3
1	F	258	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	258	TYR	2.3
1	C	42	GLY	2.3
1	F	113	VAL	2.3
1	G	21	ALA	2.3
1	H	256	GLY	2.3
1	F	112	LEU	2.3
1	D	49	CYS	2.3
1	H	32	GLY	2.2
1	C	43	VAL	2.2
1	H	54	PHE	2.2
1	F	2	VAL	2.2
1	G	265	GLY	2.2
1	F	72	ILE	2.2
1	H	94	SER	2.2
1	H	2	VAL	2.1
1	F	100	THR	2.1
1	H	69	PHE	2.1
1	H	255	ALA	2.1
1	F	92	GLY	2.1
1	G	85	LEU	2.1
1	F	45	LEU	2.1
1	E	146	TYR	2.1
1	F	41	VAL	2.1
1	E	10	ALA	2.1
1	E	91	TYR	2.1
1	A	116	GLN	2.0
1	F	71	VAL	2.0
1	D	140	ALA	2.0
1	A	38	SER	2.0
1	F	36	PRO	2.0
1	F	49	CYS	2.0
1	F	90	GLN	2.0
1	F	117	VAL	2.0
1	H	142	VAL	2.0
1	C	48	LEU	2.0
1	A	50	GLY	2.0
1	E	36	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	F	1004	5/5	0.46	0.17	88,106,115,116	0
3	SO4	A	1005	5/5	0.54	0.15	93,96,115,116	0
3	SO4	E	1004	5/5	0.71	0.21	65,78,82,96	0
3	SO4	F	1005	5/5	0.71	0.19	66,69,78,80	0
3	SO4	C	1003	5/5	0.73	0.17	75,89,101,102	0
3	SO4	H	1005	5/5	0.74	0.24	77,77,91,91	0
3	SO4	A	1004	5/5	0.75	0.11	89,98,104,113	0
3	SO4	E	1003	5/5	0.77	0.18	90,92,94,98	0
3	SO4	G	1004	5/5	0.78	0.15	90,91,103,112	0
2	NAD	A	1001	44/44	0.78	0.14	61,75,84,86	0
3	SO4	A	1002	5/5	0.79	0.14	68,72,79,80	0
3	SO4	H	1003	5/5	0.79	0.19	116,125,136,138	0
3	SO4	F	1003	5/5	0.79	0.14	53,72,78,83	0
3	SO4	G	1003	5/5	0.80	0.20	85,90,96,96	0
3	SO4	H	1004	5/5	0.80	0.14	75,76,84,92	0
3	SO4	C	1005	5/5	0.80	0.24	89,90,91,96	0
4	7FN	C	1006	11/11	0.82	0.10	50,57,60,61	0
3	SO4	B	1003	5/5	0.84	0.14	59,63,77,77	0
4	7FN	F	1002	11/11	0.84	0.10	33,42,46,49	0
3	SO4	D	1003	5/5	0.87	0.14	60,63,66,69	0
4	7FN	D	1002	11/11	0.88	0.10	30,36,39,40	0
4	7FN	E	1002	11/11	0.89	0.10	34,36,40,41	0
4	7FN	B	1002	11/11	0.89	0.10	27,29,31,31	0
3	SO4	A	1003	5/5	0.90	0.13	61,62,65,67	0
2	NAD	E	1001	44/44	0.90	0.10	34,51,62,68	0
4	7FN	G	1002	11/11	0.90	0.11	29,35,40,42	0
2	NAD	F	1001	44/44	0.91	0.10	31,50,81,86	0
4	7FN	C	1002	11/11	0.92	0.09	28,36,39,39	0
4	7FN	H	1002	11/11	0.92	0.09	33,37,46,47	0
2	NAD	G	1001	44/44	0.93	0.08	32,40,51,54	0
3	SO4	C	1004	5/5	0.93	0.10	55,58,64,67	0
2	NAD	C	1001	44/44	0.95	0.08	30,38,41,43	0

Continued on next page...

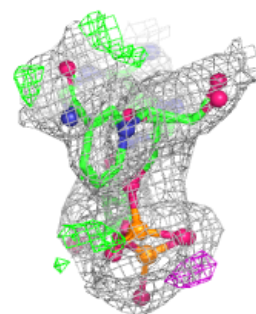
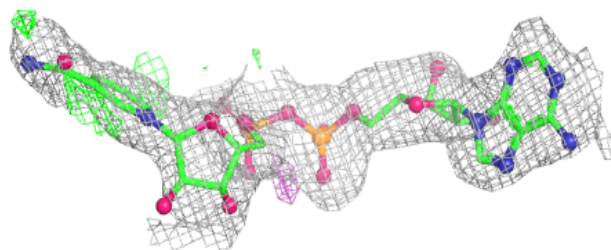
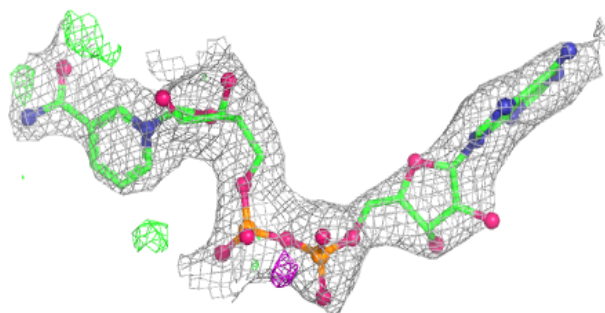
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	1001	44/44	0.95	0.07	26,33,40,42	0
2	NAD	H	1001	44/44	0.95	0.07	26,35,41,47	0
2	NAD	D	1001	44/44	0.96	0.07	25,36,40,42	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.

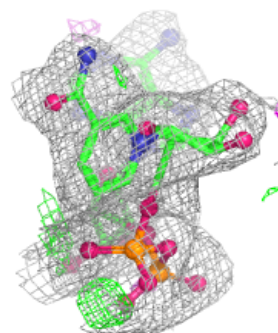
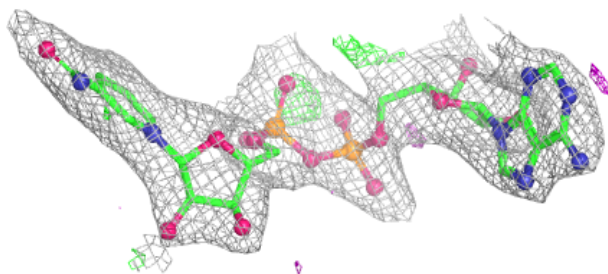
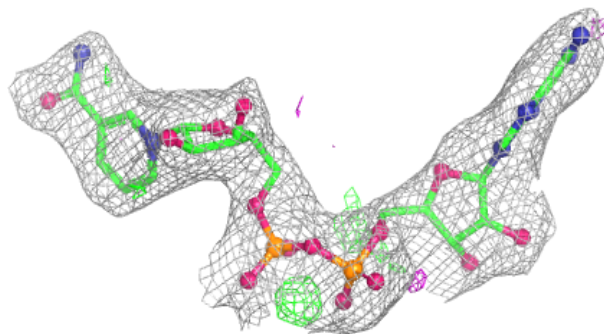
Electron density around NAD A 1001:

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

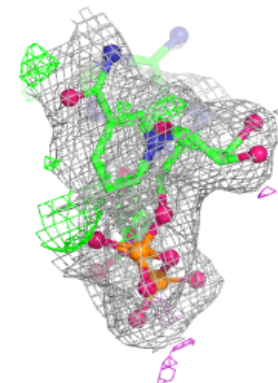
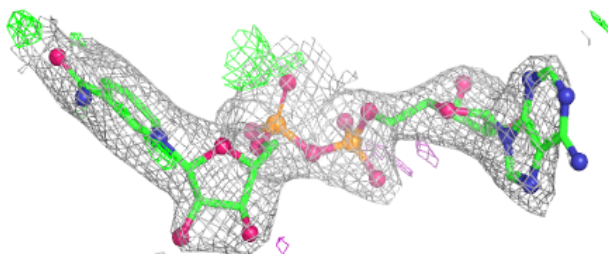
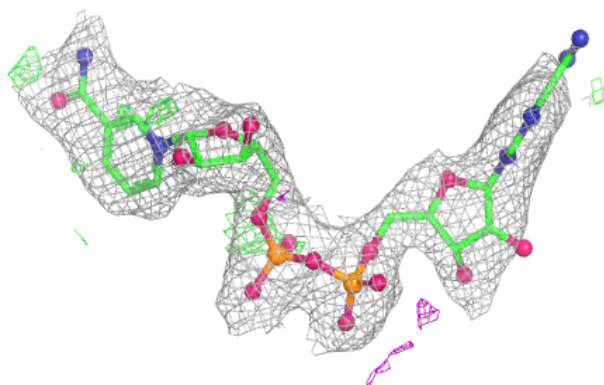


Electron density around NAD E 1001:

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

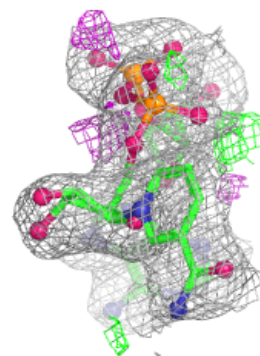
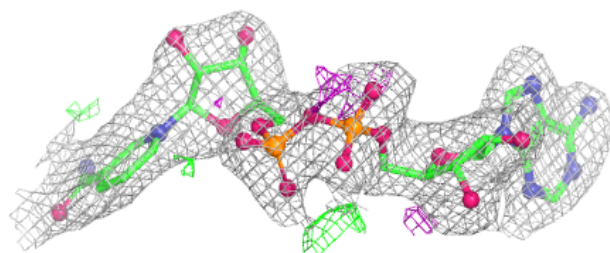
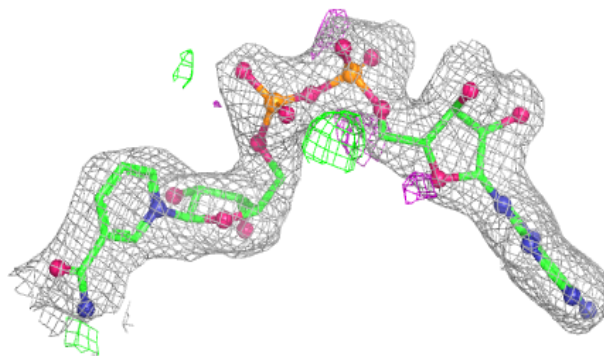
**Electron density around NAD F 1001:**

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

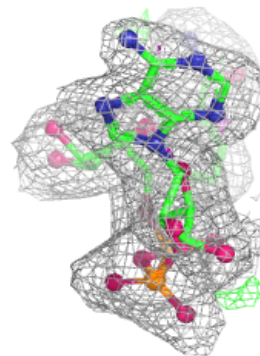
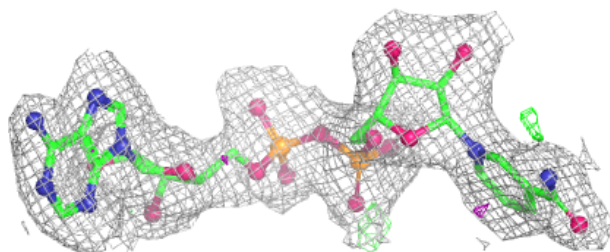
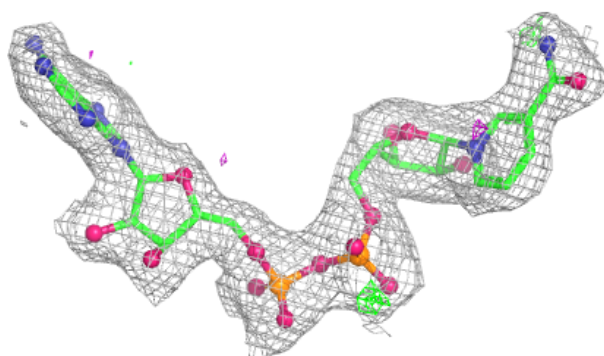


Electron density around NAD G 1001:

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

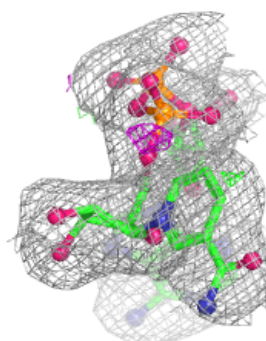
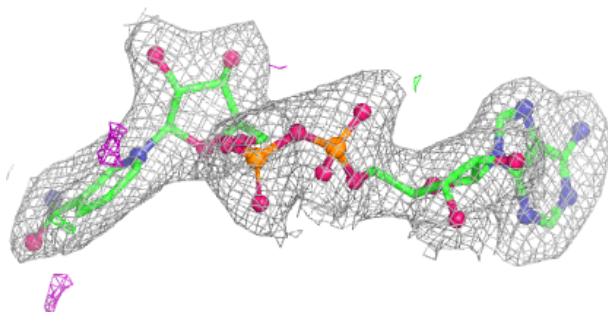
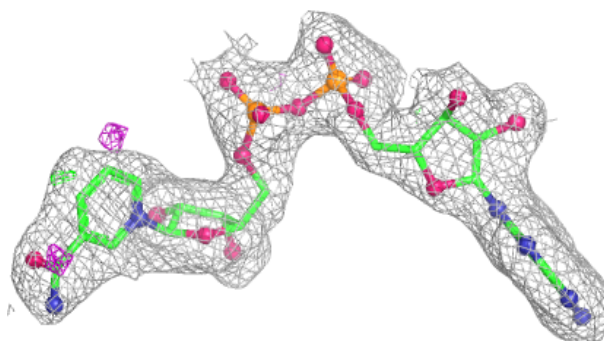
**Electron density around NAD C 1001:**

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

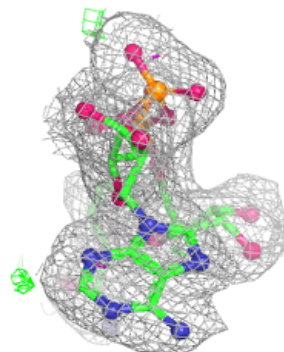
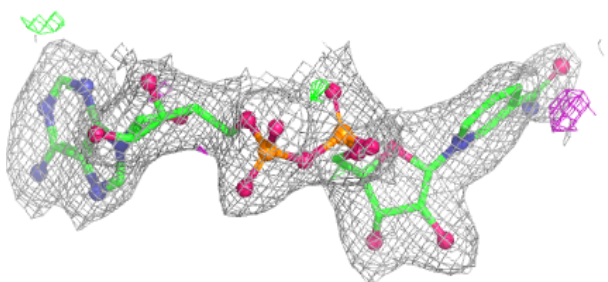
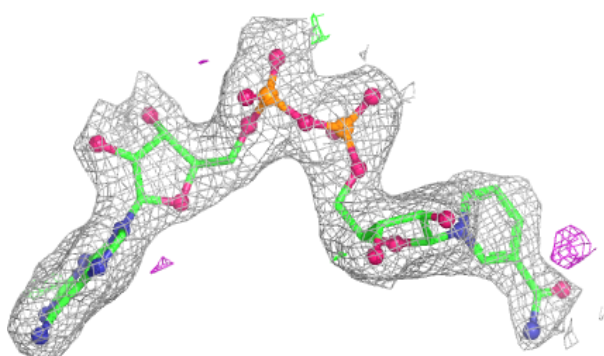


Electron density around NAD B 1001:

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

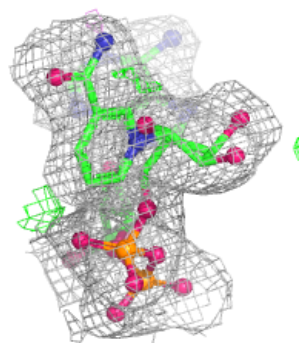
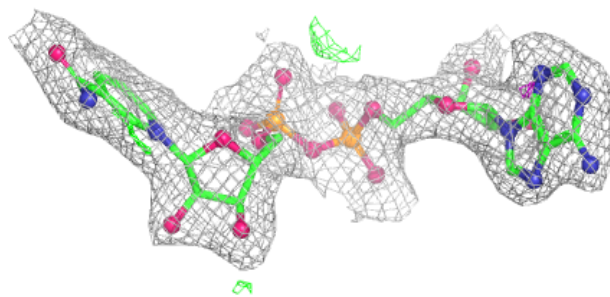
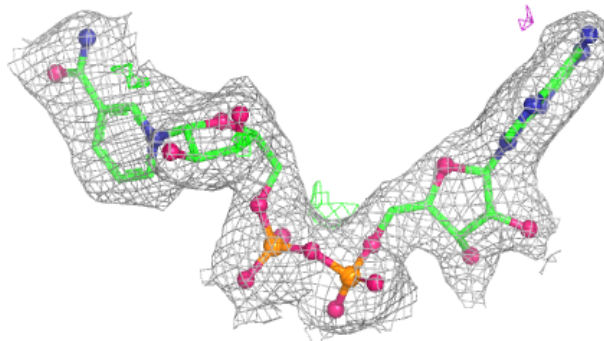
**Electron density around NAD H 1001:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.