



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:22 AM UTC

PDB ID : 1O00 / pdb_00001o00
Title : Human mitochondrial aldehyde dehydrogenase complexed with NAD⁺ and Mg²⁺ showing dual NAD(H) conformations
Authors : Perez-Miller, S.J.; Hurley, T.D.
Deposited on : 2003-02-20
Resolution : 2.60 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

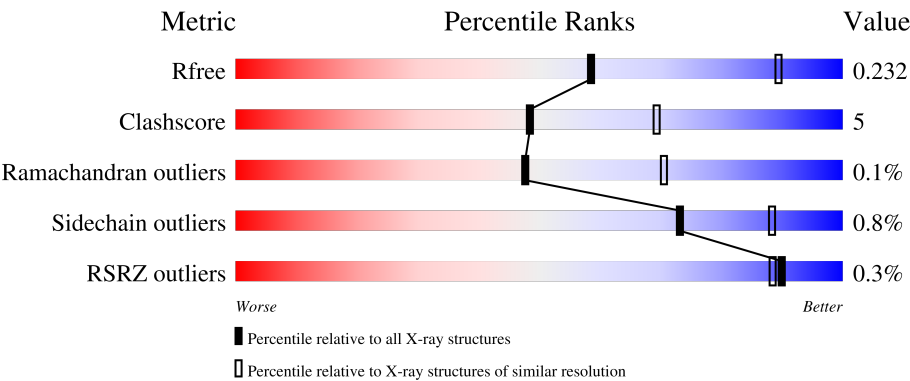
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	500	84%14%..
1	B	500	85%13%..
1	C	500	85%13%..
1	D	500	%86%13%.
1	E	500	85%13%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	500	84% 14% ..
1	G	500	86% 12% ..
1	H	500	% 84% 15% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32876 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	717	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

Continued on next page...

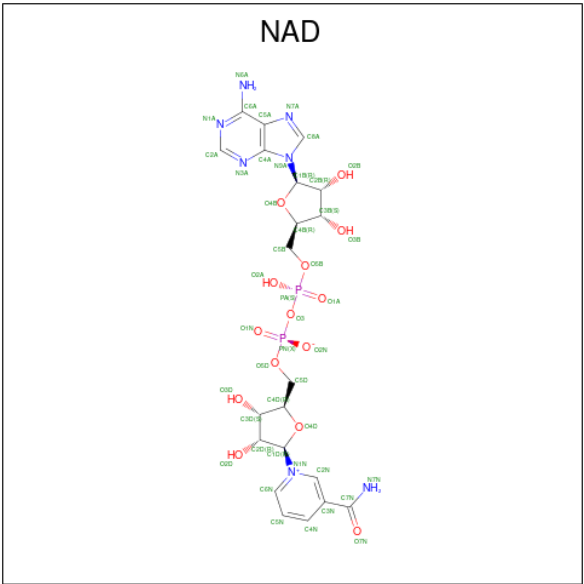
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	E	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	F	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	G	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	H	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

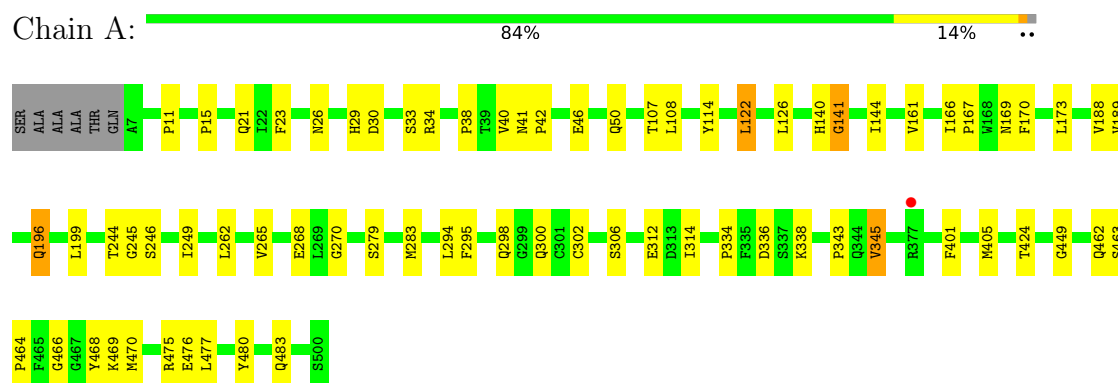
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total	O	0	0
			250	250		
5	B	241	Total	O	0	0
			241	241		
5	C	209	Total	O	0	0
			209	209		
5	D	199	Total	O	0	0
			199	199		
5	E	252	Total	O	0	0
			252	252		
5	F	234	Total	O	0	0
			234	234		
5	G	199	Total	O	0	0
			199	199		
5	H	188	Total	O	0	0
			188	188		

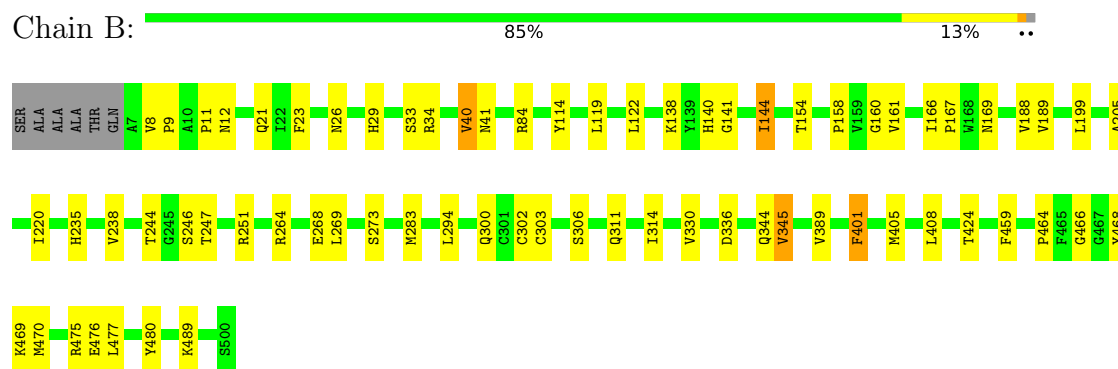
3 Residue-property plots

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.

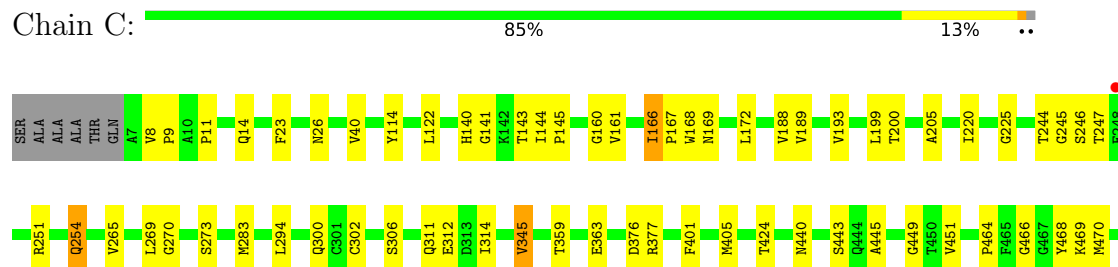
• Molecule 1: Aldehyde dehydrogenase

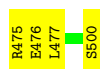


• Molecule 1: Aldehyde dehydrogenase

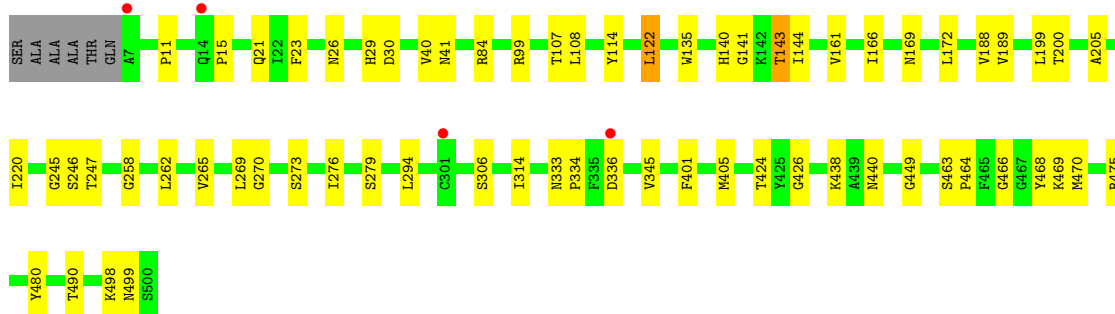
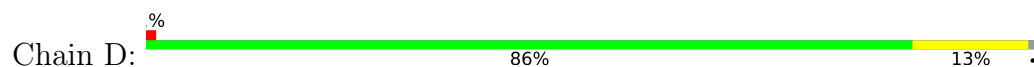


• Molecule 1: Aldehyde dehydrogenase

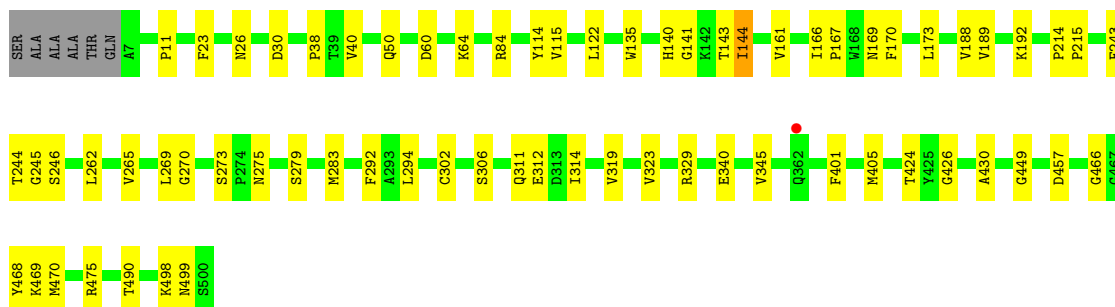
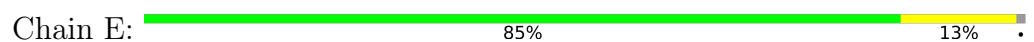




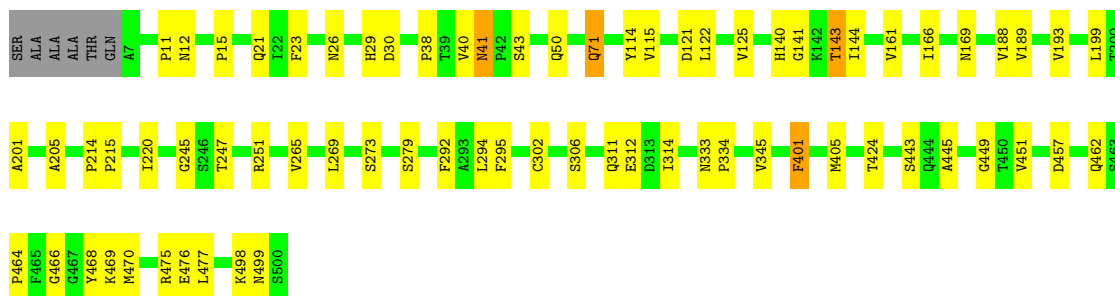
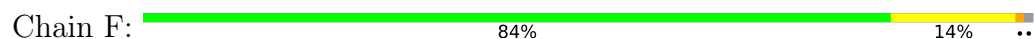
• Molecule 1: Aldehyde dehydrogenase



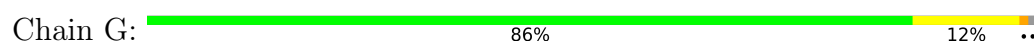
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase

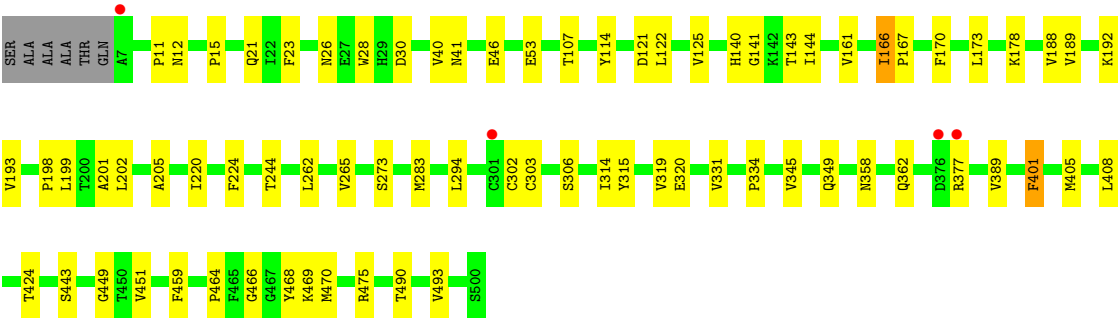
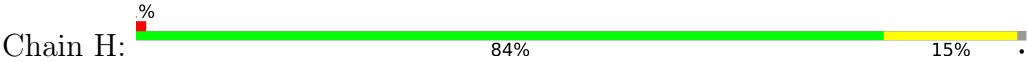


• Molecule 1: Aldehyde dehydrogenase





● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.91Å 150.67Å 177.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.60 29.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.81-2.60) 94.8 (29.81-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.232 0.192 , 0.232	Depositor DCC
R_{free} test set	5567 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtrriage
Anisotropy	1.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32876	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.80 % 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 1.9385e-05. 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: MG, NAD, NA

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	0.40	0/3882	0.94	13/5267 (0.2%)
1	B	0.41	0/3882	0.94	17/5267 (0.3%)
1	C	0.40	0/3882	0.95	16/5267 (0.3%)
1	D	0.40	0/3882	0.94	17/5267 (0.3%)
1	E	0.40	0/3882	0.93	15/5267 (0.3%)
1	F	0.42	0/3882	0.95	17/5267 (0.3%)
1	G	0.41	0/3882	0.96	15/5267 (0.3%)
1	H	0.40	0/3882	0.95	14/5267 (0.3%)
All	All	0.41	0/31056	0.94	124/42136 (0.3%)

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	ILE	N-CA-C	9.62	118.37	107.89
1	H	144	ILE	N-CA-C	9.09	117.80	107.89
1	G	8	VAL	N-CA-C	8.98	117.68	107.89
1	F	199	LEU	N-CA-C	8.96	121.94	111.02
1	D	144	ILE	N-CA-C	8.92	117.62	107.89
1	E	144	ILE	N-CA-C	8.87	117.56	107.89
1	B	166	ILE	N-CA-C	8.76	117.57	107.84
1	F	166	ILE	N-CA-C	8.72	117.53	107.84
1	C	144	ILE	N-CA-C	8.60	117.27	107.89
1	A	199	LEU	N-CA-C	8.40	121.27	111.02
1	G	199	LEU	N-CA-C	8.37	121.23	111.02
1	C	199	LEU	N-CA-C	8.21	121.03	111.02
1	A	166	ILE	N-CA-C	8.18	116.92	107.84
1	A	144	ILE	N-CA-C	8.12	117.63	108.05
1	D	199	LEU	N-CA-C	8.06	120.85	111.02
1	B	199	LEU	N-CA-C	8.01	120.79	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	144	ILE	N-CA-C	7.96	116.57	107.89
1	H	166	ILE	N-CA-C	7.90	116.61	107.84
1	A	189	VAL	N-CA-C	7.84	120.14	108.46
1	C	166	ILE	N-CA-C	7.64	116.32	107.84
1	H	199	LEU	N-CA-C	7.64	120.34	111.02
1	G	189	VAL	N-CA-C	7.61	119.80	108.46
1	C	189	VAL	N-CA-C	7.58	119.75	108.46
1	B	189	VAL	N-CA-C	7.34	119.40	108.46
1	E	166	ILE	N-CA-C	7.34	115.99	107.84
1	G	166	ILE	N-CA-C	7.28	115.92	107.84
1	D	189	VAL	N-CA-C	7.24	119.25	108.46
1	D	166	ILE	N-CA-C	7.20	115.83	107.84
1	B	144	ILE	N-CA-C	7.16	116.50	108.05
1	E	189	VAL	N-CA-C	7.13	119.08	108.46
1	C	141	GLY	N-CA-C	-7.11	102.83	112.57
1	B	345	VAL	N-CA-C	7.07	117.83	110.62
1	H	189	VAL	N-CA-C	7.06	118.99	108.46
1	G	140	HIS	N-CA-C	6.97	119.83	110.35
1	F	312	GLU	N-CA-C	6.95	119.73	111.33
1	A	141	GLY	N-CA-C	-6.90	103.12	112.57
1	F	189	VAL	N-CA-C	6.89	118.73	108.46
1	G	345	VAL	N-CA-C	6.87	118.45	110.62
1	D	140	HIS	N-CA-C	6.86	119.68	110.35
1	E	140	HIS	N-CA-C	6.68	119.44	110.35
1	D	141	GLY	N-CA-C	-6.66	102.43	112.41
1	A	140	HIS	N-CA-C	6.65	119.40	110.35
1	G	41	ASN	N-CA-C	-6.65	100.00	109.24
1	H	140	HIS	N-CA-C	6.64	119.39	110.35
1	C	312	GLU	N-CA-C	6.57	119.28	111.33
1	A	312	GLU	N-CA-C	6.56	120.15	111.75
1	A	345	VAL	N-CA-C	6.47	117.15	110.36
1	E	141	GLY	N-CA-C	-6.33	102.92	112.41
1	H	273	SER	N-CA-C	6.32	118.58	109.48
1	C	140	HIS	N-CA-C	6.29	118.91	110.35
1	F	140	HIS	N-CA-C	6.28	118.89	110.35
1	H	141	GLY	N-CA-C	-6.28	102.99	112.41
1	G	30	ASP	N-CA-C	-6.20	102.53	110.53
1	F	273	SER	N-CA-C	6.19	118.39	109.48
1	F	141	GLY	N-CA-C	-6.16	103.18	112.41
1	B	141	GLY	N-CA-C	-6.07	103.31	112.41
1	H	345	VAL	N-CA-C	6.07	117.53	110.62
1	G	141	GLY	N-CA-C	-6.02	103.37	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	345	VAL	N-CA-C	5.99	117.45	110.62
1	E	468	TYR	N-CA-C	-5.85	101.81	110.46
1	D	468	TYR	N-CA-C	-5.84	101.82	110.46
1	D	84	ARG	N-CA-C	-5.83	105.00	111.36
1	B	468	TYR	N-CA-C	-5.80	101.88	110.46
1	F	143	THR	N-CA-C	-5.79	99.08	108.52
1	C	160	GLY	N-CA-C	5.75	117.19	111.21
1	C	273	SER	N-CA-C	5.75	117.77	109.48
1	E	312	GLU	N-CA-C	5.70	119.05	111.75
1	G	468	TYR	N-CA-C	-5.69	101.60	110.42
1	E	84	ARG	N-CA-C	-5.69	105.17	111.71
1	E	345	VAL	N-CA-C	5.68	117.10	110.62
1	E	30	ASP	N-CA-C	-5.68	102.88	110.55
1	D	273	SER	N-CA-C	5.67	117.65	109.48
1	D	265	VAL	N-CA-C	5.67	116.90	108.46
1	A	468	TYR	N-CA-C	-5.63	101.69	110.42
1	B	160	GLY	N-CA-C	5.61	117.04	111.21
1	G	469	LYS	CB-CA-C	-5.60	110.10	116.54
1	H	468	TYR	N-CA-C	-5.60	102.18	110.46
1	C	143	THR	N-CA-C	-5.58	99.42	108.52
1	B	273	SER	N-CA-C	5.58	117.52	109.48
1	D	345	VAL	N-CA-C	5.55	116.95	110.62
1	B	344	GLN	N-CA-C	-5.52	103.09	110.55
1	G	273	SER	N-CA-C	5.50	117.41	109.48
1	H	30	ASP	N-CA-C	-5.50	103.12	110.55
1	F	30	ASP	N-CA-C	-5.50	102.62	110.59
1	F	265	VAL	N-CA-C	5.45	116.57	108.46
1	C	468	TYR	N-CA-C	-5.44	102.41	110.46
1	C	265	VAL	N-CA-C	5.43	116.55	108.46
1	C	345	VAL	N-CA-C	5.42	116.80	110.62
1	F	468	TYR	N-CA-C	-5.42	102.44	110.46
1	A	469	LYS	CB-CA-C	-5.42	110.31	116.54
1	A	30	ASP	N-CA-C	-5.41	103.24	110.55
1	H	493	VAL	N-CA-C	5.41	115.74	108.17
1	F	295	PHE	N-CA-C	5.40	119.71	113.18
1	F	469	LYS	CB-CA-C	-5.39	110.34	116.54
1	B	12	ASN	N-CA-C	-5.37	99.76	108.41
1	F	40	VAL	N-CA-C	5.36	117.28	108.97
1	B	469	LYS	CB-CA-C	-5.36	110.38	116.54
1	C	445	ALA	N-CA-C	5.35	117.19	111.36
1	D	469	LYS	CB-CA-C	-5.33	110.41	116.54
1	E	273	SER	N-CA-C	5.31	117.13	109.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	ASP	N-CA-C	-5.31	103.38	110.55
1	E	265	VAL	N-CA-C	5.31	116.37	108.46
1	B	140	HIS	N-CA-C	5.30	117.55	110.35
1	E	469	LYS	CB-CA-C	-5.28	110.46	116.54
1	D	143	THR	N-CA-C	-5.26	99.84	108.41
1	F	445	ALA	N-CA-C	5.21	117.04	111.36
1	C	40	VAL	N-CA-C	5.21	117.04	108.97
1	H	143	THR	N-CA-C	-5.16	100.11	108.52
1	H	469	LYS	CB-CA-C	-5.16	110.61	116.54
1	D	276	ILE	N-CA-C	5.15	116.11	108.23
1	E	40	VAL	N-CA-C	5.14	116.93	108.97
1	A	295	PHE	N-CA-C	5.12	119.38	113.18
1	G	295	PHE	N-CA-C	5.11	119.36	113.18
1	H	265	VAL	N-CA-C	5.11	116.07	108.46
1	C	469	LYS	CB-CA-C	-5.10	110.68	116.54
1	G	40	VAL	N-CA-C	5.09	116.86	108.97
1	B	84	ARG	N-CA-C	-5.09	105.73	111.28
1	B	119	LEU	N-CA-C	5.08	117.71	111.82
1	D	144	ILE	CA-C-N	5.07	126.18	119.84
1	D	144	ILE	C-N-CA	5.07	126.18	119.84
1	A	265	VAL	N-CA-C	5.05	115.99	108.46
1	E	143	THR	N-CA-C	-5.03	100.20	108.41
1	B	330	VAL	N-CA-C	5.02	115.47	108.84
1	B	40	VAL	N-CA-C	5.00	116.72	108.97

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	3798	0	3745	55	0
1	B	3798	0	3745	43	0
1	C	3798	0	3745	52	0
1	D	3798	0	3745	39	0
1	E	3798	0	3745	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	48	0
1	G	3798	0	3745	37	0
1	H	3798	0	3745	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	88	0	52	15	0
4	B	88	0	52	8	0
4	C	88	0	52	21	0
4	D	88	0	52	8	0
4	E	88	0	52	11	0
4	F	88	0	52	7	0
4	G	88	0	52	5	0
4	H	88	0	52	5	0
5	A	250	0	0	1	0
5	B	241	0	0	3	0
5	C	209	0	0	3	0
5	D	199	0	0	1	0
5	E	252	0	0	2	0
5	F	234	0	0	3	0
5	G	199	0	0	1	0
5	H	188	0	0	3	0
All	All	32876	0	30376	336	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 5.

All (336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:HD21	4:C:3502[B]:NAD:H5N	1.22	1.05
1:F:71:GLN:HE21	1:F:71:GLN:HA	1.22	0.98
1:A:196:GLN:H	1:A:196:GLN:HE21	1.17	0.91
1:D:270:GLY:HA2	4:D:4502[B]:NAD:O2D	1.76	0.86
1:C:246:SER:HA	4:C:3502[B]:NAD:O3D	1.77	0.85
1:A:169:ASN:HD21	4:A:1502[B]:NAD:H5N	1.41	0.85
1:F:333:ASN:HD22	1:F:334:PRO:HD2	1.49	0.76
1:C:302:CYS:HB3	4:C:3502[B]:NAD:C4N	2.15	0.76
1:D:246:SER:HA	4:D:4502[B]:NAD:O3D	1.85	0.75
1:E:169:ASN:HD21	4:E:5502[B]:NAD:H5N	1.50	0.75
1:C:245:GLY:O	4:C:3502[B]:NAD:H1D	1.86	0.74
1:F:424:THR:HB	1:F:470:MET:HE3	1.68	0.74
1:C:424:THR:HB	1:C:470:MET:HE3	1.70	0.72
1:C:14:GLN:HE21	1:C:14:GLN:HA	1.55	0.72
1:G:363:GLU:HB2	5:G:1438:HOH:O	1.89	0.71
1:C:300:GLN:HE22	1:C:345:VAL:H	1.36	0.71
1:G:424:THR:HB	1:G:470:MET:HE3	1.71	0.71
1:D:464:PRO:HG3	1:D:480:TYR:CD1	2.26	0.71
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.73	0.71
1:F:279:SER:HB3	1:F:311:GLN:OE1	1.91	0.70
1:G:347:GLU:HG2	1:G:351:LYS:HE2	1.74	0.70
1:B:300:GLN:HE22	1:B:345:VAL:H	1.40	0.70
1:D:245:GLY:O	4:D:4502[B]:NAD:H1D	1.93	0.69
1:B:464:PRO:HG3	1:B:480:TYR:CD1	2.28	0.69
1:F:71:GLN:HA	1:F:71:GLN:NE2	2.03	0.68
1:F:169:ASN:HD21	4:F:6502[B]:NAD:H5N	1.57	0.68
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.75	0.67
1:H:401:PHE:CZ	4:H:8502[B]:NAD:H2D	2.29	0.67
1:A:246:SER:HA	4:A:1502[B]:NAD:O3D	1.95	0.67
1:C:169:ASN:ND2	4:C:3502[B]:NAD:H5N	2.03	0.67
1:F:401:PHE:CZ	4:F:6502[B]:NAD:H2D	2.30	0.67
1:A:270:GLY:HA2	4:A:1502[B]:NAD:O2D	1.95	0.67
1:A:294:LEU:HD22	1:A:405:MET:HB2	1.75	0.67
1:D:424:THR:HB	1:D:470:MET:HE3	1.78	0.66
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.78	0.66
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.78	0.66
1:A:464:PRO:HG3	1:A:480:TYR:CD1	2.31	0.66
1:A:302:CYS:HB3	4:A:1502[B]:NAD:C3N	2.26	0.65
1:A:300:GLN:HE22	1:A:345:VAL:H	1.43	0.65
1:B:424:THR:HB	1:B:470:MET:HE3	1.78	0.65
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.79	0.65
1:E:270:GLY:HA2	4:E:5502[B]:NAD:O2D	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:C	1:F:41:ASN:HD22	2.06	0.63
1:A:302:CYS:SG	4:A:1502[B]:NAD:C4N	2.87	0.63
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.34	0.62
1:D:333:ASN:HB3	1:D:336:ASP:OD2	1.99	0.62
1:F:169:ASN:HD21	4:F:6502[B]:NAD:C5N	2.12	0.62
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.81	0.62
1:A:283:MET:HE1	1:A:314:ILE:HB	1.82	0.62
1:B:246:SER:HB3	4:B:2502[A]:NAD:O4D	1.99	0.62
1:E:246:SER:HA	4:E:5502[B]:NAD:O3D	1.99	0.62
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.35	0.61
1:G:9:PRO:HG3	1:G:100:THR:HG22	1.82	0.61
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.35	0.61
1:B:336:ASP:HB3	5:B:2871:HOH:O	1.99	0.61
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.81	0.61
1:G:401:PHE:CZ	4:G:7502[B]:NAD:H2D	2.36	0.61
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.36	0.60
1:H:178:LYS:HD3	5:H:8689:HOH:O	2.01	0.60
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.83	0.60
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.36	0.60
1:F:41:ASN:ND2	1:F:43:SER:H	2.00	0.60
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.84	0.59
1:C:14:GLN:HA	1:C:14:GLN:NE2	2.17	0.59
1:A:169:ASN:ND2	4:A:1502[B]:NAD:H5N	2.16	0.59
1:C:302:CYS:HB3	4:C:3502[B]:NAD:C5N	2.33	0.59
1:H:424:THR:HB	1:H:470:MET:HE3	1.85	0.59
1:A:294:LEU:HD12	1:A:306:SER:HA	1.85	0.58
1:D:169:ASN:HD21	4:D:4502[B]:NAD:H5N	1.66	0.58
1:E:245:GLY:O	4:E:5502[B]:NAD:H1D	2.03	0.58
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.85	0.58
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.84	0.58
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.86	0.58
1:H:358:ASN:O	1:H:362:GLN:HG2	2.04	0.58
1:B:401:PHE:CZ	4:B:2502[B]:NAD:H2D	2.39	0.57
1:H:294:LEU:HD12	1:H:306:SER:HA	1.86	0.57
1:B:311:GLN:HG3	5:B:2934:HOH:O	2.03	0.57
1:E:115:VAL:HG23	5:E:840:HOH:O	2.05	0.57
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.40	0.57
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.05	0.57
1:F:294:LEU:HD13	5:F:1044:HOH:O	2.04	0.57
1:C:245:GLY:C	4:C:3502[B]:NAD:H1D	2.29	0.57
1:C:246:SER:CA	4:C:3502[B]:NAD:O3D	2.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.40	0.56
1:A:302:CYS:HB3	4:A:1502[B]:NAD:C2N	2.35	0.56
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.88	0.56
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.41	0.56
1:B:247:THR:HA	1:B:269:LEU:HD13	1.87	0.56
1:E:424:THR:HB	1:E:470:MET:HE3	1.88	0.56
1:D:294:LEU:HD12	1:D:306:SER:HA	1.89	0.55
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.89	0.55
1:F:169:ASN:ND2	4:F:6502[B]:NAD:H5N	2.21	0.55
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.42	0.55
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.41	0.55
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.30	0.54
1:C:270:GLY:HA2	4:C:3502[B]:NAD:O2D	2.08	0.54
1:E:329:ARG:HA	1:E:340:GLU:OE2	2.08	0.54
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.89	0.54
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.90	0.54
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.90	0.54
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.89	0.54
1:C:302:CYS:SG	4:C:3502[B]:NAD:C4N	2.96	0.53
1:D:270:GLY:HA2	4:D:4502[B]:NAD:HO2N	1.73	0.53
1:A:196:GLN:HE21	1:A:196:GLN:N	1.98	0.53
1:E:319:VAL:O	1:E:323:VAL:HG23	2.08	0.53
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.91	0.53
1:A:424:THR:HB	1:A:470:MET:HE3	1.91	0.53
1:D:246:SER:HB3	4:D:4502[A]:NAD:O4D	2.08	0.53
1:C:294:LEU:HD12	1:C:306:SER:HA	1.91	0.53
1:C:302:CYS:CB	4:C:3502[B]:NAD:C4N	2.86	0.53
1:D:161:VAL:HA	1:D:188:VAL:HG23	1.89	0.53
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.44	0.52
1:C:302:CYS:HB3	4:C:3502[B]:NAD:C3N	2.40	0.52
1:F:41:ASN:HD22	1:F:43:SER:H	1.56	0.52
1:C:167:PRO:HD3	1:C:244:THR:HB	1.91	0.52
1:F:311:GLN:NE2	5:F:1053:HOH:O	2.41	0.52
1:A:279:SER:HA	1:A:314:ILE:HD13	1.91	0.52
1:G:443:SER:HA	1:G:451:VAL:HG11	1.92	0.52
1:H:362:GLN:OE1	1:H:362:GLN:HA	2.10	0.52
1:A:338:LYS:NZ	1:H:331:VAL:O	2.42	0.51
1:G:247:THR:HA	1:G:269:LEU:HD13	1.90	0.51
1:A:302:CYS:CB	4:A:1502[B]:NAD:C3N	2.87	0.51
1:G:169:ASN:HD21	4:G:7502[B]:NAD:H5N	1.75	0.51
1:A:161:VAL:HA	1:A:188:VAL:HG23	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.11	0.51
1:A:38:PRO:HB3	1:A:50:GLN:HE22	1.75	0.50
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.10	0.50
1:A:302:CYS:SG	4:A:1502[B]:NAD:C7N	2.99	0.50
1:H:408:LEU:HD12	1:H:408:LEU:N	2.26	0.50
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.46	0.50
1:C:251:ARG:HA	1:D:262:LEU:HD21	1.92	0.50
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.46	0.50
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.93	0.50
1:A:15:PRO:HD2	1:A:108:LEU:HD22	1.92	0.50
1:C:270:GLY:CA	4:C:3502[B]:NAD:O2D	2.60	0.50
1:B:302:CYS:HB3	4:B:2502[A]:NAD:O7N	2.12	0.50
1:C:246:SER:HB3	4:C:3502[A]:NAD:O4D	2.12	0.50
1:E:167:PRO:HD3	1:E:244:THR:HB	1.93	0.50
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.94	0.49
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.93	0.49
1:G:283:MET:HE1	1:G:314:ILE:HB	1.93	0.49
1:B:21:GLN:HB3	1:B:29:HIS:O	2.12	0.49
1:B:294:LEU:HD12	1:B:306:SER:HA	1.93	0.49
1:G:294:LEU:HD13	1:G:405:MET:HA	1.95	0.49
1:F:302:CYS:HB3	4:F:6502[B]:NAD:C3N	2.43	0.49
1:B:294:LEU:HD13	1:B:405:MET:HA	1.95	0.49
1:H:46:GLU:OE1	1:H:46:GLU:HA	2.13	0.49
1:B:302:CYS:HB3	4:B:2502[B]:NAD:C2N	2.43	0.48
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.47	0.48
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.95	0.48
1:A:336:ASP:OD2	1:A:338:LYS:HB2	2.13	0.48
1:C:168:TRP:NE1	4:C:3502[A]:NAD:O2N	2.44	0.48
1:D:15:PRO:HD2	1:D:108:LEU:HD22	1.94	0.48
1:D:270:GLY:CA	4:D:4502[B]:NAD:O2D	2.57	0.48
1:E:169:ASN:ND2	4:E:5502[B]:NAD:H5N	2.23	0.48
1:A:122:LEU:O	1:A:126:LEU:HG	2.13	0.48
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.14	0.48
1:H:166:ILE:HD11	1:H:193:VAL:HG12	1.95	0.48
1:C:254:GLN:HG2	1:D:258:GLY:CA	2.44	0.48
1:D:246:SER:N	4:D:4502[B]:NAD:H4D	2.29	0.48
1:F:294:LEU:HD12	1:F:306:SER:HA	1.95	0.48
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.48
1:G:294:LEU:HD12	1:G:306:SER:HA	1.96	0.48
1:H:443:SER:HA	1:H:451:VAL:HG11	1.96	0.48
1:B:283:MET:HE1	1:B:314:ILE:HB	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:THR:HA	1:C:269:LEU:HD13	1.96	0.47
1:E:60:ASP:O	1:E:64:LYS:HG3	2.14	0.47
1:H:302:CYS:HB3	4:H:8502[B]:NAD:C2N	2.44	0.47
1:A:302:CYS:SG	4:A:1502[B]:NAD:C3N	3.02	0.47
1:C:449:GLY:HA3	1:C:466:GLY:O	2.15	0.47
1:G:408:LEU:N	1:G:408:LEU:HD12	2.29	0.47
1:A:483:GLN:HB3	5:A:2709:HOH:O	2.14	0.47
1:F:443:SER:HA	1:F:451:VAL:HG11	1.97	0.47
1:A:245:GLY:O	4:A:1502[B]:NAD:H1D	2.14	0.47
1:C:245:GLY:HA2	4:C:3502[B]:NAD:O4D	2.14	0.47
1:C:246:SER:HA	4:C:3502[B]:NAD:HO3N	1.79	0.47
1:G:449:GLY:HA3	1:G:466:GLY:O	2.14	0.47
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.49	0.47
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.95	0.47
1:A:246:SER:HB3	4:A:1502[A]:NAD:O4D	2.15	0.46
1:E:294:LEU:HD12	1:E:306:SER:HA	1.97	0.46
1:C:283:MET:HE1	1:C:314:ILE:HB	1.97	0.46
1:D:498:LYS:HG2	1:D:499:ASN:N	2.30	0.46
1:C:311:GLN:HG3	5:C:3682:HOH:O	2.14	0.46
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.50	0.46
1:D:464:PRO:HG3	1:D:480:TYR:HD1	1.78	0.46
1:B:11:PRO:HB3	1:B:114:TYR:CE1	2.51	0.46
1:B:167:PRO:HD3	1:B:244:THR:HB	1.98	0.46
1:C:376:ASP:OD1	1:C:377:ARG:N	2.49	0.46
1:H:53:GLU:CD	1:H:224:PHE:HE1	2.24	0.46
1:F:143:THR:OG1	1:G:141:GLY:HA3	2.16	0.46
1:G:9:PRO:CG	1:G:100:THR:HG22	2.45	0.46
1:B:33:SER:O	1:B:34:ARG:HB2	2.14	0.46
1:G:169:ASN:HD21	4:G:7502[B]:NAD:C5N	2.29	0.46
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.16	0.46
1:H:121:ASP:O	1:H:125:VAL:HG23	2.15	0.46
1:F:279:SER:HB3	1:F:311:GLN:CD	2.40	0.45
1:H:377:ARG:NH1	5:H:8681:HOH:O	2.49	0.45
1:H:167:PRO:HD3	1:H:244:THR:HB	1.99	0.45
1:E:269:LEU:C	4:E:5502[A]:NAD:N7N	2.74	0.45
1:B:158:PRO:HD3	1:C:500:SER:OXT	2.16	0.45
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.51	0.45
1:B:169:ASN:HD21	4:B:2502[B]:NAD:H5N	1.81	0.45
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.98	0.45
1:C:359:THR:O	1:C:363:GLU:HG2	2.16	0.45
1:A:107:THR:HG23	1:A:334:PRO:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:HB3	4:B:2502[B]:NAD:C3N	2.47	0.45
1:B:303:CYS:HG	1:B:459:PHE:HZ	1.63	0.45
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.51	0.45
1:F:401:PHE:CE1	4:F:6502[B]:NAD:H2D	2.51	0.45
1:G:168:TRP:CD1	4:G:7502[B]:NAD:O2N	2.70	0.45
1:E:302:CYS:HB3	4:E:5502[B]:NAD:C3N	2.47	0.45
1:F:449:GLY:HA3	1:F:466:GLY:O	2.17	0.45
1:G:121:ASP:O	1:G:125:VAL:HG23	2.17	0.45
1:E:449:GLY:HA3	1:E:466:GLY:O	2.17	0.44
1:F:476:GLU:O	1:F:477:LEU:HB2	2.17	0.44
1:A:463:SER:HA	1:A:464:PRO:HD3	1.84	0.44
1:D:464:PRO:CG	1:D:480:TYR:CD1	2.97	0.44
1:D:438:LYS:HE2	5:D:4644:HOH:O	2.17	0.44
1:G:109:ASP:OD2	1:G:197:THR:HA	2.18	0.44
1:H:167:PRO:HG3	1:H:244:THR:HG22	1.99	0.44
1:A:302:CYS:HB3	4:A:1502[B]:NAD:C4N	2.47	0.44
1:B:401:PHE:CE1	4:B:2502[B]:NAD:H2D	2.53	0.44
1:C:172:LEU:HD21	1:C:200:THR:HB	2.00	0.44
1:A:196:GLN:H	1:A:196:GLN:NE2	1.99	0.44
1:D:107:THR:HG23	1:D:334:PRO:HB2	1.99	0.44
1:H:193:VAL:HG11	1:H:201:ALA:CB	2.48	0.44
1:A:167:PRO:HD3	1:A:244:THR:HB	1.99	0.43
1:C:294:LEU:HD13	5:C:3606:HOH:O	2.18	0.43
1:H:449:GLY:HA3	1:H:466:GLY:O	2.18	0.43
1:A:33:SER:O	1:A:34:ARG:HB2	2.17	0.43
1:C:302:CYS:SG	4:C:3502[B]:NAD:H4N	2.57	0.43
1:H:302:CYS:HB3	4:H:8502[B]:NAD:C3N	2.47	0.43
1:A:42:PRO:HG3	1:A:345:VAL:O	2.18	0.43
1:E:169:ASN:HD21	4:E:5502[B]:NAD:C5N	2.26	0.43
1:C:443:SER:HA	1:C:451:VAL:HG11	2.00	0.43
1:E:214:PRO:HA	1:E:215:PRO:HD3	1.91	0.43
1:H:198:PRO:O	1:H:202:LEU:HG	2.18	0.43
1:H:389:VAL:HB	1:H:408:LEU:HG	2.01	0.43
1:A:141:GLY:HA3	1:D:143:THR:OG1	2.19	0.43
1:E:262:LEU:HD21	1:F:251:ARG:HA	2.00	0.43
1:H:40:VAL:HG12	1:H:41:ASN:N	2.33	0.43
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.41	0.43
1:F:12:ASN:O	1:F:15:PRO:HD3	2.19	0.43
1:G:401:PHE:CE1	4:G:7502[B]:NAD:H2D	2.53	0.43
1:E:38:PRO:HB3	1:E:50:GLN:HE22	1.84	0.43
1:A:476:GLU:O	1:A:477:LEU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLN:HG3	5:E:1150:HOH:O	2.18	0.43
1:H:315:TYR:O	1:H:319:VAL:HG23	2.19	0.43
1:A:21:GLN:HB3	1:A:29:HIS:O	2.18	0.43
1:A:262:LEU:HD21	1:B:251:ARG:HA	2.00	0.43
1:D:172:LEU:HD21	1:D:200:THR:HB	2.00	0.43
1:A:167:PRO:CB	4:A:1502[A]:NAD:H4N	2.48	0.42
1:A:464:PRO:CG	1:A:480:TYR:CD1	3.02	0.42
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.53	0.42
1:B:268:GLU:OE2	1:B:476:GLU:HG3	2.19	0.42
1:D:21:GLN:HB3	1:D:29:HIS:O	2.19	0.42
1:G:164:GLN:CD	1:G:178:LYS:HB3	2.44	0.42
1:G:389:VAL:HB	1:G:408:LEU:HG	2.00	0.42
1:H:21:GLN:NE2	1:H:28:TRP:HB3	2.34	0.42
1:C:269:LEU:C	4:C:3502[A]:NAD:N7N	2.77	0.42
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.53	0.42
1:D:449:GLY:HA3	1:D:466:GLY:O	2.19	0.42
1:E:170:PHE:HB3	1:E:173:LEU:HB3	2.00	0.42
1:E:283:MET:HE1	1:E:314:ILE:HB	2.02	0.42
1:D:498:LYS:HE2	1:D:498:LYS:HB3	1.90	0.42
1:E:243:PHE:HE1	4:E:5502[B]:NAD:O4B	2.03	0.42
1:F:38:PRO:HB3	1:F:50:GLN:NE2	2.34	0.42
1:H:283:MET:HE1	1:H:314:ILE:HB	2.00	0.42
1:A:170:PHE:HB3	1:A:173:LEU:HB3	2.02	0.42
1:H:170:PHE:HB3	1:H:173:LEU:HB3	2.01	0.42
1:H:349:GLN:HE22	4:H:8502[A]:NAD:H52N	1.84	0.42
1:B:235:HIS:HB3	1:B:238:VAL:HG23	2.02	0.42
1:B:389:VAL:HB	1:B:408:LEU:HG	2.00	0.42
1:E:279:SER:HA	1:E:314:ILE:HD13	2.02	0.42
1:A:268:GLU:HG3	1:A:476:GLU:OE1	2.20	0.42
1:A:38:PRO:HB3	1:A:50:GLN:NE2	2.34	0.42
1:E:498:LYS:HG2	1:E:499:ASN:N	2.34	0.42
1:C:225:GLY:HA3	4:C:3502[B]:NAD:C8A	2.50	0.42
1:F:21:GLN:HB3	1:F:29:HIS:O	2.20	0.42
1:F:121:ASP:O	1:F:125:VAL:HG23	2.20	0.42
1:H:466:GLY:HA3	1:H:475:ARG:HD3	2.02	0.42
1:A:249:ILE:HG13	4:A:1502[A]:NAD:O2A	2.20	0.42
1:A:462:GLN:HB3	1:B:144:ILE:CG2	2.48	0.42
1:B:154:THR:HA	1:B:489:LYS:O	2.20	0.41
1:A:40:VAL:HG12	1:A:41:ASN:N	2.35	0.41
1:A:298:GLN:HG2	1:A:343:PRO:O	2.20	0.41
1:B:40:VAL:HG12	1:B:41:ASN:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ASN:ND2	1:E:430:ALA:HB3	2.35	0.41
1:A:268:GLU:OE2	1:A:476:GLU:HG3	2.20	0.41
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.95	0.41
1:B:264:ARG:HA	5:B:2839:HOH:O	2.20	0.41
1:E:269:LEU:C	4:E:5502[A]:NAD:H72N	2.28	0.41
1:F:498:LYS:HG2	1:F:499:ASN:N	2.35	0.41
1:G:251:ARG:HA	1:H:262:LEU:HD21	2.01	0.41
1:C:166:ILE:HD11	1:C:193:VAL:HG12	2.01	0.41
1:F:292:PHE:HE1	1:F:457:ASP:HB2	1.85	0.41
1:G:170:PHE:HB3	1:G:173:LEU:HB3	2.02	0.41
1:D:463:SER:HA	1:D:464:PRO:HD3	1.87	0.41
1:E:243:PHE:HE1	4:E:5502[A]:NAD:O4B	2.03	0.41
1:F:71:GLN:HE21	1:F:71:GLN:CA	2.04	0.41
1:F:247:THR:HA	1:F:269:LEU:HD13	2.03	0.41
1:D:440:ASN:HD22	1:D:440:ASN:HA	1.69	0.41
1:F:11:PRO:HB3	1:F:114:TYR:CE2	2.56	0.41
1:F:245:GLY:O	1:F:269:LEU:HA	2.20	0.41
1:F:333:ASN:HD22	1:F:334:PRO:CD	2.24	0.41
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.88	0.41
1:G:247:THR:O	1:G:251:ARG:HG3	2.21	0.41
1:H:12:ASN:O	1:H:15:PRO:HD3	2.21	0.41
1:H:294:LEU:HD13	5:H:8621:HOH:O	2.20	0.41
1:B:464:PRO:HG3	1:B:480:TYR:HD1	1.84	0.41
1:C:225:GLY:HA3	4:C:3502[A]:NAD:C8A	2.51	0.41
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.51	0.41
1:F:279:SER:HA	1:F:314:ILE:HD13	2.02	0.41
1:D:247:THR:HA	1:D:269:LEU:HD13	2.03	0.41
1:D:279:SER:HA	1:D:314:ILE:HD13	2.04	0.41
1:G:498:LYS:HG2	1:G:499:ASN:N	2.36	0.41
1:F:214:PRO:HA	1:F:215:PRO:HD3	1.91	0.40
1:G:71:GLN:HA	1:G:71:GLN:OE1	2.20	0.40
1:B:476:GLU:O	1:B:477:LEU:HB2	2.20	0.40
1:C:145:PRO:HA	5:C:3653:HOH:O	2.21	0.40
1:D:40:VAL:HG12	1:D:41:ASN:N	2.36	0.40
1:D:99:ARG:HG3	1:D:122:LEU:HD22	2.03	0.40
1:C:440:ASN:HD22	1:C:440:ASN:HA	1.71	0.40
1:E:144:ILE:CG2	1:F:462:GLN:HB3	2.52	0.40
1:E:292:PHE:HE1	1:E:457:ASP:HB2	1.86	0.40
1:F:169:ASN:OD1	4:F:6502[B]:NAD:H5N	2.21	0.40
1:H:107:THR:HG23	1:H:334:PRO:HB2	2.04	0.40
1:A:449:GLY:HA3	1:A:466:GLY:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:HD21	4:B:2502[B]:NAD:C5N	2.35	0.40
1:H:244:THR:HG23	4:H:8502[B]:NAD:C3N	2.51	0.40
1:A:294:LEU:CD1	1:A:306:SER:HA	2.51	0.40
1:C:8:VAL:HA	1:C:9:PRO:HD3	1.91	0.40
1:C:205:ALA:HB2	1:C:220:ILE:HD12	2.04	0.40
1:C:476:GLU:O	1:C:477:LEU:HB2	2.22	0.40
1:F:115:VAL:HG23	5:F:1014:HOH:O	2.22	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	492/500 (98%)	474 (96%)	18 (4%)	0	100	100
1	B	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	C	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	D	492/500 (98%)	477 (97%)	14 (3%)	1 (0%)	43	66
1	E	492/500 (98%)	474 (96%)	17 (4%)	1 (0%)	43	66
1	F	492/500 (98%)	475 (96%)	17 (4%)	0	100	100
1	G	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	H	492/500 (98%)	472 (96%)	20 (4%)	0	100	100
All	All	3936/4000 (98%)	3797 (96%)	137 (4%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	426	GLY
1	E	426	GLY

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	399/402 (99%)	396 (99%)	3 (1%)	73	88
1	B	399/402 (99%)	397 (100%)	2 (0%)	81	92
1	C	399/402 (99%)	396 (99%)	3 (1%)	73	88
1	D	399/402 (99%)	397 (100%)	2 (0%)	81	92
1	E	399/402 (99%)	396 (99%)	3 (1%)	73	88
1	F	399/402 (99%)	395 (99%)	4 (1%)	68	86
1	G	399/402 (99%)	395 (99%)	4 (1%)	68	86
1	H	399/402 (99%)	395 (99%)	4 (1%)	68	86
All	All	3192/3216 (99%)	3167 (99%)	25 (1%)	73	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	196	GLN
1	A	401	PHE
1	B	122	LEU
1	B	401	PHE
1	C	122	LEU
1	C	254	GLN
1	C	401	PHE
1	D	122	LEU
1	D	401	PHE
1	E	122	LEU
1	E	192	LYS
1	E	401	PHE
1	F	41	ASN
1	F	71	GLN
1	F	122	LEU
1	F	401	PHE
1	G	122	LEU
1	G	362	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	401	PHE
1	G	408	LEU
1	H	122	LEU
1	H	192	LYS
1	H	320	GLU
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	26	ASN
1	A	50	GLN
1	A	175	GLN
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	A	362	GLN
1	A	390	GLN
1	B	25	ASN
1	B	50	GLN
1	B	83	HIS
1	B	164	GLN
1	B	254	GLN
1	B	275	ASN
1	B	289	GLN
1	B	300	GLN
1	C	14	GLN
1	C	50	GLN
1	C	300	GLN
1	C	358	ASN
1	C	440	ASN
1	C	483	GLN
1	D	50	GLN
1	D	89	ASN
1	D	175	GLN
1	D	254	GLN
1	D	275	ASN
1	D	440	ASN
1	E	21	GLN
1	E	26	ASN
1	E	29	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	50	GLN
1	E	254	GLN
1	E	275	ASN
1	E	349	GLN
1	E	440	ASN
1	F	13	GLN
1	F	25	ASN
1	F	41	ASN
1	F	50	GLN
1	F	71	GLN
1	F	275	ASN
1	F	333	ASN
1	G	25	ASN
1	G	26	ASN
1	G	29	HIS
1	G	50	GLN
1	G	164	GLN
1	G	254	GLN
1	G	275	ASN
1	G	362	GLN
1	G	440	ASN
1	H	21	GLN
1	H	25	ASN
1	H	89	ASN
1	H	164	GLN
1	H	254	GLN
1	H	275	ASN
1	H	349	GLN
1	H	483	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

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	D	4502[B]	2	46,48,48	2.30	11 (23%)	64,73,73	1.54	10 (15%)
4	NAD	B	2502[A]	2	46,48,48	2.40	10 (21%)	64,73,73	1.57	11 (17%)
4	NAD	E	5502[A]	2	46,48,48	2.47	10 (21%)	64,73,73	1.62	13 (20%)
4	NAD	H	8502[A]	2	46,48,48	2.44	12 (26%)	64,73,73	1.52	11 (17%)
4	NAD	B	2502[B]	2	46,48,48	2.33	12 (26%)	64,73,73	1.40	8 (12%)
4	NAD	F	6502[A]	2	46,48,48	2.49	13 (28%)	64,73,73	1.52	11 (17%)
4	NAD	G	7502[A]	2	46,48,48	2.39	10 (21%)	64,73,73	1.58	11 (17%)
4	NAD	G	7502[B]	2	46,48,48	2.26	10 (21%)	64,73,73	1.48	9 (14%)
4	NAD	H	8502[B]	2	46,48,48	2.23	12 (26%)	64,73,73	1.48	8 (12%)
4	NAD	A	1502[A]	2	46,48,48	2.41	11 (23%)	64,73,73	1.50	9 (14%)
4	NAD	F	6502[B]	2	46,48,48	2.26	11 (23%)	64,73,73	1.48	8 (12%)
4	NAD	C	3502[A]	2	46,48,48	2.53	13 (28%)	64,73,73	1.51	11 (17%)
4	NAD	E	5502[B]	2	46,48,48	2.26	10 (21%)	64,73,73	1.47	8 (12%)
4	NAD	D	4502[A]	2	46,48,48	2.44	12 (26%)	64,73,73	1.54	10 (15%)
4	NAD	A	1502[B]	2	46,48,48	2.19	9 (19%)	64,73,73	1.47	7 (10%)
4	NAD	C	3502[B]	2	46,48,48	2.34	12 (26%)	64,73,73	1.52	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	D	4502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	B	2502[A]	2	-	2/30/62/62	0/5/5/5
4	NAD	E	5502[A]	2	-	6/30/62/62	0/5/5/5
4	NAD	H	8502[A]	2	-	2/30/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	B	2502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	F	6502[A]	2	-	5/30/62/62	0/5/5/5
4	NAD	G	7502[A]	2	-	2/30/62/62	0/5/5/5
4	NAD	G	7502[B]	2	-	6/30/62/62	0/5/5/5
4	NAD	H	8502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	A	1502[A]	2	-	10/30/62/62	0/5/5/5
4	NAD	F	6502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	C	3502[A]	2	-	2/30/62/62	0/5/5/5
4	NAD	E	5502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	D	4502[A]	2	-	6/30/62/62	0/5/5/5
4	NAD	A	1502[B]	2	-	5/30/62/62	0/5/5/5
4	NAD	C	3502[B]	2	-	5/30/62/62	0/5/5/5

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3502[A]	NAD	C3N-C7N	-12.09	1.32	1.50
4	E	5502[A]	NAD	C3N-C7N	-11.86	1.32	1.50
4	F	6502[A]	NAD	C3N-C7N	-11.70	1.33	1.50
4	A	1502[A]	NAD	C3N-C7N	-11.45	1.33	1.50
4	B	2502[A]	NAD	C3N-C7N	-11.44	1.33	1.50
4	H	8502[A]	NAD	C3N-C7N	-11.37	1.33	1.50
4	D	4502[A]	NAD	C3N-C7N	-11.25	1.33	1.50
4	G	7502[A]	NAD	C3N-C7N	-11.16	1.34	1.50
4	C	3502[B]	NAD	C3N-C7N	-10.82	1.34	1.50
4	D	4502[B]	NAD	C3N-C7N	-10.81	1.34	1.50
4	B	2502[B]	NAD	C3N-C7N	-10.66	1.34	1.50
4	F	6502[B]	NAD	C3N-C7N	-10.44	1.35	1.50
4	G	7502[B]	NAD	C3N-C7N	-10.32	1.35	1.50
4	E	5502[B]	NAD	C3N-C7N	-10.29	1.35	1.50
4	H	8502[B]	NAD	C3N-C7N	-10.17	1.35	1.50
4	A	1502[B]	NAD	C3N-C7N	-10.02	1.35	1.50
4	D	4502[B]	NAD	C8A-N7A	4.61	1.40	1.31
4	E	5502[A]	NAD	C8A-N7A	4.51	1.40	1.31
4	D	4502[A]	NAD	C8A-N7A	4.47	1.40	1.31
4	E	5502[B]	NAD	C8A-N7A	4.47	1.40	1.31
4	G	7502[B]	NAD	C8A-N7A	4.44	1.40	1.31
4	A	1502[B]	NAD	C8A-N7A	4.44	1.40	1.31
4	E	5502[A]	NAD	C4N-C3N	-4.36	1.32	1.39
4	G	7502[A]	NAD	C8A-N7A	4.35	1.40	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	8502[B]	NAD	C8A-N7A	4.31	1.40	1.31
4	D	4502[A]	NAD	C4N-C3N	-4.29	1.32	1.39
4	B	2502[B]	NAD	C8A-N7A	4.28	1.39	1.31
4	C	3502[B]	NAD	C8A-N7A	4.26	1.39	1.31
4	F	6502[B]	NAD	C8A-N7A	4.24	1.39	1.31
4	E	5502[B]	NAD	PN-O3	4.23	1.64	1.59
4	B	2502[A]	NAD	C4N-C3N	-4.21	1.33	1.39
4	A	1502[A]	NAD	C8A-N7A	4.21	1.39	1.31
4	E	5502[A]	NAD	O4D-C1D	4.18	1.46	1.40
4	F	6502[A]	NAD	C8A-N7A	4.17	1.39	1.31
4	B	2502[B]	NAD	PN-O3	4.13	1.64	1.59
4	C	3502[A]	NAD	C8A-N7A	4.13	1.39	1.31
4	G	7502[A]	NAD	O4D-C1D	4.13	1.46	1.40
4	C	3502[A]	NAD	C4N-C3N	-4.10	1.33	1.39
4	G	7502[A]	NAD	C4N-C3N	-4.09	1.33	1.39
4	B	2502[A]	NAD	C8A-N7A	4.08	1.39	1.31
4	H	8502[A]	NAD	C4N-C3N	-4.08	1.33	1.39
4	A	1502[A]	NAD	C4N-C3N	-4.06	1.33	1.39
4	H	8502[A]	NAD	C8A-N7A	4.05	1.39	1.31
4	F	6502[A]	NAD	C4N-C3N	-4.01	1.33	1.39
4	B	2502[A]	NAD	C5N-C4N	-3.96	1.32	1.38
4	C	3502[B]	NAD	C4N-C3N	-3.89	1.33	1.39
4	H	8502[A]	NAD	O4D-C1D	3.83	1.45	1.40
4	F	6502[B]	NAD	C5N-C4N	-3.81	1.32	1.38
4	F	6502[A]	NAD	C5N-C4N	-3.79	1.32	1.38
4	E	5502[A]	NAD	C5N-C4N	-3.78	1.32	1.38
4	D	4502[B]	NAD	C4N-C3N	-3.74	1.33	1.39
4	G	7502[B]	NAD	C2A-N1A	3.72	1.40	1.33
4	G	7502[A]	NAD	C5N-C4N	-3.72	1.32	1.38
4	C	3502[A]	NAD	C5N-C4N	-3.68	1.32	1.38
4	C	3502[A]	NAD	C2A-N3A	3.68	1.40	1.33
4	F	6502[B]	NAD	C4N-C3N	-3.66	1.33	1.39
4	H	8502[A]	NAD	C2A-N3A	3.65	1.40	1.33
4	G	7502[A]	NAD	C2A-N3A	3.65	1.40	1.33
4	G	7502[B]	NAD	C5N-C4N	-3.64	1.32	1.38
4	D	4502[A]	NAD	C5N-C4N	-3.63	1.32	1.38
4	E	5502[B]	NAD	C2A-N1A	3.63	1.40	1.33
4	B	2502[B]	NAD	C2A-N1A	3.62	1.40	1.33
4	G	7502[B]	NAD	PA-O3	3.60	1.63	1.59
4	G	7502[B]	NAD	C4N-C3N	-3.60	1.34	1.39
4	C	3502[B]	NAD	C2A-N1A	3.59	1.40	1.33
4	C	3502[B]	NAD	C5N-C4N	-3.59	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6502[A]	NAD	O4D-C1D	3.58	1.45	1.40
4	G	7502[A]	NAD	C2A-N1A	3.57	1.40	1.33
4	H	8502[B]	NAD	C4N-C3N	-3.57	1.34	1.39
4	H	8502[A]	NAD	C5N-C4N	-3.57	1.32	1.38
4	E	5502[B]	NAD	C4N-C3N	-3.56	1.34	1.39
4	B	2502[B]	NAD	C4N-C3N	-3.55	1.34	1.39
4	A	1502[B]	NAD	C2A-N1A	3.50	1.40	1.33
4	C	3502[B]	NAD	PN-O3	3.50	1.63	1.59
4	A	1502[A]	NAD	C5N-C4N	-3.49	1.32	1.38
4	F	6502[B]	NAD	C2A-N1A	3.49	1.40	1.33
4	H	8502[B]	NAD	C2A-N1A	3.49	1.40	1.33
4	D	4502[B]	NAD	PN-O3	3.48	1.63	1.59
4	D	4502[A]	NAD	O4D-C1D	3.47	1.45	1.40
4	D	4502[B]	NAD	C2A-N1A	3.47	1.40	1.33
4	A	1502[B]	NAD	C5N-C4N	-3.47	1.33	1.38
4	B	2502[A]	NAD	O4D-C1D	3.47	1.45	1.40
4	B	2502[A]	NAD	C2A-N3A	3.47	1.40	1.33
4	B	2502[A]	NAD	C2A-N1A	3.46	1.40	1.33
4	H	8502[B]	NAD	C2A-N3A	3.44	1.40	1.33
4	E	5502[A]	NAD	C2A-N1A	3.43	1.40	1.33
4	A	1502[A]	NAD	C2A-N3A	3.43	1.40	1.33
4	F	6502[A]	NAD	C2A-N1A	3.41	1.40	1.33
4	G	7502[B]	NAD	C2A-N3A	3.39	1.40	1.33
4	D	4502[A]	NAD	PN-O3	3.39	1.63	1.59
4	B	2502[B]	NAD	C5N-C4N	-3.38	1.33	1.38
4	F	6502[A]	NAD	C2A-N3A	3.37	1.39	1.33
4	B	2502[B]	NAD	C2A-N3A	3.35	1.39	1.33
4	A	1502[A]	NAD	O4D-C1D	3.35	1.45	1.40
4	D	4502[B]	NAD	C5N-C4N	-3.34	1.33	1.38
4	C	3502[B]	NAD	C2A-N3A	3.34	1.39	1.33
4	C	3502[A]	NAD	O4D-C1D	3.34	1.45	1.40
4	D	4502[A]	NAD	C2A-N1A	3.34	1.39	1.33
4	A	1502[B]	NAD	C2A-N3A	3.33	1.39	1.33
4	H	8502[A]	NAD	C2A-N1A	3.31	1.39	1.33
4	D	4502[A]	NAD	C2A-N3A	3.31	1.39	1.33
4	A	1502[A]	NAD	C2A-N1A	3.29	1.39	1.33
4	A	1502[B]	NAD	C4N-C3N	-3.28	1.34	1.39
4	E	5502[B]	NAD	C5N-C4N	-3.27	1.33	1.38
4	C	3502[A]	NAD	C2A-N1A	3.26	1.39	1.33
4	E	5502[A]	NAD	C2A-N3A	3.25	1.39	1.33
4	F	6502[B]	NAD	C2A-N3A	3.18	1.39	1.33
4	A	1502[B]	NAD	PN-O3	3.17	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4502[B]	NAD	C2A-N3A	3.16	1.39	1.33
4	H	8502[B]	NAD	C5N-C4N	-3.11	1.33	1.38
4	A	1502[A]	NAD	PN-O3	3.11	1.62	1.59
4	E	5502[B]	NAD	C2A-N3A	3.08	1.39	1.33
4	C	3502[A]	NAD	PN-O3	2.99	1.62	1.59
4	C	3502[A]	NAD	PA-O3	2.94	1.62	1.59
4	H	8502[A]	NAD	PN-O3	2.94	1.62	1.59
4	F	6502[A]	NAD	PA-O3	2.92	1.62	1.59
4	G	7502[A]	NAD	C4A-N3A	2.90	1.39	1.34
4	H	8502[B]	NAD	PN-O3	2.88	1.62	1.59
4	H	8502[A]	NAD	C4A-N3A	2.88	1.39	1.34
4	B	2502[A]	NAD	C4A-N3A	2.88	1.39	1.34
4	C	3502[B]	NAD	PA-O3	2.86	1.62	1.59
4	H	8502[B]	NAD	C4A-N3A	2.82	1.39	1.34
4	F	6502[B]	NAD	PN-O3	2.80	1.62	1.59
4	F	6502[B]	NAD	C5A-C4A	-2.80	1.34	1.39
4	B	2502[B]	NAD	C4A-N3A	2.76	1.39	1.34
4	H	8502[A]	NAD	PA-O3	2.76	1.62	1.59
4	F	6502[A]	NAD	C2N-C3N	-2.69	1.34	1.39
4	D	4502[B]	NAD	C5A-C4A	-2.68	1.34	1.39
4	D	4502[A]	NAD	C5A-C4A	-2.68	1.34	1.39
4	A	1502[B]	NAD	C5A-C4A	-2.67	1.34	1.39
4	H	8502[B]	NAD	C5A-C4A	-2.66	1.34	1.39
4	E	5502[A]	NAD	C4A-N3A	2.66	1.39	1.34
4	D	4502[A]	NAD	C4A-N3A	2.66	1.39	1.34
4	B	2502[A]	NAD	C5A-C4A	-2.65	1.34	1.39
4	F	6502[A]	NAD	C5A-C4A	-2.64	1.34	1.39
4	C	3502[A]	NAD	C2N-C3N	-2.64	1.34	1.39
4	E	5502[B]	NAD	C5A-C4A	-2.64	1.34	1.39
4	H	8502[B]	NAD	PA-O3	2.63	1.62	1.59
4	F	6502[A]	NAD	C4A-N3A	2.63	1.39	1.34
4	E	5502[A]	NAD	C5A-C4A	-2.62	1.34	1.39
4	B	2502[B]	NAD	C5A-C4A	-2.61	1.34	1.39
4	A	1502[B]	NAD	C4A-N3A	2.61	1.39	1.34
4	A	1502[A]	NAD	C4A-N3A	2.61	1.39	1.34
4	B	2502[B]	NAD	PA-O3	2.61	1.62	1.59
4	C	3502[A]	NAD	C4A-N3A	2.60	1.39	1.34
4	G	7502[B]	NAD	C4A-N3A	2.59	1.39	1.34
4	D	4502[B]	NAD	C4A-N3A	2.57	1.39	1.34
4	C	3502[B]	NAD	C4A-N3A	2.56	1.39	1.34
4	C	3502[A]	NAD	C5A-C4A	-2.56	1.34	1.39
4	C	3502[B]	NAD	C5A-C4A	-2.55	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	7502[B]	NAD	C5A-C4A	-2.55	1.34	1.39
4	A	1502[A]	NAD	C5A-C4A	-2.55	1.34	1.39
4	H	8502[A]	NAD	C5A-C4A	-2.55	1.34	1.39
4	G	7502[A]	NAD	C5A-C4A	-2.53	1.34	1.39
4	F	6502[B]	NAD	C4A-N3A	2.53	1.39	1.34
4	G	7502[B]	NAD	O4D-C1D	2.47	1.44	1.40
4	E	5502[B]	NAD	C4A-N3A	2.45	1.39	1.34
4	F	6502[A]	NAD	PN-O3	2.44	1.62	1.59
4	F	6502[B]	NAD	PA-O3	2.42	1.62	1.59
4	A	1502[A]	NAD	C2N-C3N	-2.39	1.35	1.39
4	F	6502[A]	NAD	C2N-N1N	-2.34	1.32	1.35
4	F	6502[B]	NAD	O4D-C1D	2.31	1.43	1.40
4	D	4502[A]	NAD	PA-O3	2.31	1.62	1.59
4	D	4502[B]	NAD	C2N-C3N	-2.31	1.35	1.39
4	C	3502[B]	NAD	C6N-N1N	-2.29	1.30	1.35
4	B	2502[B]	NAD	C2N-C3N	-2.28	1.35	1.39
4	C	3502[A]	NAD	C2N-N1N	-2.26	1.32	1.35
4	D	4502[A]	NAD	C2N-C3N	-2.24	1.35	1.39
4	H	8502[A]	NAD	C2N-C3N	-2.21	1.35	1.39
4	H	8502[B]	NAD	C2N-C3N	-2.17	1.35	1.39
4	E	5502[B]	NAD	C2N-C3N	-2.16	1.35	1.39
4	D	4502[B]	NAD	C6N-N1N	-2.16	1.30	1.35
4	B	2502[A]	NAD	C2N-C3N	-2.15	1.35	1.39
4	C	3502[B]	NAD	C2N-C3N	-2.14	1.35	1.39
4	H	8502[B]	NAD	O4D-C1D	2.13	1.43	1.40
4	B	2502[B]	NAD	O4D-C1D	2.07	1.43	1.40
4	G	7502[A]	NAD	C2N-C3N	-2.06	1.35	1.39
4	E	5502[A]	NAD	PN-O3	2.00	1.61	1.59

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5502[A]	NAD	C5A-C4A-N9A	5.24	111.52	105.81
4	D	4502[A]	NAD	C5A-C4A-N9A	4.96	111.22	105.81
4	D	4502[B]	NAD	C5A-C4A-N9A	4.90	111.16	105.81
4	E	5502[B]	NAD	C5A-C4A-N9A	4.85	111.10	105.81
4	F	6502[B]	NAD	C5A-C4A-N9A	4.82	111.06	105.81
4	G	7502[B]	NAD	C5A-C4A-N9A	4.81	111.05	105.81
4	F	6502[A]	NAD	C5A-C4A-N9A	4.80	111.05	105.81
4	A	1502[B]	NAD	C5A-C4A-N9A	4.80	111.04	105.81
4	C	3502[B]	NAD	C5A-C4A-N9A	4.75	110.99	105.81
4	G	7502[A]	NAD	C5A-C4A-N9A	4.68	110.92	105.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1502[A]	NAD	C5A-C4A-N9A	4.65	110.88	105.81
4	H	8502[B]	NAD	C5A-C4A-N9A	4.62	110.85	105.81
4	B	2502[A]	NAD	C5A-C4A-N9A	4.58	110.80	105.81
4	C	3502[A]	NAD	C5A-C4A-N9A	4.51	110.73	105.81
4	B	2502[B]	NAD	C5A-C4A-N9A	4.46	110.67	105.81
4	G	7502[A]	NAD	C6A-C5A-C4A	4.41	123.20	117.18
4	C	3502[A]	NAD	C6A-C5A-C4A	4.38	123.15	117.18
4	H	8502[A]	NAD	C6A-C5A-C4A	4.32	123.08	117.18
4	D	4502[A]	NAD	C6A-C5A-C4A	4.29	123.04	117.18
4	B	2502[A]	NAD	C6A-C5A-C4A	4.29	123.03	117.18
4	A	1502[A]	NAD	C6A-C5A-C4A	4.23	122.96	117.18
4	E	5502[A]	NAD	C6A-C5A-C4A	4.22	122.95	117.18
4	F	6502[A]	NAD	C6A-C5A-C4A	4.21	122.92	117.18
4	H	8502[A]	NAD	C5A-C4A-N9A	4.17	110.36	105.81
4	E	5502[A]	NAD	C6N-N1N-C2N	-4.16	118.33	121.88
4	D	4502[B]	NAD	C6A-C5A-C4A	4.03	122.68	117.18
4	G	7502[B]	NAD	C6A-C5A-C4A	3.99	122.63	117.18
4	F	6502[B]	NAD	C6A-C5A-C4A	3.99	122.62	117.18
4	C	3502[B]	NAD	C6A-C5A-C4A	3.99	122.62	117.18
4	H	8502[B]	NAD	C6A-C5A-C4A	3.98	122.61	117.18
4	E	5502[B]	NAD	C6A-C5A-C4A	3.96	122.58	117.18
4	A	1502[B]	NAD	C6A-C5A-C4A	3.94	122.55	117.18
4	B	2502[B]	NAD	C6A-C5A-C4A	3.89	122.48	117.18
4	G	7502[B]	NAD	O7N-C7N-N7N	-3.83	117.08	122.62
4	H	8502[B]	NAD	O7N-C7N-N7N	-3.78	117.16	122.62
4	C	3502[B]	NAD	O7N-C7N-N7N	-3.76	117.19	122.62
4	E	5502[B]	NAD	O7N-C7N-N7N	-3.71	117.26	122.62
4	D	4502[B]	NAD	C2D-C3D-C4D	-3.61	95.63	102.61
4	A	1502[A]	NAD	C6N-N1N-C2N	-3.58	118.83	121.88
4	F	6502[B]	NAD	O7N-C7N-N7N	-3.58	117.45	122.62
4	H	8502[B]	NAD	N3A-C2A-N1A	-3.56	123.19	128.58
4	G	7502[A]	NAD	C6N-N1N-C2N	-3.54	118.86	121.88
4	H	8502[A]	NAD	C6N-N1N-C2N	-3.42	118.97	121.88
4	D	4502[B]	NAD	O7N-C7N-N7N	-3.39	117.72	122.62
4	B	2502[A]	NAD	C6N-N1N-C2N	-3.37	119.01	121.88
4	A	1502[B]	NAD	N3A-C2A-N1A	-3.36	123.50	128.58
4	C	3502[A]	NAD	C6N-N1N-C2N	-3.28	119.08	121.88
4	D	4502[B]	NAD	N3A-C2A-N1A	-3.24	123.68	128.58
4	F	6502[A]	NAD	C6N-N1N-C2N	-3.24	119.12	121.88
4	H	8502[B]	NAD	C3N-C7N-N7N	3.21	121.69	117.74
4	F	6502[B]	NAD	N3A-C2A-N1A	-3.20	123.74	128.58
4	F	6502[B]	NAD	C3N-C7N-N7N	3.19	121.67	117.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5502[B]	NAD	N3A-C2A-N1A	-3.19	123.76	128.58
4	G	7502[A]	NAD	C5A-C4A-N3A	-3.19	122.33	126.72
4	A	1502[B]	NAD	O7N-C7N-N7N	-3.18	118.02	122.62
4	H	8502[A]	NAD	N3A-C2A-N1A	-3.17	123.79	128.58
4	C	3502[B]	NAD	C4D-O4D-C1D	-3.16	107.03	109.92
4	D	4502[A]	NAD	C3N-C7N-N7N	3.11	121.57	117.74
4	B	2502[B]	NAD	O7N-C7N-N7N	-3.10	118.13	122.62
4	D	4502[A]	NAD	C6N-N1N-C2N	-3.10	119.24	121.88
4	G	7502[A]	NAD	C6A-C5A-N7A	-3.09	126.13	132.09
4	E	5502[A]	NAD	N3A-C2A-N1A	-3.08	123.92	128.58
4	C	3502[B]	NAD	C3N-C7N-N7N	3.05	121.50	117.74
4	H	8502[A]	NAD	C5A-C4A-N3A	-3.04	122.53	126.72
4	B	2502[B]	NAD	C3N-C7N-N7N	3.03	121.48	117.74
4	D	4502[A]	NAD	N3A-C2A-N1A	-3.03	123.99	128.58
4	H	8502[A]	NAD	C6A-C5A-N7A	-3.03	126.25	132.09
4	G	7502[B]	NAD	N3A-C2A-N1A	-3.02	124.01	128.58
4	F	6502[A]	NAD	N3A-C2A-N1A	-2.99	124.05	128.58
4	G	7502[B]	NAD	C3N-C7N-N7N	2.98	121.40	117.74
4	A	1502[B]	NAD	C3N-C7N-N7N	2.97	121.40	117.74
4	A	1502[A]	NAD	N3A-C2A-N1A	-2.95	124.11	128.58
4	H	8502[B]	NAD	C5A-C4A-N3A	-2.94	122.66	126.72
4	E	5502[B]	NAD	C3N-C7N-N7N	2.92	121.34	117.74
4	B	2502[A]	NAD	C6A-C5A-N7A	-2.90	126.50	132.09
4	B	2502[B]	NAD	N3A-C2A-N1A	-2.90	124.20	128.58
4	A	1502[B]	NAD	C5A-C4A-N3A	-2.88	122.76	126.72
4	D	4502[B]	NAD	C3N-C7N-N7N	2.87	121.27	117.74
4	C	3502[A]	NAD	C6A-C5A-N7A	-2.86	126.57	132.09
4	F	6502[A]	NAD	C5A-C4A-N3A	-2.84	122.81	126.72
4	D	4502[A]	NAD	C6A-C5A-N7A	-2.82	126.65	132.09
4	F	6502[B]	NAD	C5A-C4A-N3A	-2.82	122.84	126.72
4	F	6502[A]	NAD	C6A-C5A-N7A	-2.79	126.70	132.09
4	A	1502[A]	NAD	C6A-C5A-N7A	-2.79	126.71	132.09
4	D	4502[A]	NAD	C5A-C4A-N3A	-2.77	122.90	126.72
4	D	4502[B]	NAD	C5A-C4A-N3A	-2.77	122.91	126.72
4	B	2502[A]	NAD	N3A-C2A-N1A	-2.76	124.41	128.58
4	C	3502[B]	NAD	N3A-C2A-N1A	-2.75	124.42	128.58
4	E	5502[A]	NAD	C5A-C4A-N3A	-2.74	122.94	126.72
4	E	5502[A]	NAD	C6A-C5A-N7A	-2.74	126.81	132.09
4	A	1502[A]	NAD	C5A-C4A-N3A	-2.71	122.99	126.72
4	G	7502[A]	NAD	C3N-C7N-N7N	2.70	121.06	117.74
4	D	4502[B]	NAD	C6A-C5A-N7A	-2.69	126.91	132.09
4	C	3502[A]	NAD	C5A-C4A-N3A	-2.68	123.02	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5502[B]	NAD	C6A-C5A-N7A	-2.68	126.93	132.09
4	G	7502[B]	NAD	C6A-C5A-N7A	-2.66	126.96	132.09
4	H	8502[A]	NAD	C4D-O4D-C1D	-2.66	107.49	109.92
4	E	5502[B]	NAD	C5A-C4A-N3A	-2.65	123.06	126.72
4	G	7502[B]	NAD	C5A-C4A-N3A	-2.65	123.07	126.72
4	C	3502[A]	NAD	O7N-C7N-N7N	-2.65	118.79	122.62
4	G	7502[A]	NAD	N3A-C2A-N1A	-2.62	124.61	128.58
4	F	6502[B]	NAD	C6A-C5A-N7A	-2.59	127.10	132.09
4	G	7502[A]	NAD	C4D-O4D-C1D	-2.56	107.58	109.92
4	C	3502[B]	NAD	C5A-C4A-N3A	-2.55	123.20	126.72
4	B	2502[B]	NAD	C6A-C5A-N7A	-2.55	127.18	132.09
4	B	2502[B]	NAD	C5A-C4A-N3A	-2.53	123.24	126.72
4	A	1502[B]	NAD	C6A-C5A-N7A	-2.52	127.23	132.09
4	E	5502[A]	NAD	C4A-N9A-C8A	-2.52	103.09	105.74
4	C	3502[B]	NAD	C6A-C5A-N7A	-2.51	127.25	132.09
4	G	7502[A]	NAD	C4A-N9A-C8A	-2.49	103.12	105.74
4	B	2502[A]	NAD	C5A-C4A-N3A	-2.49	123.29	126.72
4	H	8502[B]	NAD	C6A-C5A-N7A	-2.48	127.31	132.09
4	D	4502[A]	NAD	O7N-C7N-N7N	-2.46	119.06	122.62
4	C	3502[A]	NAD	N3A-C2A-N1A	-2.45	124.88	128.58
4	C	3502[A]	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
4	C	3502[A]	NAD	C2N-C3N-C4N	2.44	121.09	118.26
4	H	8502[A]	NAD	N6A-C6A-N1A	2.41	123.75	118.38
4	E	5502[A]	NAD	O7N-C7N-N7N	-2.39	119.17	122.62
4	B	2502[A]	NAD	N6A-C6A-N1A	2.38	123.69	118.38
4	E	5502[B]	NAD	C4A-N9A-C8A	-2.38	103.24	105.74
4	E	5502[A]	NAD	C2N-C3N-C4N	2.34	120.98	118.26
4	F	6502[A]	NAD	C2N-C3N-C4N	2.34	120.98	118.26
4	E	5502[A]	NAD	C3N-C7N-N7N	2.34	120.62	117.74
4	F	6502[A]	NAD	C3N-C7N-N7N	2.31	120.58	117.74
4	A	1502[A]	NAD	N6A-C6A-N1A	2.31	123.51	118.38
4	D	4502[B]	NAD	C4A-N9A-C8A	-2.30	103.32	105.74
4	B	2502[A]	NAD	C2N-C3N-C4N	2.27	120.89	118.26
4	B	2502[A]	NAD	C4D-O4D-C1D	-2.26	107.85	109.92
4	F	6502[A]	NAD	O7N-C7N-N7N	-2.26	119.36	122.62
4	D	4502[A]	NAD	N6A-C6A-N1A	2.25	123.39	118.38
4	E	5502[A]	NAD	C1B-N9A-C8A	2.23	132.05	127.09
4	C	3502[A]	NAD	N6A-C6A-N1A	2.22	123.33	118.38
4	B	2502[A]	NAD	C3N-C7N-N7N	2.20	120.45	117.74
4	F	6502[A]	NAD	N6A-C6A-N1A	2.20	123.27	118.38
4	G	7502[B]	NAD	C4A-N9A-C8A	-2.19	103.44	105.74
4	A	1502[A]	NAD	C3N-C7N-N7N	2.19	120.44	117.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	7502[A]	NAD	O7N-C7N-N7N	-2.18	119.46	122.62
4	H	8502[A]	NAD	O7N-C7N-N7N	-2.15	119.51	122.62
4	F	6502[B]	NAD	C4A-N9A-C8A	-2.14	103.49	105.74
4	E	5502[A]	NAD	N6A-C6A-N1A	2.13	123.11	118.38
4	G	7502[B]	NAD	C6N-N1N-C2N	-2.12	120.07	121.88
4	H	8502[A]	NAD	C2N-C3N-C4N	2.12	120.73	118.26
4	G	7502[A]	NAD	N6A-C6A-N1A	2.12	123.11	118.38
4	B	2502[A]	NAD	C2D-C3D-C4D	-2.12	98.52	102.61
4	B	2502[B]	NAD	N6A-C6A-N1A	2.09	123.04	118.38
4	H	8502[A]	NAD	C2D-C3D-C4D	-2.09	98.57	102.61
4	F	6502[A]	NAD	C4A-N9A-C8A	-2.08	103.55	105.74
4	D	4502[A]	NAD	C4A-N9A-C8A	-2.08	103.55	105.74
4	A	1502[A]	NAD	C2N-C3N-C4N	2.08	120.67	118.26
4	D	4502[B]	NAD	N6A-C6A-N1A	2.07	122.98	118.38
4	E	5502[A]	NAD	C4D-O4D-C1D	-2.06	108.04	109.92
4	C	3502[A]	NAD	C3N-C7N-N7N	2.03	120.24	117.74
4	H	8502[B]	NAD	N6A-C6A-N1A	2.02	122.88	118.38

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1502[A]	NAD	C5B-O5B-PA-O1A
4	A	1502[A]	NAD	C5B-O5B-PA-O3
4	A	1502[B]	NAD	C5B-O5B-PA-O1A
4	B	2502[B]	NAD	C5B-O5B-PA-O1A
4	C	3502[B]	NAD	C5B-O5B-PA-O1A
4	D	4502[A]	NAD	C5B-O5B-PA-O1A
4	D	4502[B]	NAD	C5B-O5B-PA-O1A
4	E	5502[A]	NAD	C5B-O5B-PA-O1A
4	E	5502[B]	NAD	C5B-O5B-PA-O1A
4	F	6502[B]	NAD	C5B-O5B-PA-O1A
4	G	7502[B]	NAD	C5B-O5B-PA-O1A
4	H	8502[B]	NAD	C5B-O5B-PA-O1A
4	A	1502[A]	NAD	C2N-C3N-C7N-O7N
4	C	3502[B]	NAD	C4D-C5D-O5D-PN
4	A	1502[A]	NAD	C4N-C3N-C7N-O7N
4	A	1502[A]	NAD	C4N-C3N-C7N-N7N
4	A	1502[A]	NAD	C2N-C3N-C7N-N7N
4	B	2502[A]	NAD	C2B-C1B-N9A-C8A
4	G	7502[B]	NAD	C4D-C5D-O5D-PN
4	F	6502[B]	NAD	C4D-C5D-O5D-PN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	8502[B]	NAD	C4D-C5D-O5D-PN
4	A	1502[A]	NAD	C2B-C1B-N9A-C8A
4	A	1502[B]	NAD	C2B-C1B-N9A-C8A
4	B	2502[B]	NAD	C2B-C1B-N9A-C8A
4	C	3502[B]	NAD	C2B-C1B-N9A-C8A
4	D	4502[B]	NAD	C2B-C1B-N9A-C8A
4	E	5502[A]	NAD	C2B-C1B-N9A-C8A
4	E	5502[B]	NAD	C2B-C1B-N9A-C8A
4	F	6502[B]	NAD	C2B-C1B-N9A-C8A
4	G	7502[B]	NAD	C2B-C1B-N9A-C8A
4	C	3502[A]	NAD	C2B-C1B-N9A-C8A
4	D	4502[A]	NAD	C2B-C1B-N9A-C8A
4	F	6502[A]	NAD	C2B-C1B-N9A-C8A
4	G	7502[A]	NAD	C2B-C1B-N9A-C8A
4	H	8502[A]	NAD	C2B-C1B-N9A-C8A
4	H	8502[B]	NAD	C2B-C1B-N9A-C8A
4	A	1502[B]	NAD	C4D-C5D-O5D-PN
4	D	4502[B]	NAD	C4D-C5D-O5D-PN
4	A	1502[A]	NAD	C5B-O5B-PA-O2A
4	D	4502[A]	NAD	C5B-O5B-PA-O2A
4	D	4502[A]	NAD	C5B-O5B-PA-O3
4	E	5502[A]	NAD	C5B-O5B-PA-O2A
4	E	5502[A]	NAD	C5B-O5B-PA-O3
4	F	6502[A]	NAD	C5B-O5B-PA-O1A
4	F	6502[A]	NAD	C5B-O5B-PA-O2A
4	G	7502[B]	NAD	C5B-O5B-PA-O3
4	H	8502[A]	NAD	C5B-O5B-PA-O2A
4	B	2502[B]	NAD	C4D-C5D-O5D-PN
4	E	5502[B]	NAD	C4D-C5D-O5D-PN
4	D	4502[A]	NAD	PN-O3-PA-O1A
4	E	5502[A]	NAD	C2B-C1B-N9A-C4A
4	F	6502[A]	NAD	C2B-C1B-N9A-C4A
4	C	3502[B]	NAD	C2B-C1B-N9A-C4A
4	E	5502[B]	NAD	C2B-C1B-N9A-C4A
4	F	6502[B]	NAD	C2B-C1B-N9A-C4A
4	A	1502[B]	NAD	O4B-C1B-N9A-C8A
4	F	6502[B]	NAD	O4B-C1B-N9A-C8A
4	C	3502[B]	NAD	O4B-C1B-N9A-C8A
4	D	4502[B]	NAD	O4B-C1B-N9A-C8A
4	E	5502[B]	NAD	O4B-C1B-N9A-C8A
4	F	6502[A]	NAD	O4B-C1B-N9A-C8A
4	G	7502[A]	NAD	O4B-C1B-N9A-C8A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	7502[B]	NAD	O4B-C1B-N9A-C8A
4	H	8502[B]	NAD	O4B-C1B-N9A-C8A
4	A	1502[A]	NAD	C2B-C1B-N9A-C4A
4	A	1502[B]	NAD	C2B-C1B-N9A-C4A
4	B	2502[B]	NAD	C2B-C1B-N9A-C4A
4	D	4502[B]	NAD	C2B-C1B-N9A-C4A
4	A	1502[A]	NAD	O4B-C1B-N9A-C8A
4	G	7502[B]	NAD	C2B-C1B-N9A-C4A
4	H	8502[B]	NAD	C2B-C1B-N9A-C4A
4	B	2502[A]	NAD	O4B-C1B-N9A-C8A
4	B	2502[B]	NAD	O4B-C1B-N9A-C8A
4	D	4502[A]	NAD	O4B-C1B-N9A-C8A
4	C	3502[A]	NAD	O4B-C1B-N9A-C8A
4	E	5502[A]	NAD	O4B-C1B-N9A-C8A

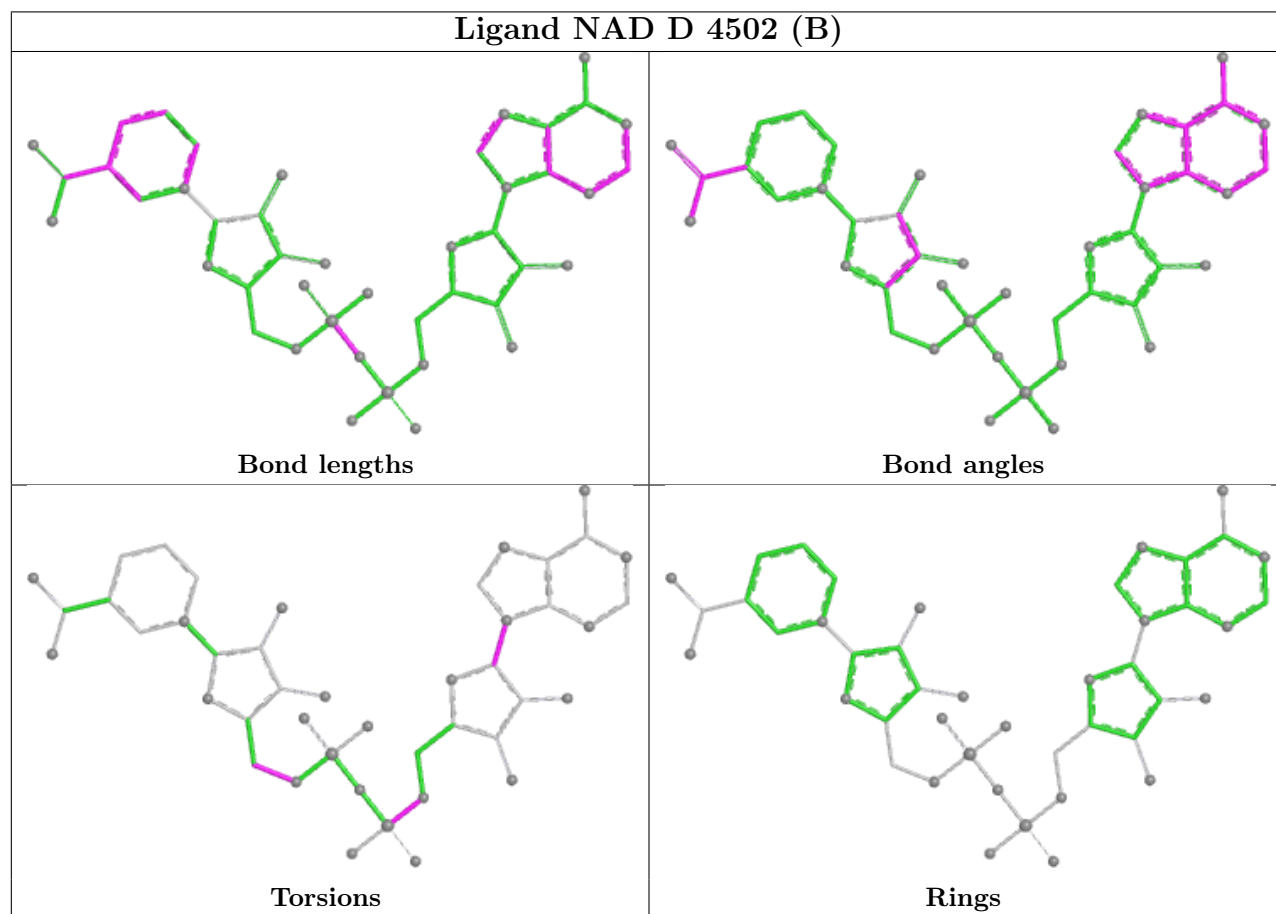
There are no ring outliers.

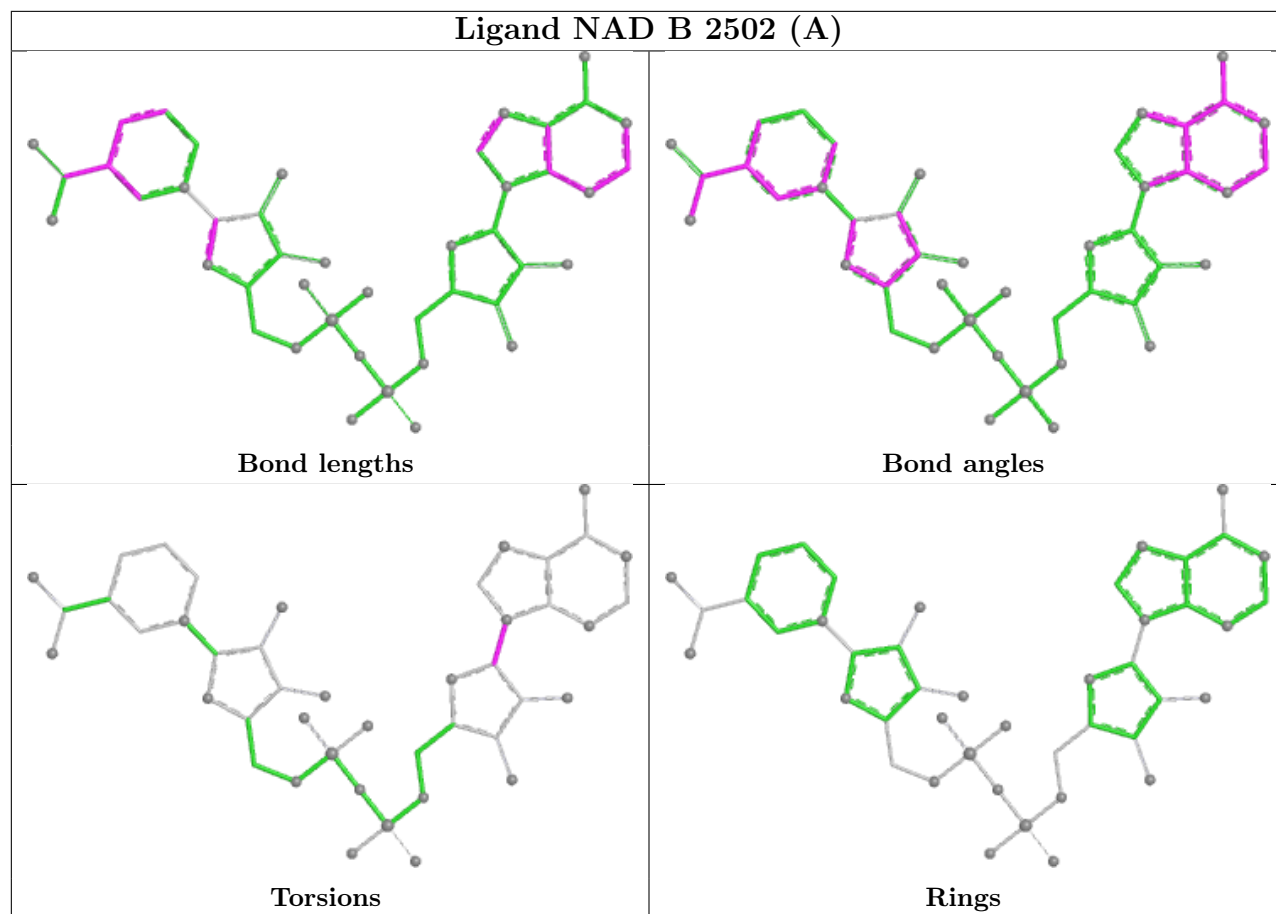
14 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4502[B]	NAD	7	0
4	B	2502[A]	NAD	2	0
4	E	5502[A]	NAD	3	0
4	H	8502[A]	NAD	1	0
4	B	2502[B]	NAD	6	0
4	G	7502[B]	NAD	5	0
4	H	8502[B]	NAD	4	0
4	A	1502[A]	NAD	3	0
4	F	6502[B]	NAD	7	0
4	C	3502[A]	NAD	4	0
4	E	5502[B]	NAD	8	0
4	D	4502[A]	NAD	1	0
4	A	1502[B]	NAD	12	0
4	C	3502[B]	NAD	17	0

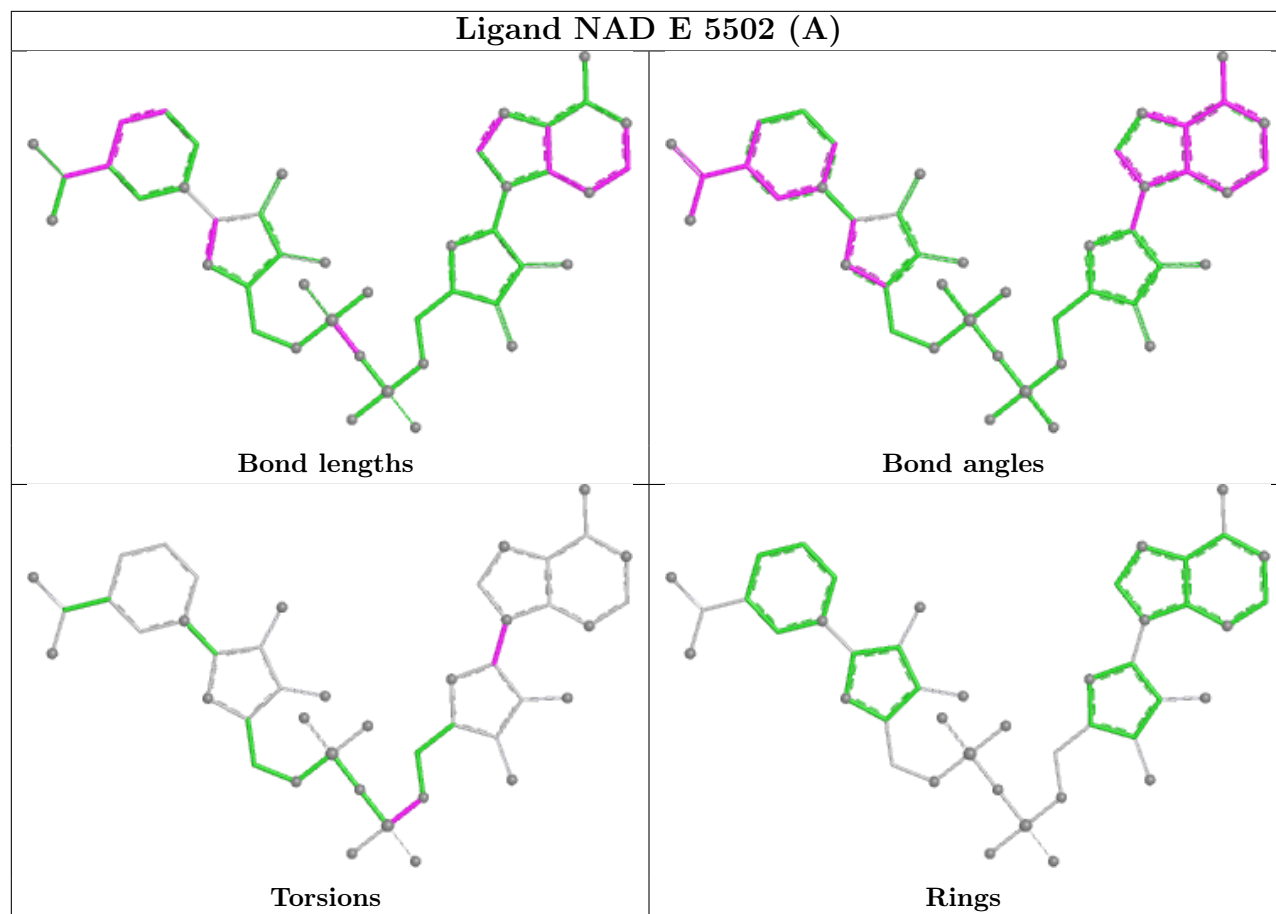
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

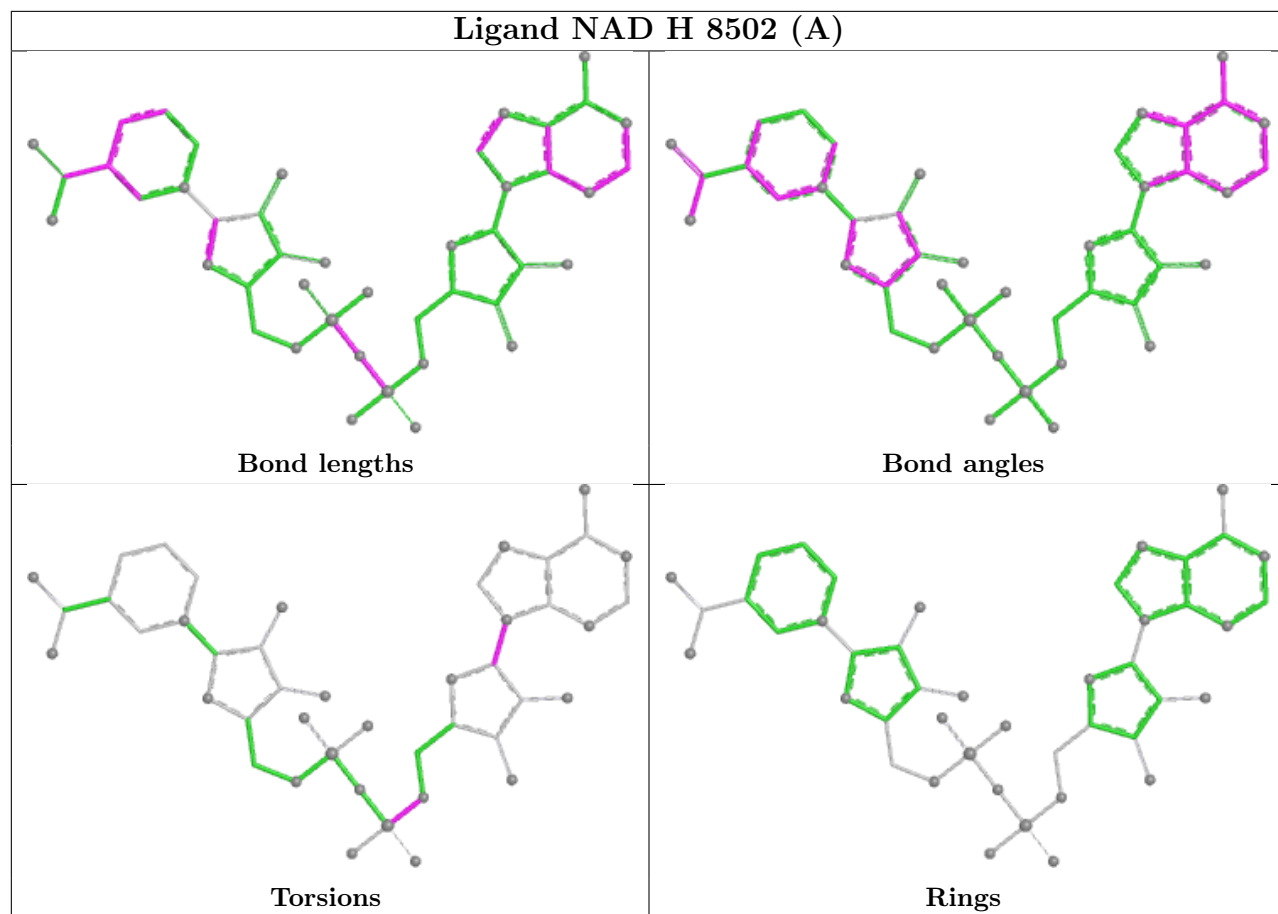




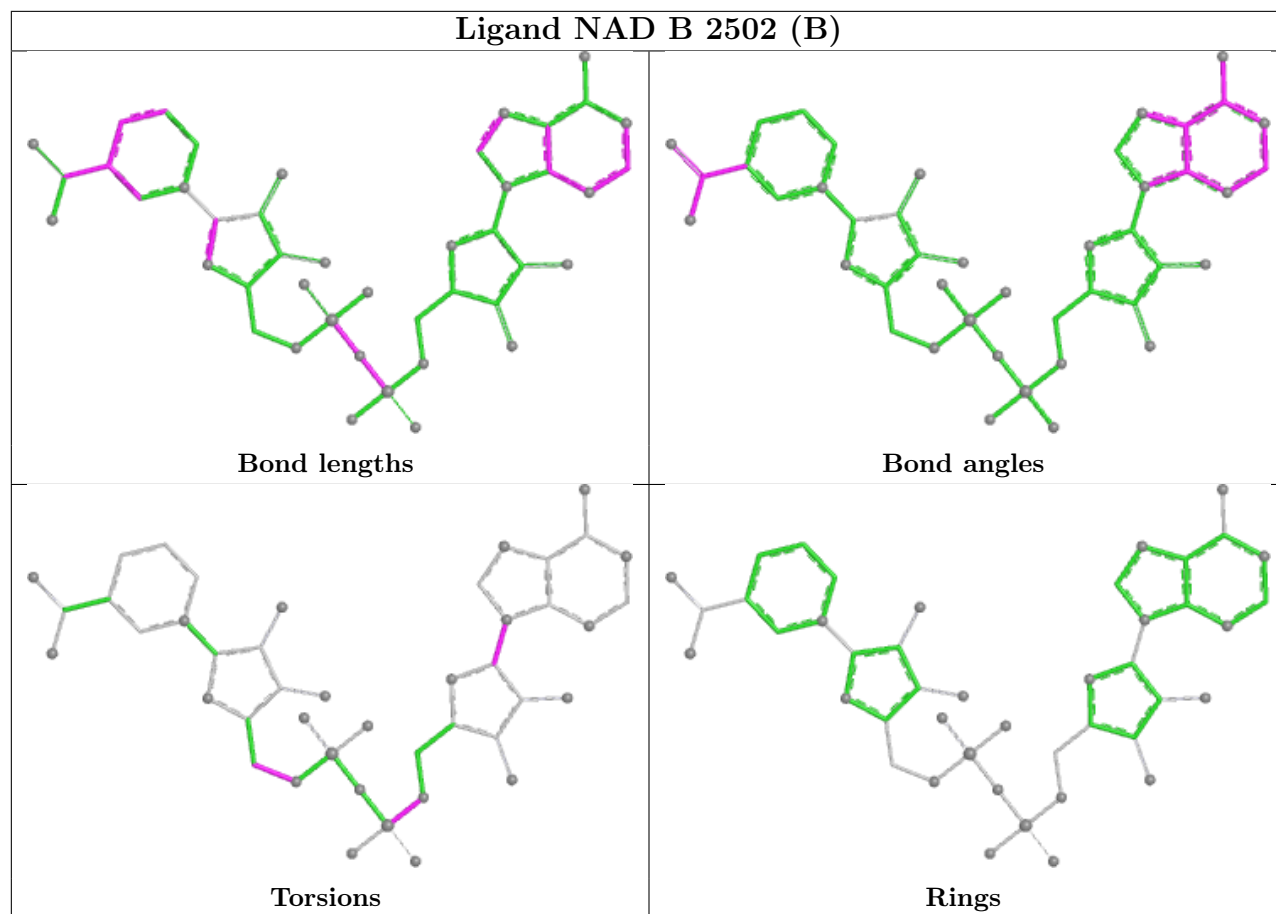
Ligand NAD E 5502 (A)



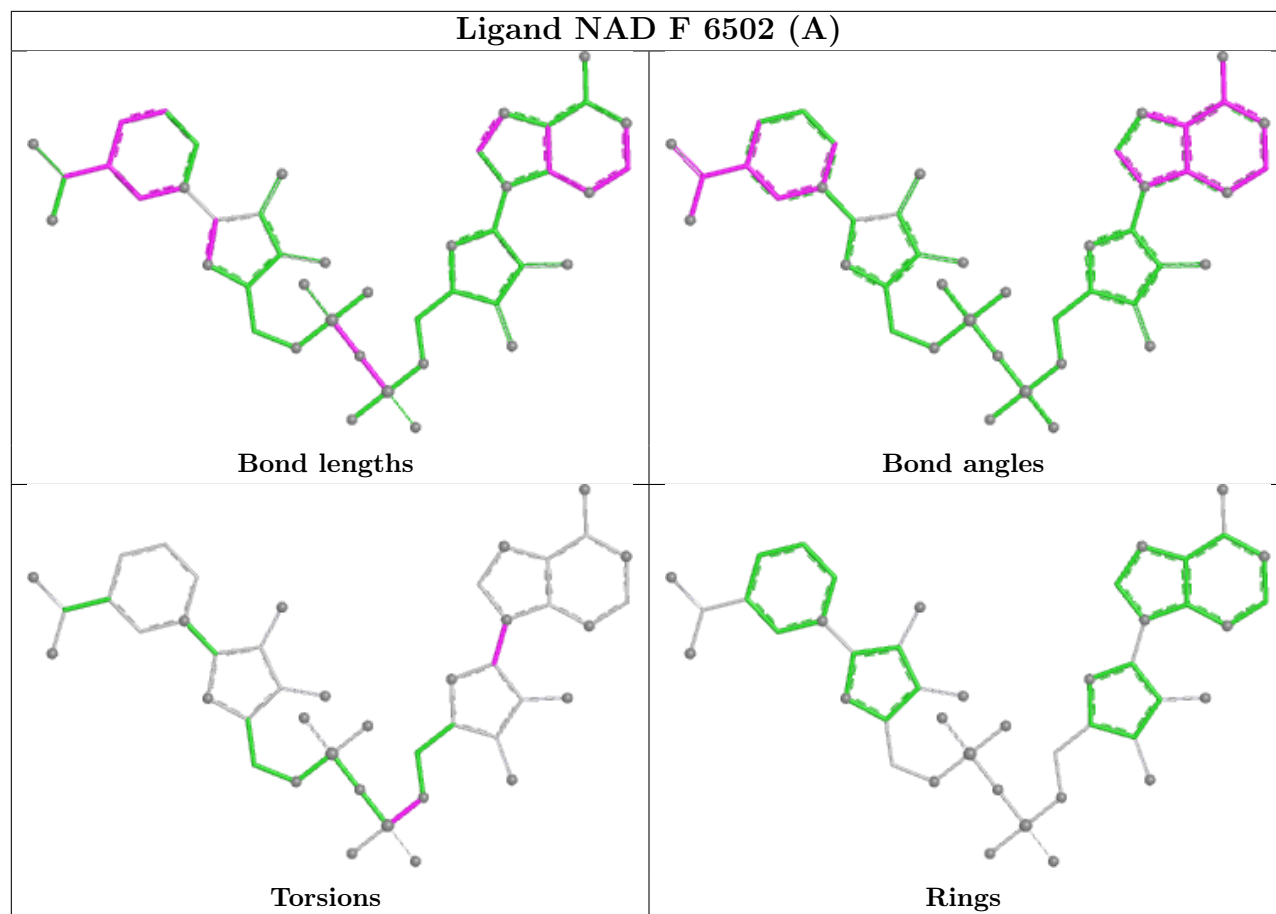
Ligand NAD H 8502 (A)



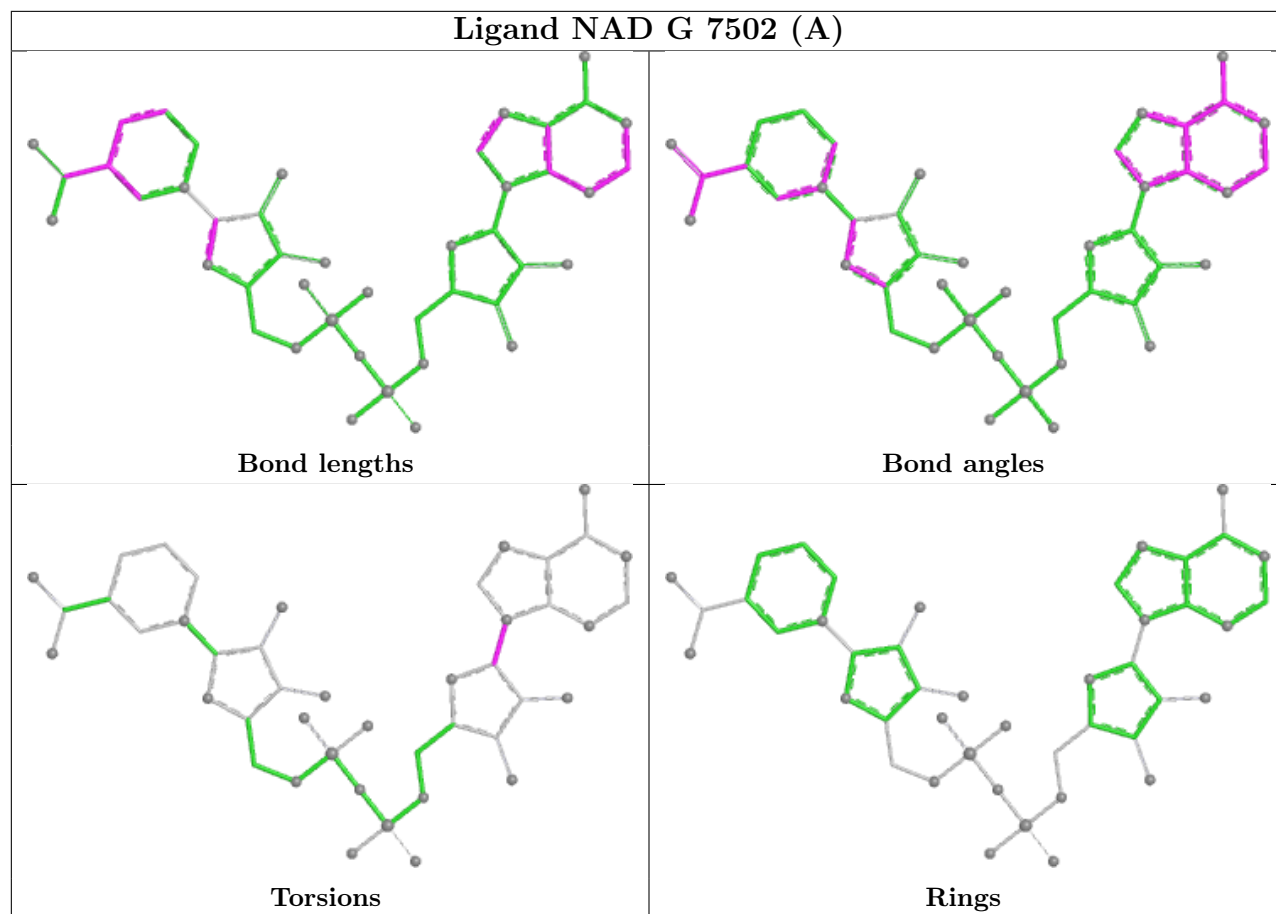
Ligand NAD B 2502 (B)



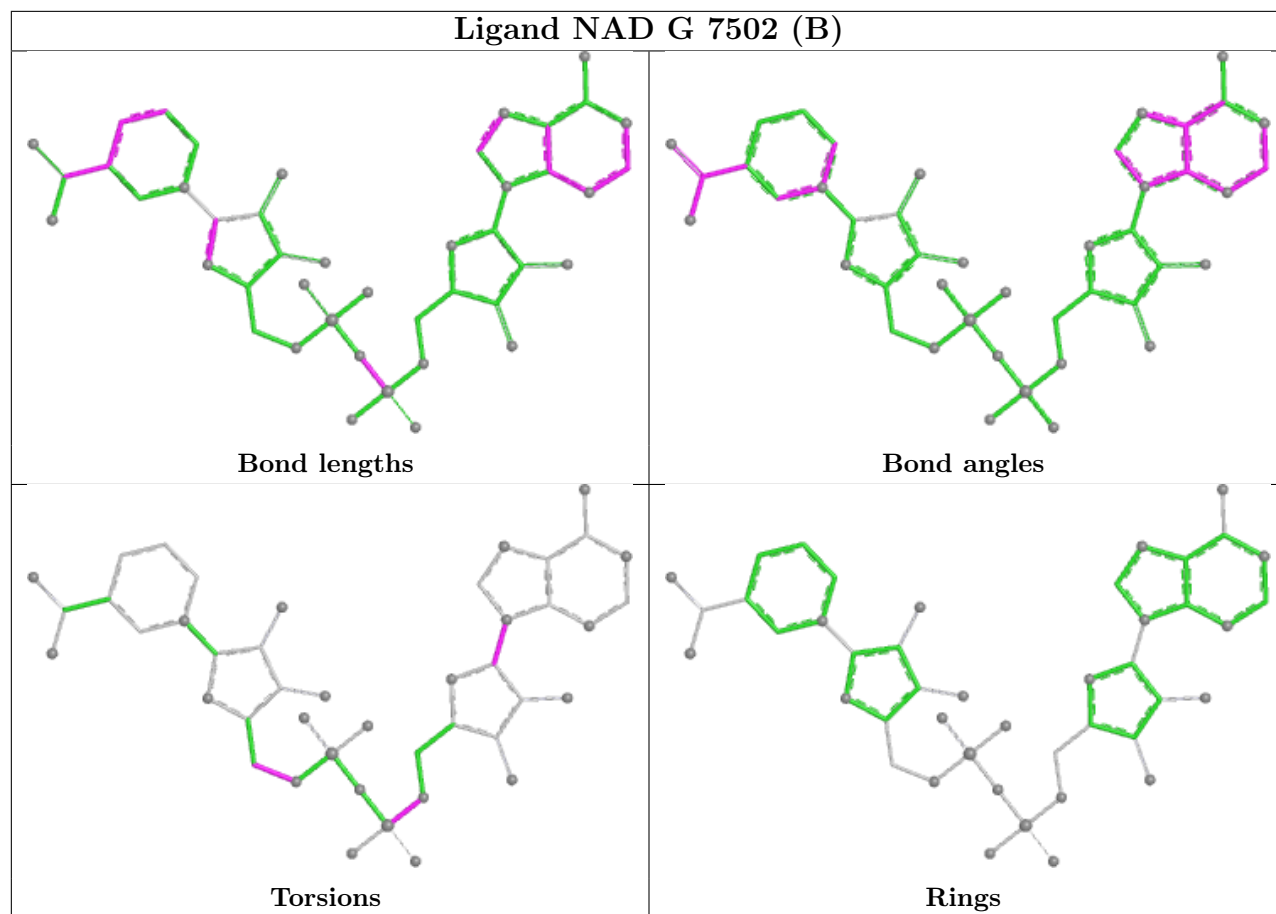
Ligand NAD F 6502 (A)



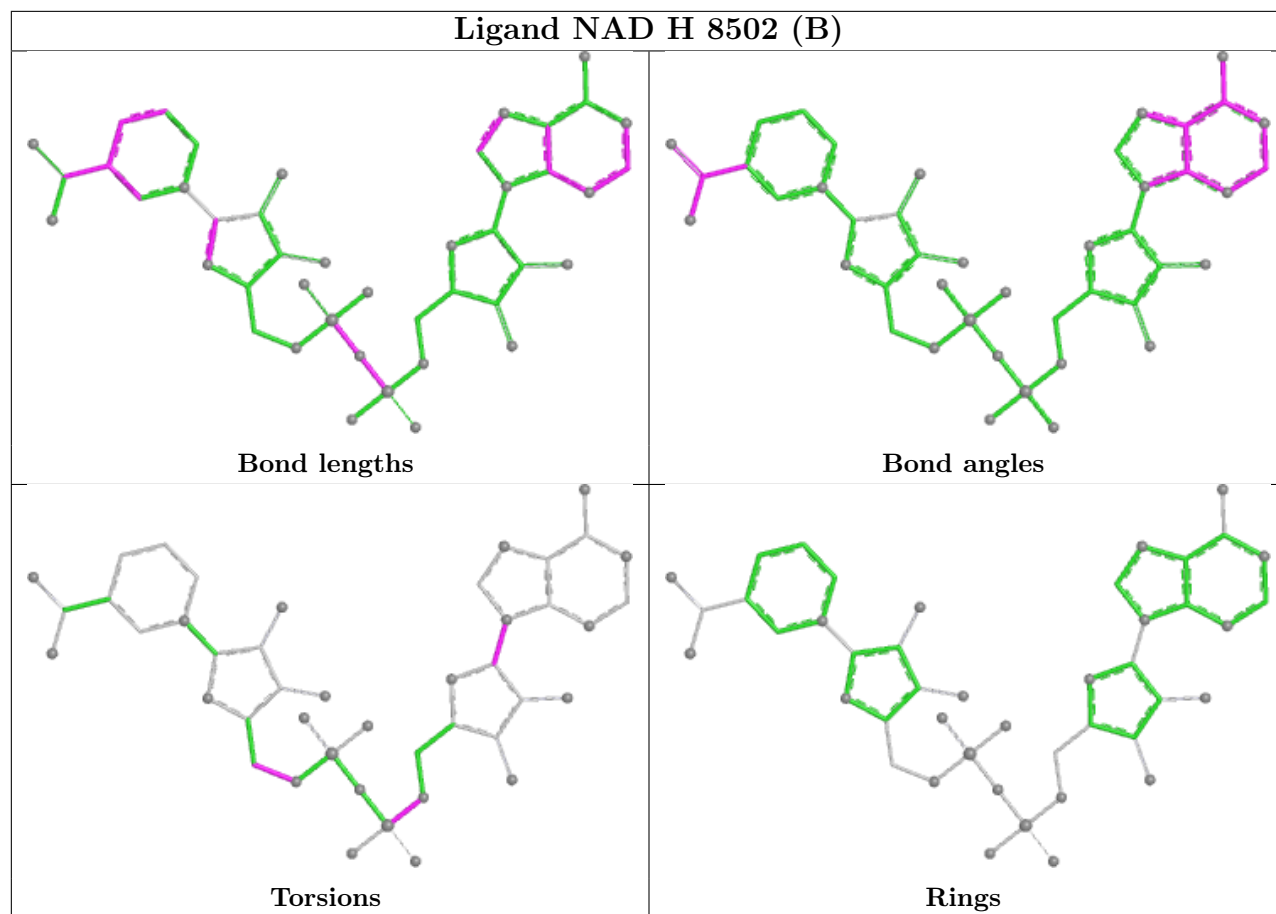
Ligand NAD G 7502 (A)



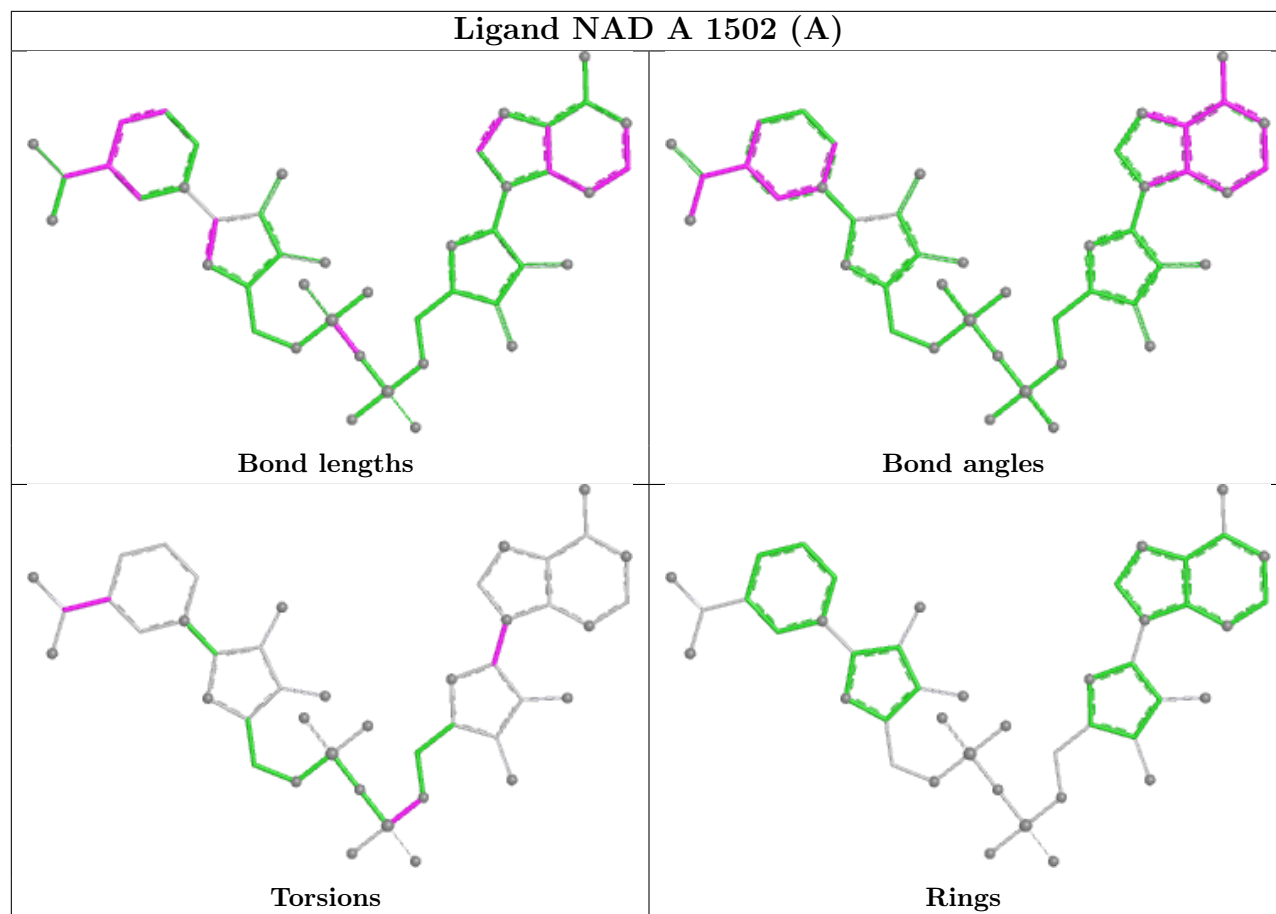
Ligand NAD G 7502 (B)



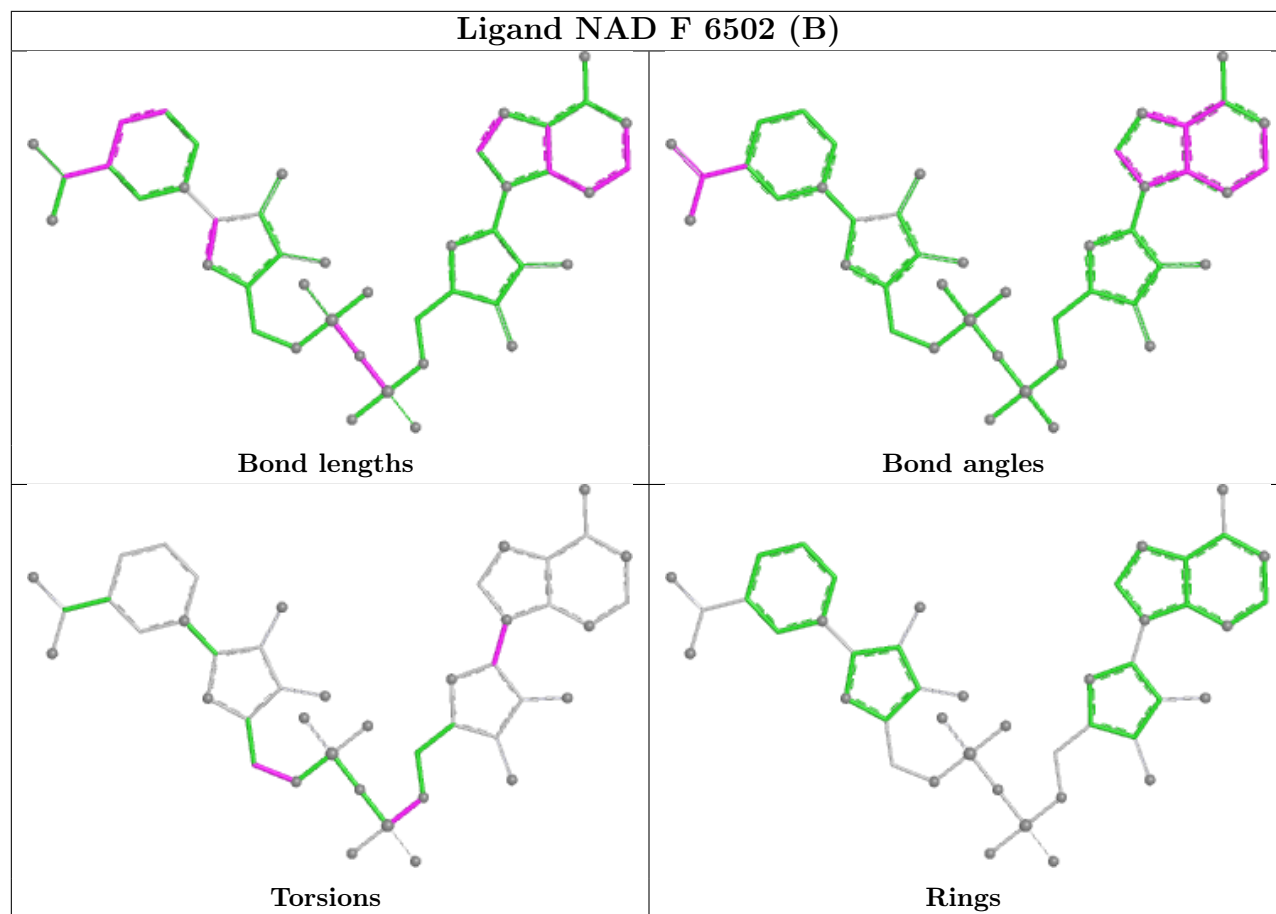
Ligand NAD H 8502 (B)



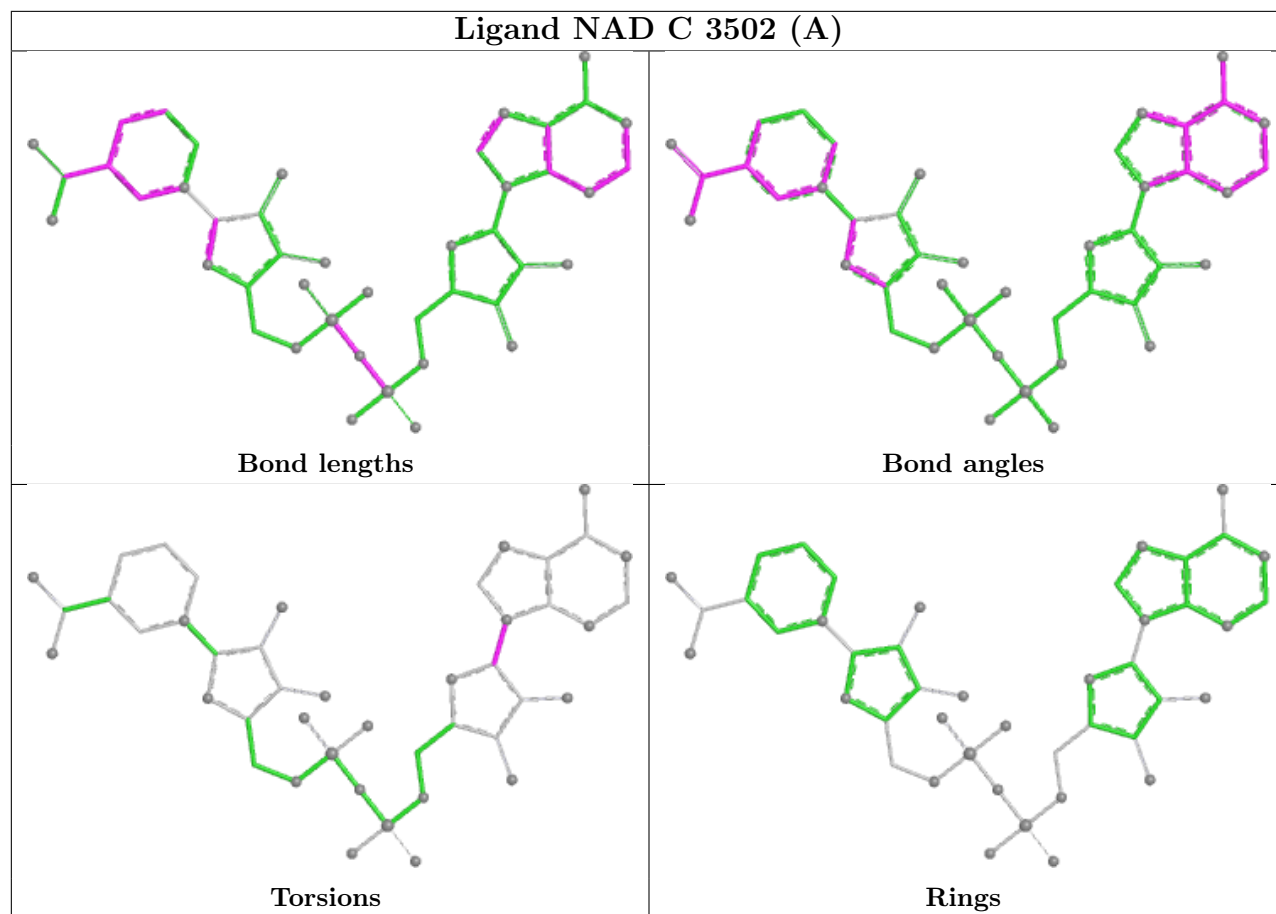
Ligand NAD A 1502 (A)



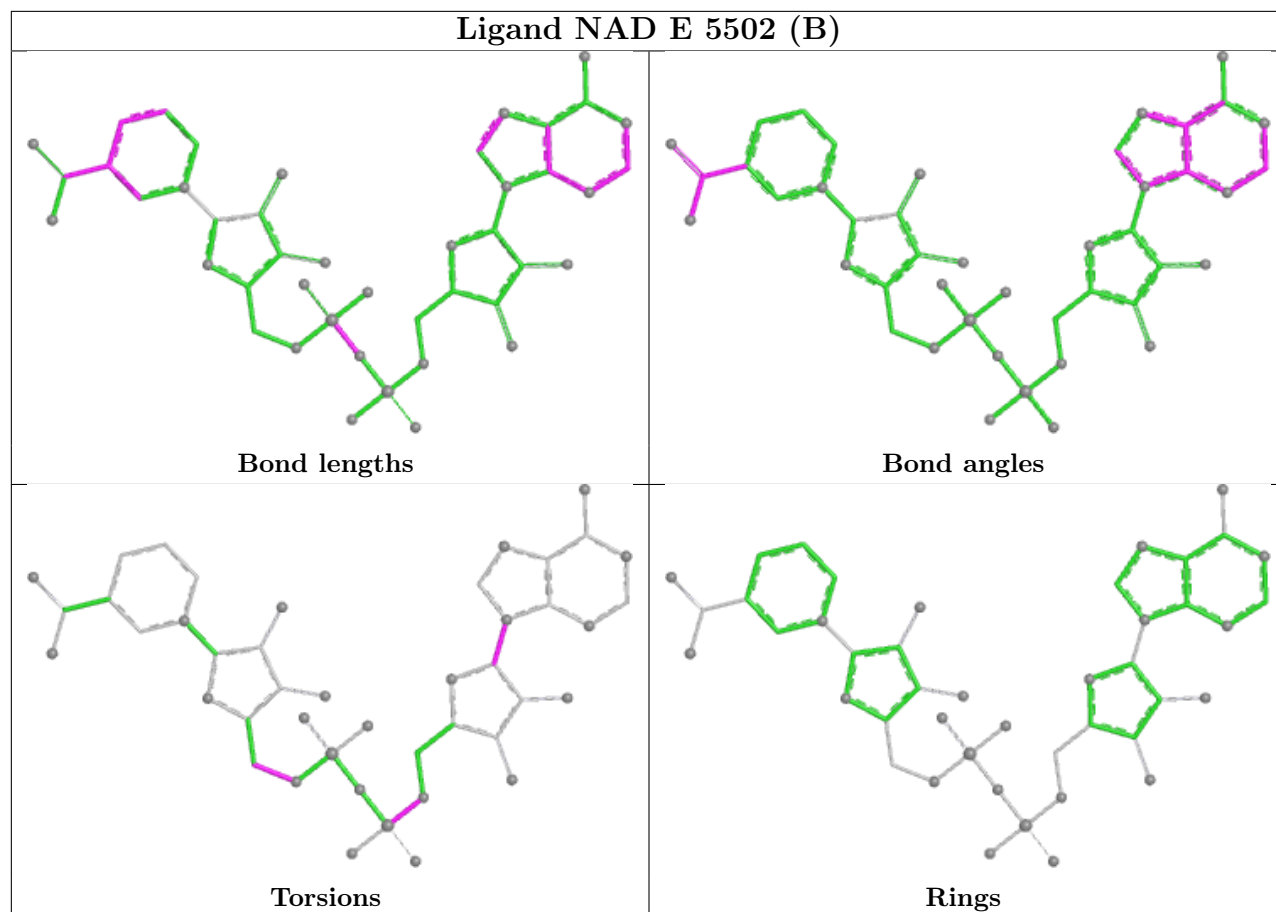
Ligand NAD F 6502 (B)



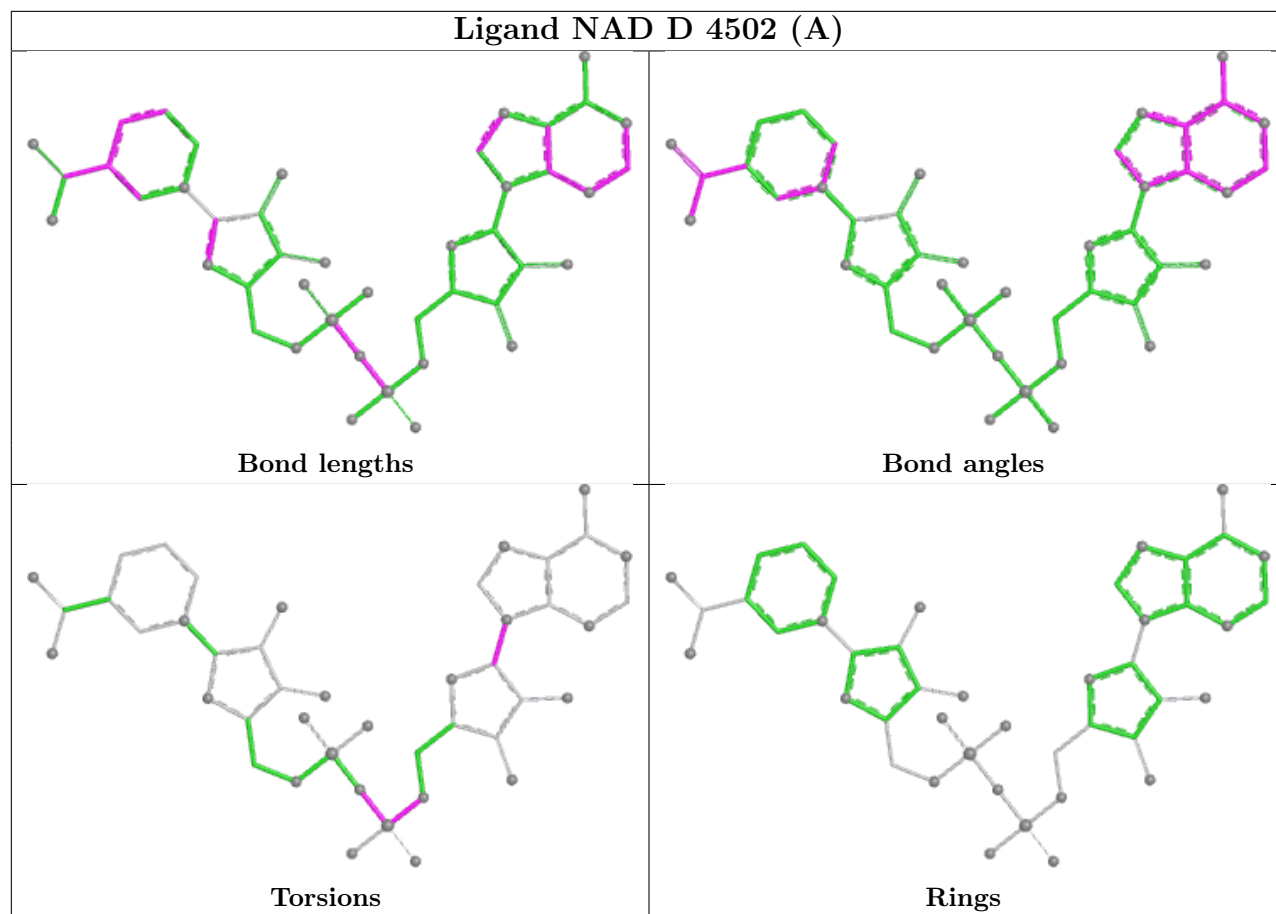
Ligand NAD C 3502 (A)



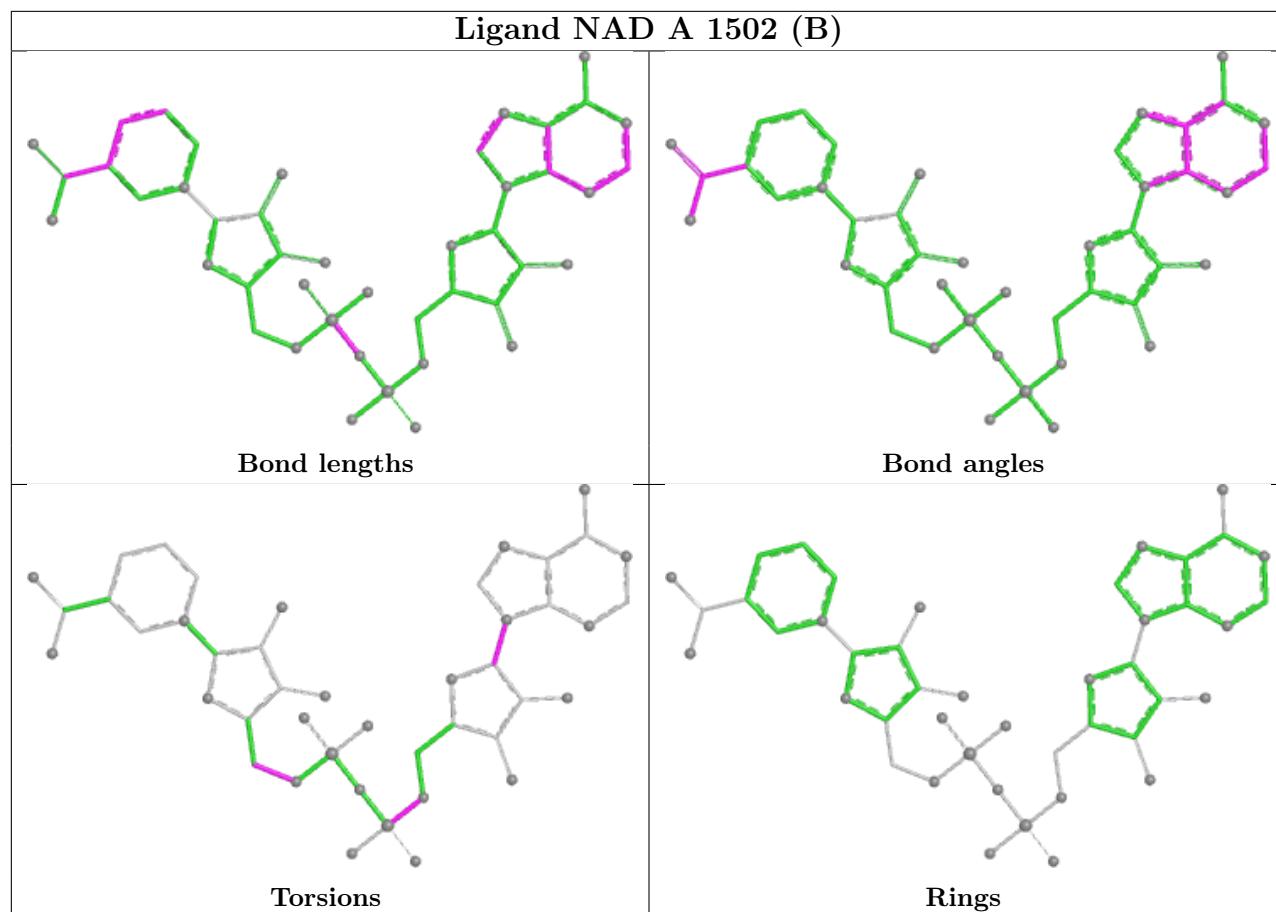
Ligand NAD E 5502 (B)

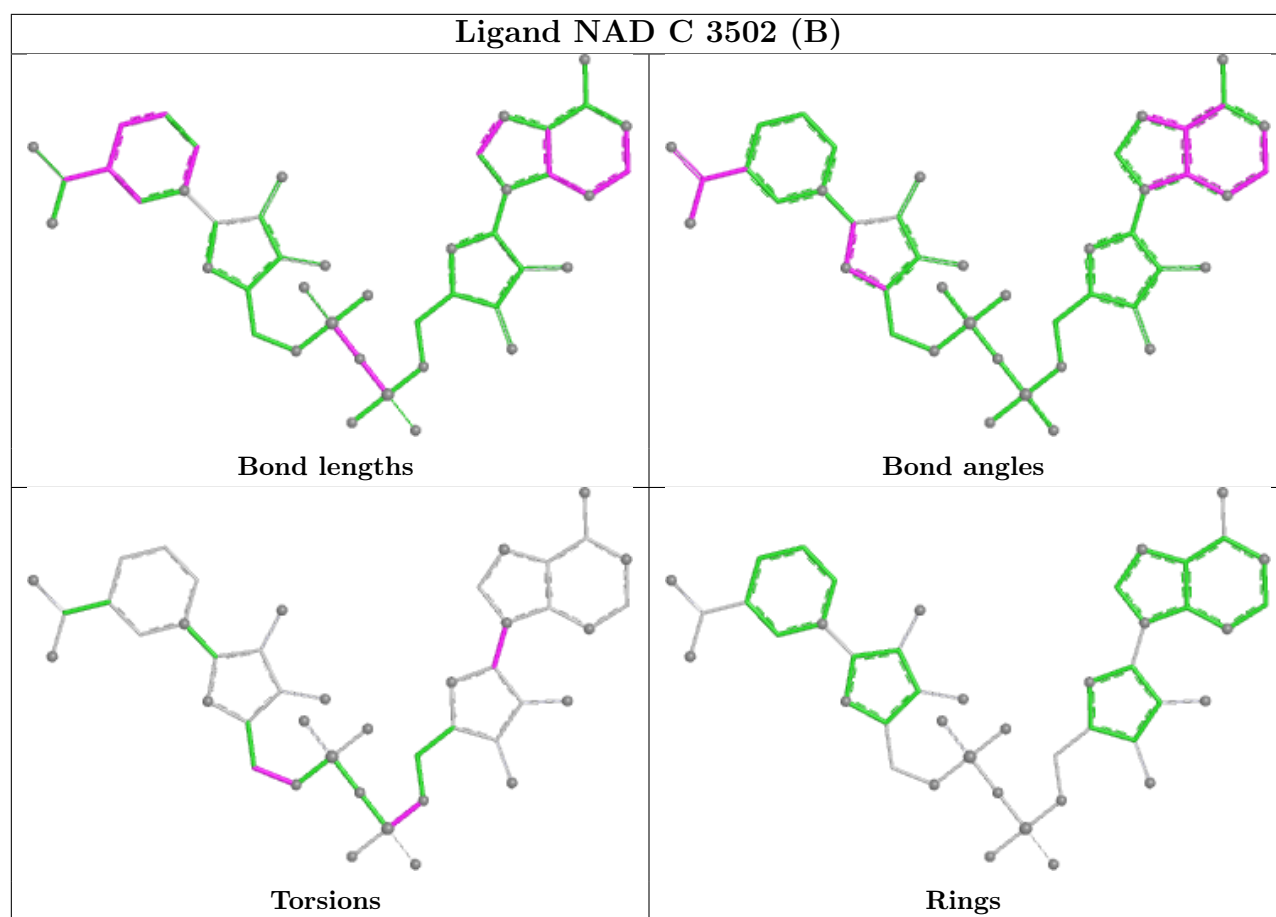


Ligand NAD D 4502 (A)



Ligand NAD A 1502 (B)





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	494/500 (98%)	-0.45	1 (0%) 91 90	5, 16, 30, 49	0
1	B	494/500 (98%)	-0.54	0 100 100	4, 14, 26, 45	0
1	C	494/500 (98%)	-0.53	1 (0%) 91 90	5, 13, 25, 42	0
1	D	494/500 (98%)	-0.40	4 (0%) 82 80	5, 16, 30, 47	0
1	E	494/500 (98%)	-0.48	1 (0%) 91 90	6, 15, 28, 46	0
1	F	494/500 (98%)	-0.54	0 100 100	4, 13, 24, 38	0
1	G	494/500 (98%)	-0.42	1 (0%) 91 90	6, 16, 30, 47	0
1	H	494/500 (98%)	-0.36	4 (0%) 82 80	7, 17, 32, 50	0
All	All	3952/4000 (98%)	-0.47	12 (0%) 90 88	4, 15, 28, 50	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	ALA	4.5
1	H	376	ASP	3.1
1	E	362	GLN	2.7
1	H	301	CYS	2.7
1	H	7	ALA	2.6
1	C	248	GLU	2.6
1	G	7	ALA	2.4
1	D	336	ASP	2.4
1	H	377	ARG	2.3
1	D	14	GLN	2.2
1	D	301	CYS	2.1
1	A	377	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	H	2608	1/1	0.56	0.19	38,38,38,38	0
2	MG	A	2601	1/1	0.61	0.25	54,54,54,54	0
2	MG	C	2603	1/1	0.69	0.19	23,23,23,23	0
3	NA	D	2704	1/1	0.69	0.15	44,44,44,44	0
3	NA	F	2706	1/1	0.74	0.16	38,38,38,38	0
3	NA	E	2705	1/1	0.77	0.10	30,30,30,30	0
3	NA	C	2703	1/1	0.77	0.23	45,45,45,45	0
2	MG	F	2606	1/1	0.78	0.14	22,22,22,22	0
3	NA	A	2701	1/1	0.79	0.12	34,34,34,34	0
4	NAD	H	8502[A]	44/44	0.79	0.17	14,31,38,38	44
4	NAD	H	8502[B]	44/44	0.79	0.17	16,29,33,34	44
4	NAD	B	2502[A]	44/44	0.80	0.16	15,28,34,34	44
4	NAD	B	2502[B]	44/44	0.80	0.16	16,27,32,32	44
4	NAD	E	5502[B]	44/44	0.81	0.14	17,26,32,32	44
2	MG	D	2604	1/1	0.81	0.20	37,37,37,37	0
4	NAD	E	5502[A]	44/44	0.81	0.14	14,27,37,37	44
3	NA	H	2708	1/1	0.82	0.11	46,46,46,46	0
4	NAD	A	1502[A]	44/44	0.84	0.14	19,26,38,38	44
4	NAD	A	1502[B]	44/44	0.84	0.14	17,29,32,32	44
4	NAD	C	3502[A]	44/44	0.84	0.13	16,25,28,30	44
4	NAD	C	3502[B]	44/44	0.84	0.13	17,28,36,37	44
4	NAD	G	7502[A]	44/44	0.85	0.14	23,36,39,39	44
4	NAD	G	7502[B]	44/44	0.85	0.14	18,28,31,31	44
4	NAD	D	4502[A]	44/44	0.85	0.14	13,23,39,40	44
4	NAD	D	4502[B]	44/44	0.85	0.14	17,25,31,32	44
2	MG	B	2602	1/1	0.86	0.25	41,41,41,41	0
4	NAD	F	6502[A]	44/44	0.88	0.12	10,17,29,30	44

Continued on next page...

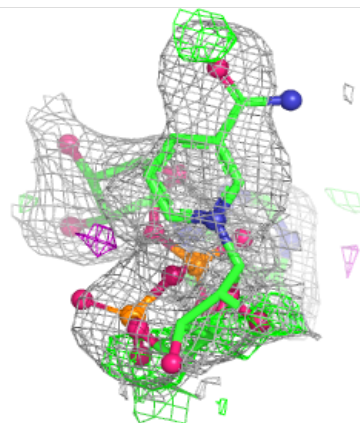
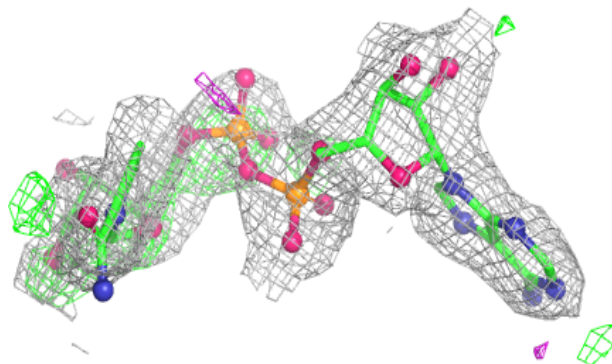
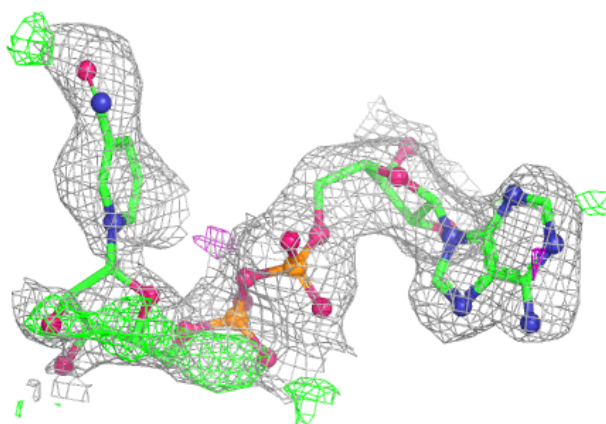
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	F	6502[B]	44/44	0.88	0.12	17,28,33,34	44
2	MG	G	2607	1/1	0.88	0.21	42,42,42,42	0
3	NA	G	2707	1/1	0.89	0.12	26,26,26,26	0
2	MG	E	2605	1/1	0.91	0.27	46,46,46,46	0
3	NA	B	2702	1/1	0.94	0.11	32,32,32,32	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.

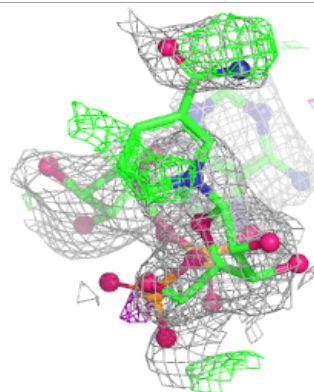
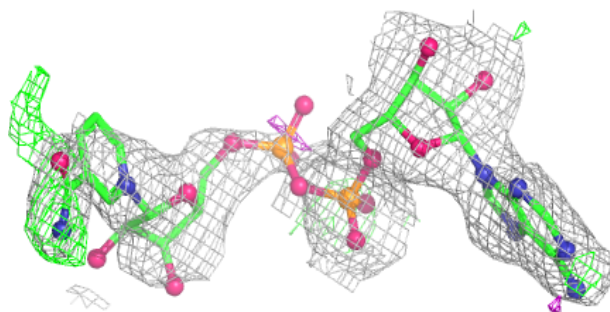
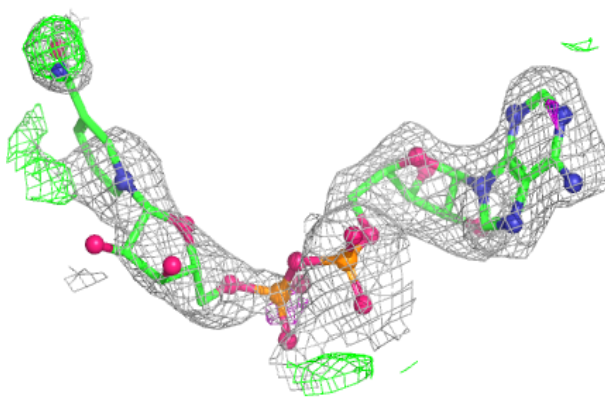
Electron density around NAD H 8502 (A):

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

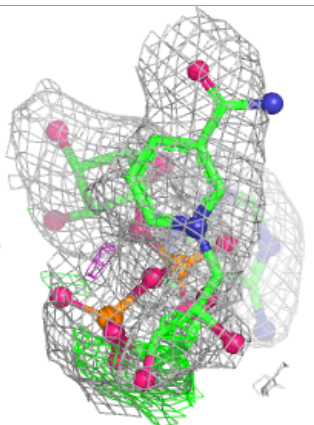
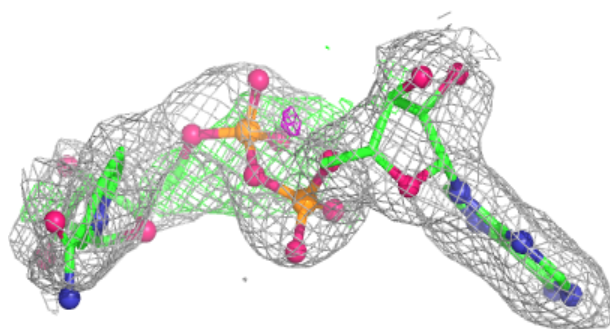
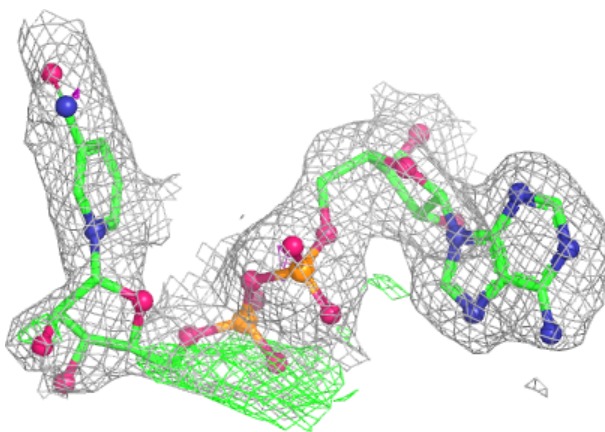


Electron density around NAD H 8502 (B):

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

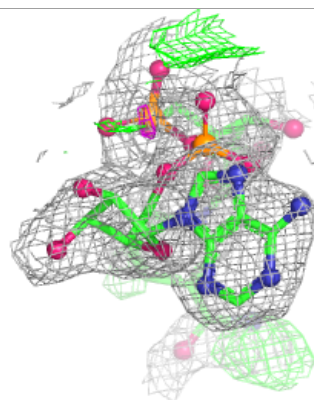
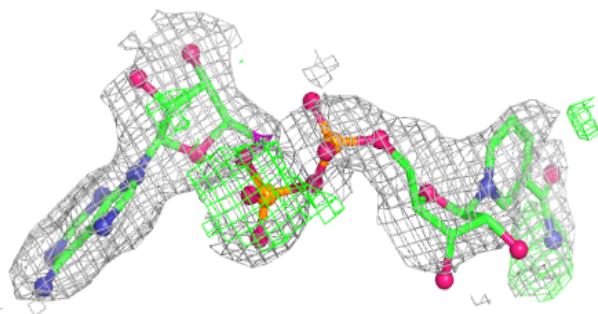
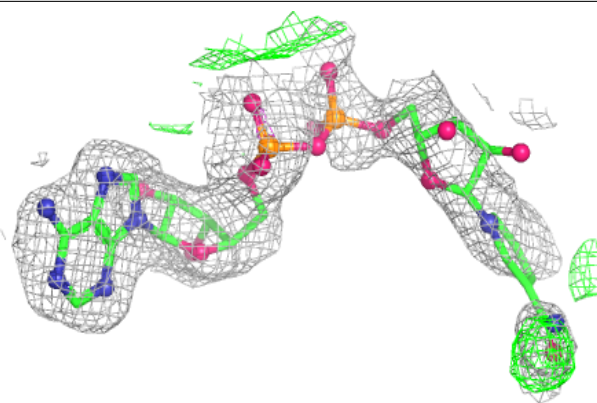
**Electron density around NAD B 2502 (A):**

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

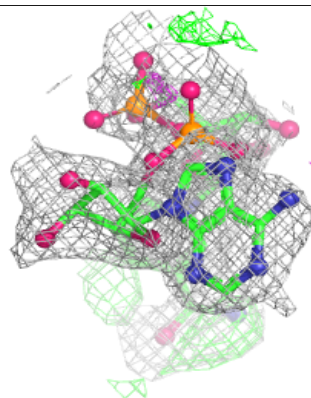
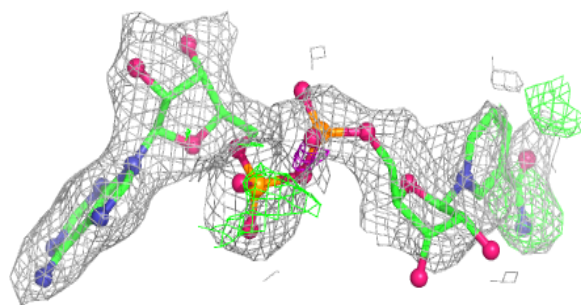
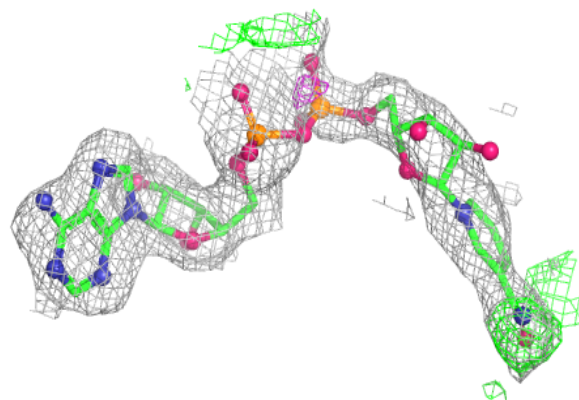


Electron density around NAD B 2502 (B):

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

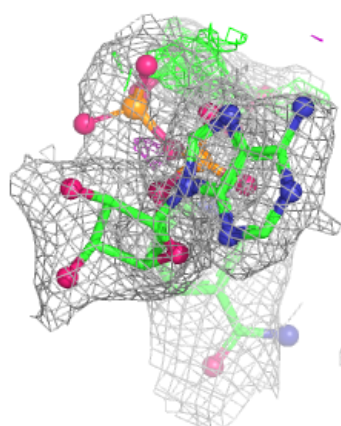
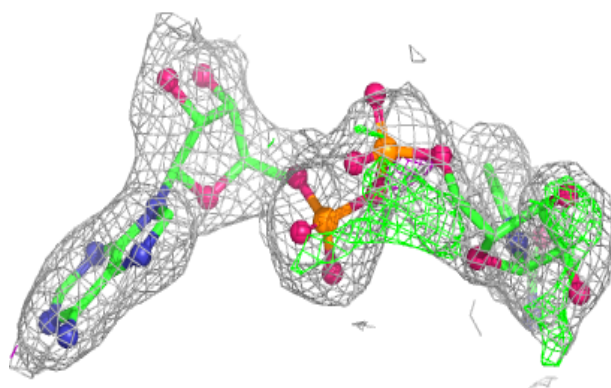
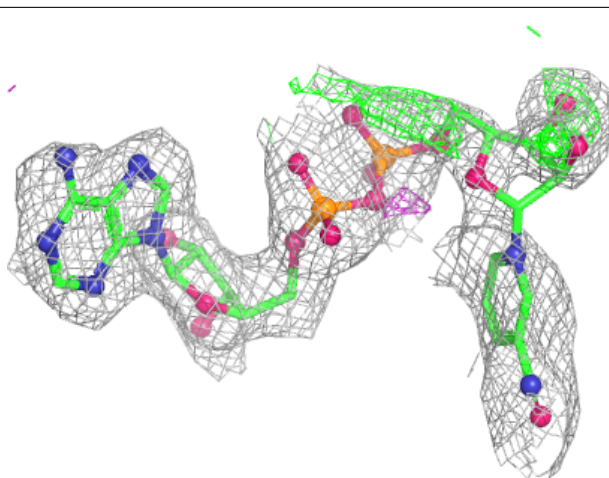
**Electron density around NAD E 5502 (B):**

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



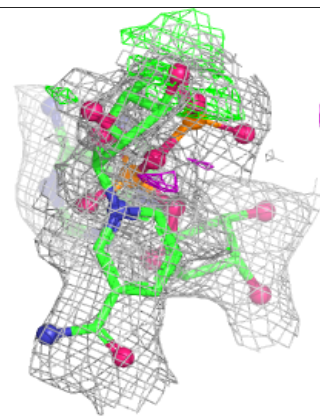
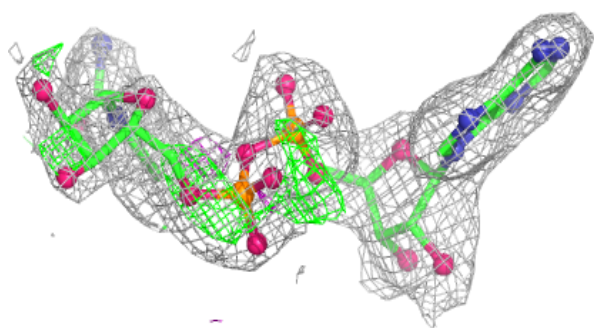
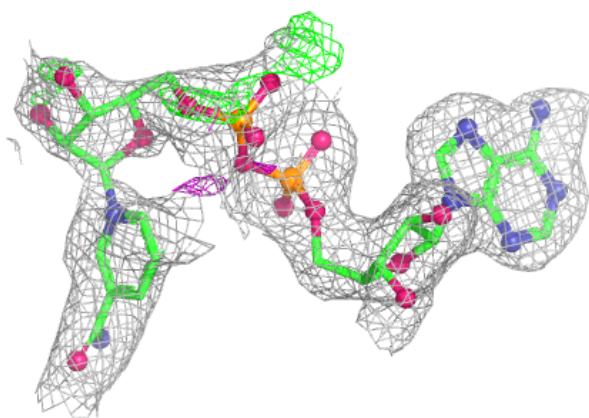
Electron density around NAD E 5502 (A):

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

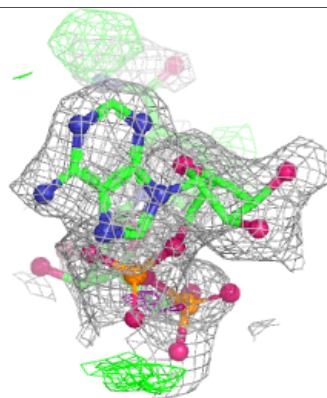
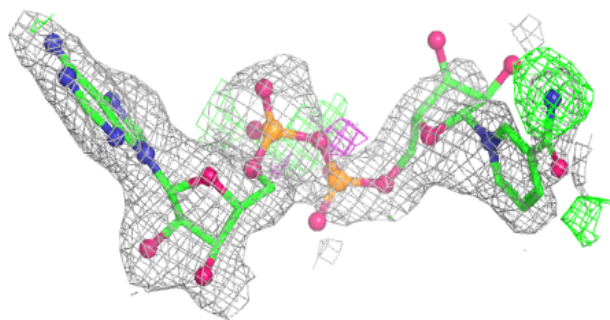
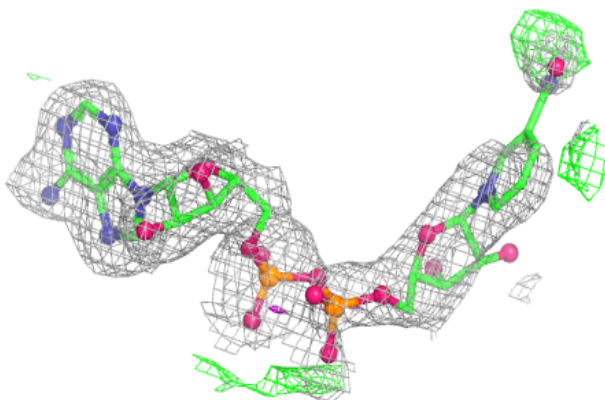


Electron density around NAD A 1502 (A):

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

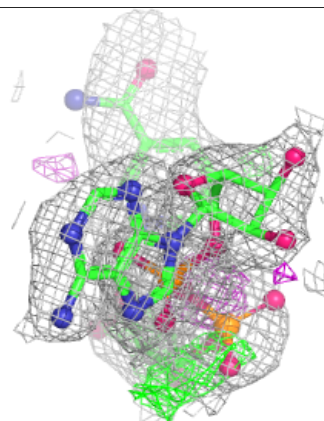
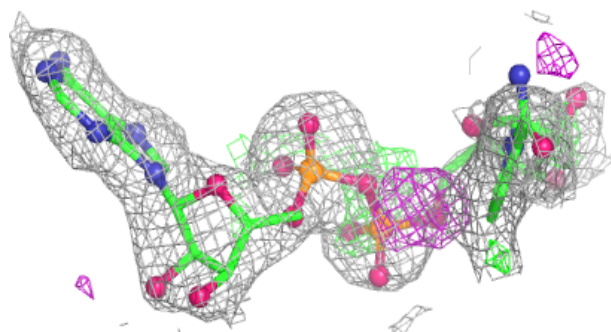
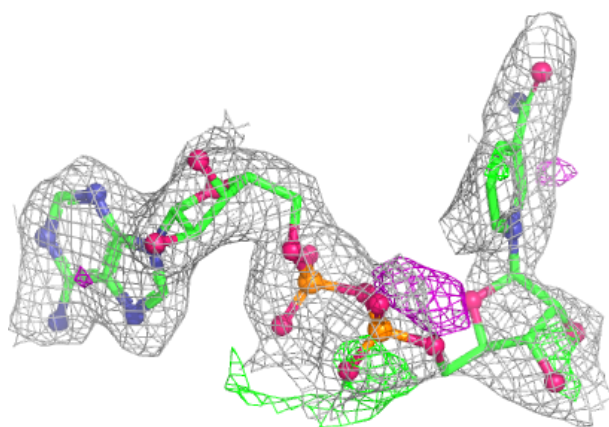
**Electron density around NAD A 1502 (B):**

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

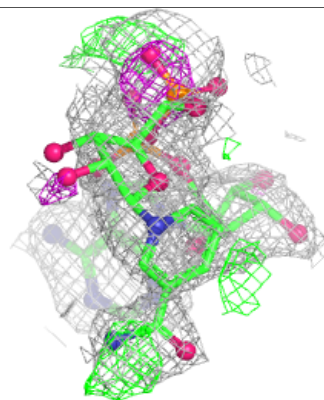
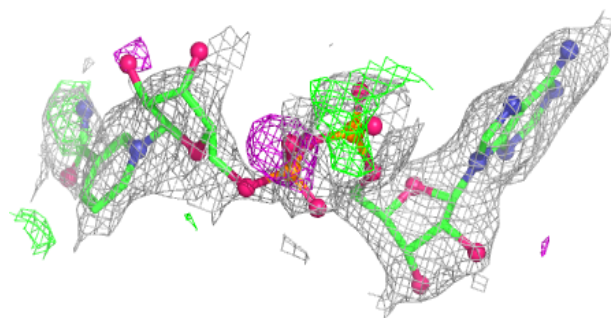
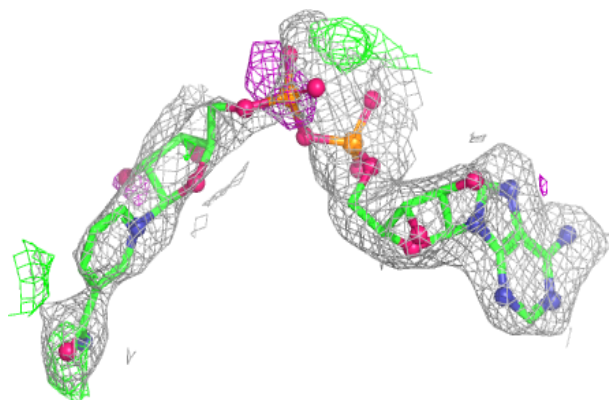


Electron density around NAD C 3502 (A):

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

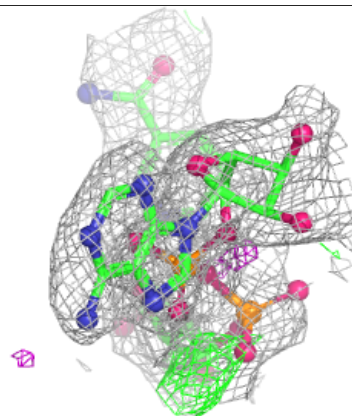
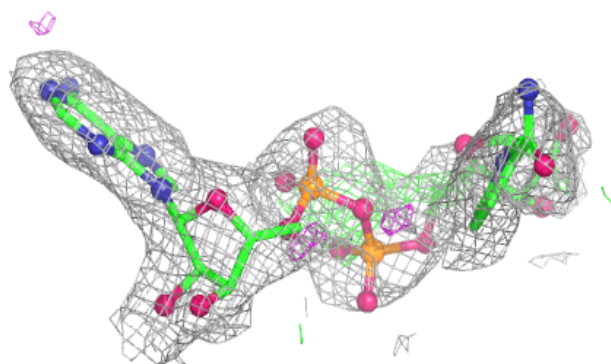
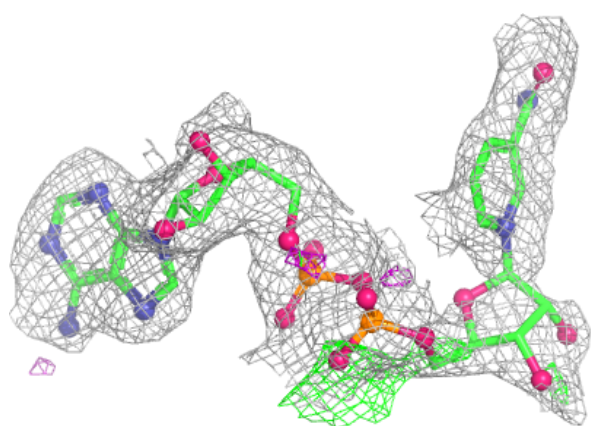
**Electron density around NAD C 3502 (B):**

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

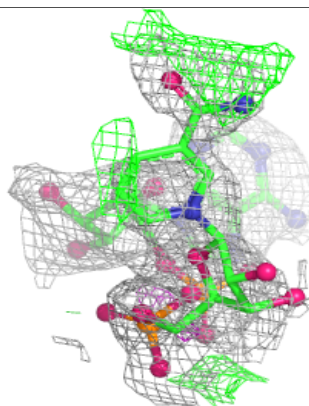
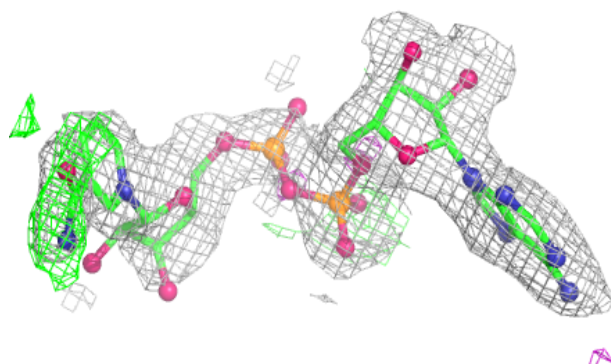
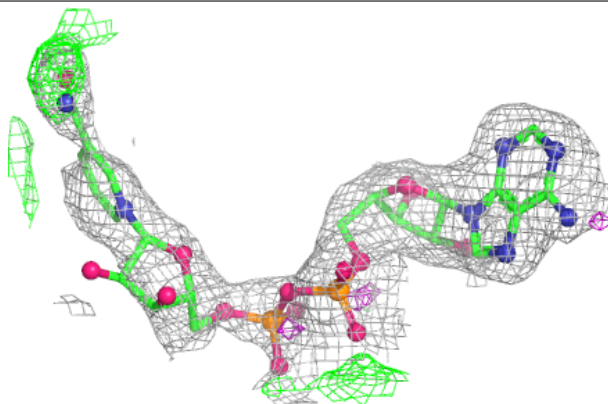


Electron density around NAD G 7502 (A):

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

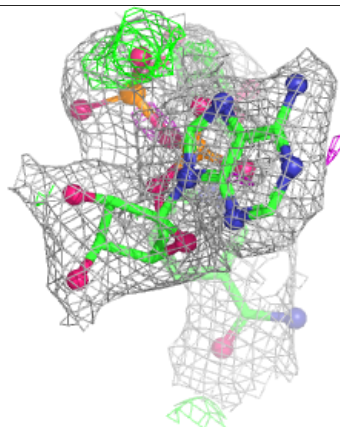
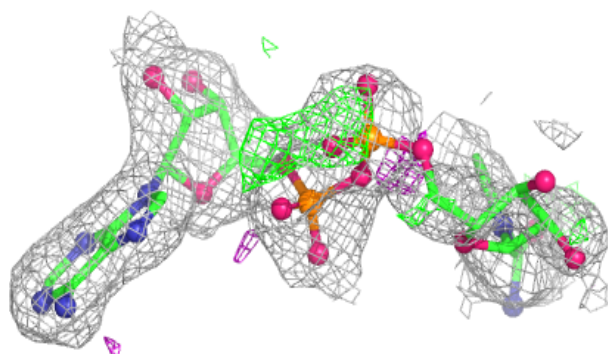
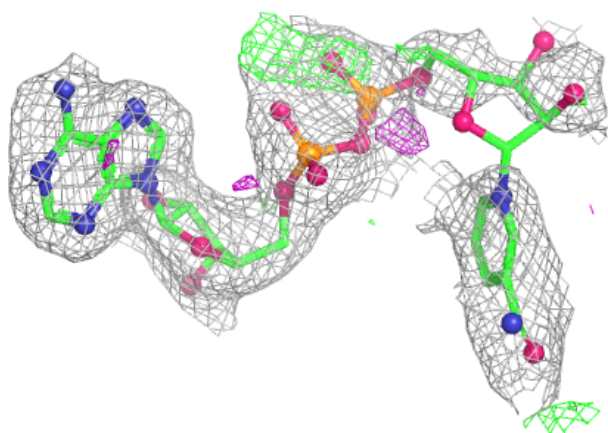
**Electron density around NAD G 7502 (B):**

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

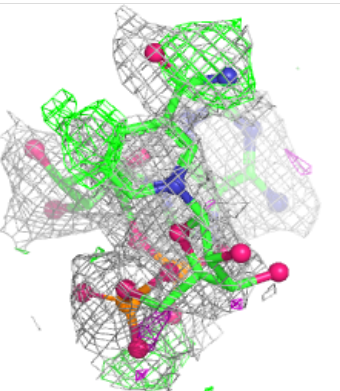
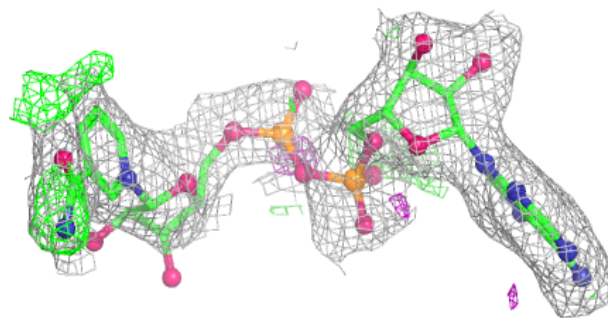
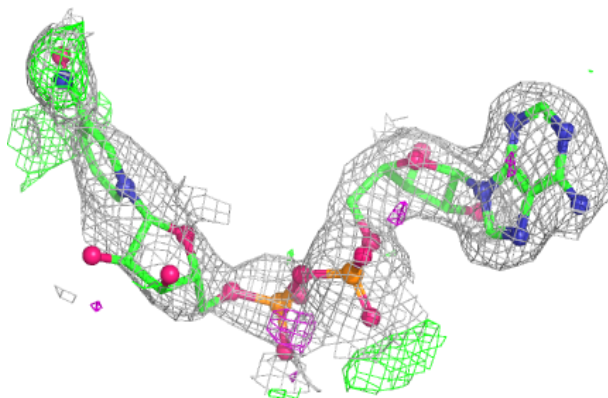


Electron density around NAD D 4502 (A):

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

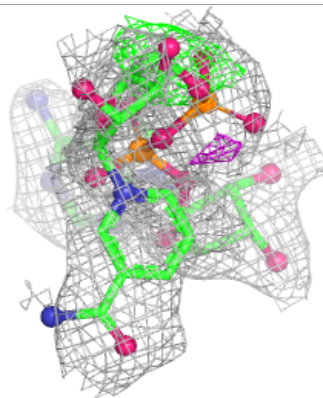
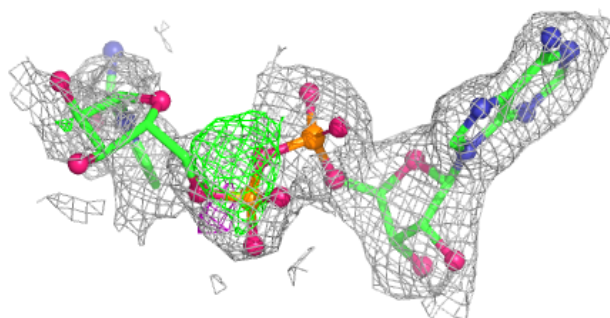
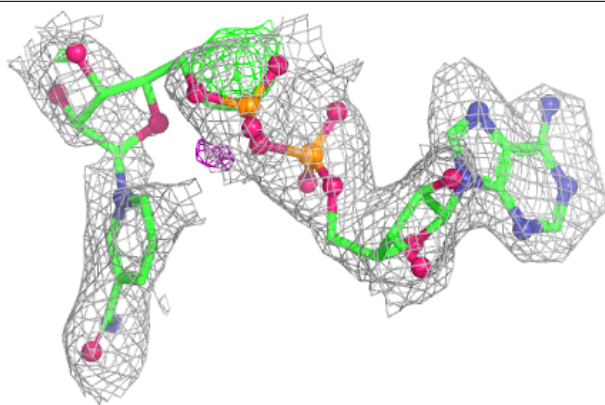
**Electron density around NAD D 4502 (B):**

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

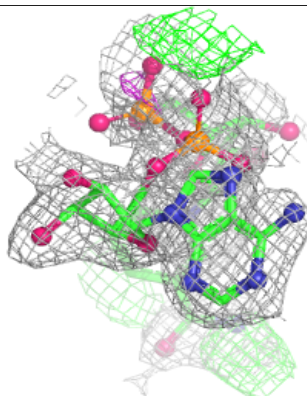
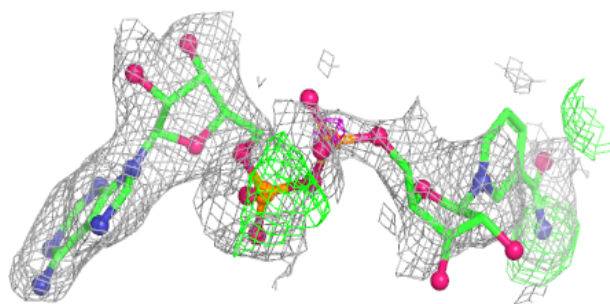
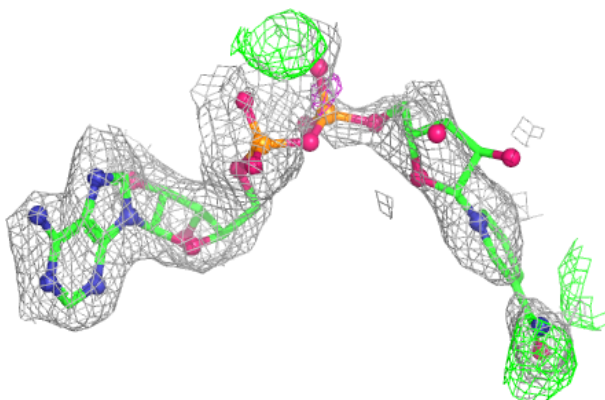


Electron density around NAD F 6502 (A):

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

**Electron density around NAD F 6502 (B):**

$2mF_o-DF_c$ (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.