



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:46 AM UTC

PDB ID : 5US6 / pdb_00005us6
Title : Structure of Dihydrodipicolinate Reductase from *Vibrio vulnificus* Bound to NADH and 2,6 Pyridine Dicarboxylic Acid with Intact Polyhistidine Tag
Authors : Mank, N.M.; Arnette, A.K.; Chruszcz, M.
Deposited on : 2017-02-13
Resolution : 2.61 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

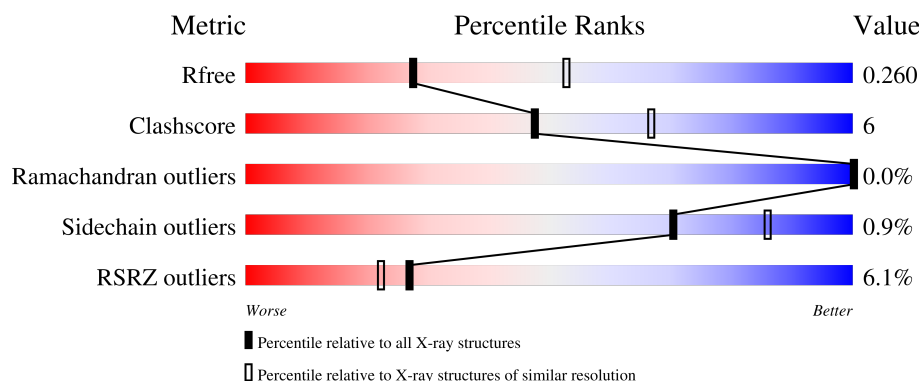
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	294	2% 81% 10% 9%
1	B	294	2% 80% 11% 10%
1	C	294	8% 78% 11% 10%
1	D	294	4% 79% 9% 12%
1	E	294	0% 80% 11% 9%

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Mol	Chain	Length	Quality of chain
1	F	294	
1	G	294	
1	H	294	
1	I	294	
1	J	294	
1	K	294	
1	L	294	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	D	304	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23790 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	267	Total	C	N	O	S	0	0	0
			1962	1228	343	378	13			
1	B	266	Total	C	N	O	S	0	0	0
			1940	1215	338	374	13			
1	C	266	Total	C	N	O	S	0	0	0
			1927	1210	337	367	13			
1	D	260	Total	C	N	O	S	0	0	0
			1876	1175	326	363	12			
1	E	267	Total	C	N	O	S	0	0	0
			1970	1234	345	378	13			
1	F	266	Total	C	N	O	S	0	0	0
			1956	1225	342	376	13			
1	G	266	Total	C	N	O	S	0	0	0
			1947	1221	341	372	13			
1	H	264	Total	C	N	O	S	0	0	0
			1900	1191	331	365	13			
1	I	267	Total	C	N	O	S	0	0	0
			1962	1228	343	378	13			
1	J	267	Total	C	N	O	S	0	0	0
			1958	1227	343	375	13			
1	K	266	Total	C	N	O	S	0	0	0
			1936	1215	341	368	12			
1	L	237	Total	C	N	O	S	0	0	0
			1676	1051	296	319	10			

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q8DEM0
A	-23	HIS	-	expression tag	UNP Q8DEM0
A	-22	HIS	-	expression tag	UNP Q8DEM0
A	-21	HIS	-	expression tag	UNP Q8DEM0
A	-20	HIS	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	expression tag	UNP Q8DEM0
A	-18	HIS	-	expression tag	UNP Q8DEM0
A	-17	SER	-	expression tag	UNP Q8DEM0
A	-16	SER	-	expression tag	UNP Q8DEM0
A	-15	GLY	-	expression tag	UNP Q8DEM0
A	-14	VAL	-	expression tag	UNP Q8DEM0
A	-13	ASP	-	expression tag	UNP Q8DEM0
A	-12	LEU	-	expression tag	UNP Q8DEM0
A	-11	GLY	-	expression tag	UNP Q8DEM0
A	-10	THR	-	expression tag	UNP Q8DEM0
A	-9	GLU	-	expression tag	UNP Q8DEM0
A	-8	ASN	-	expression tag	UNP Q8DEM0
A	-7	LEU	-	expression tag	UNP Q8DEM0
A	-6	TYR	-	expression tag	UNP Q8DEM0
A	-5	PHE	-	expression tag	UNP Q8DEM0
A	-4	GLN	-	expression tag	UNP Q8DEM0
A	-3	SER	-	expression tag	UNP Q8DEM0
A	-2	GLY	-	expression tag	UNP Q8DEM0
A	-1	SER	-	expression tag	UNP Q8DEM0
A	0	GLY	-	expression tag	UNP Q8DEM0
B	-24	MET	-	initiating methionine	UNP Q8DEM0
B	-23	HIS	-	expression tag	UNP Q8DEM0
B	-22	HIS	-	expression tag	UNP Q8DEM0
B	-21	HIS	-	expression tag	UNP Q8DEM0
B	-20	HIS	-	expression tag	UNP Q8DEM0
B	-19	HIS	-	expression tag	UNP Q8DEM0
B	-18	HIS	-	expression tag	UNP Q8DEM0
B	-17	SER	-	expression tag	UNP Q8DEM0
B	-16	SER	-	expression tag	UNP Q8DEM0
B	-15	GLY	-	expression tag	UNP Q8DEM0
B	-14	VAL	-	expression tag	UNP Q8DEM0
B	-13	ASP	-	expression tag	UNP Q8DEM0
B	-12	LEU	-	expression tag	UNP Q8DEM0
B	-11	GLY	-	expression tag	UNP Q8DEM0
B	-10	THR	-	expression tag	UNP Q8DEM0
B	-9	GLU	-	expression tag	UNP Q8DEM0
B	-8	ASN	-	expression tag	UNP Q8DEM0
B	-7	LEU	-	expression tag	UNP Q8DEM0
B	-6	TYR	-	expression tag	UNP Q8DEM0
B	-5	PHE	-	expression tag	UNP Q8DEM0
B	-4	GLN	-	expression tag	UNP Q8DEM0
B	-3	SER	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q8DEM0
B	-1	SER	-	expression tag	UNP Q8DEM0
B	0	GLY	-	expression tag	UNP Q8DEM0
C	-24	MET	-	initiating methionine	UNP Q8DEM0
C	-23	HIS	-	expression tag	UNP Q8DEM0
C	-22	HIS	-	expression tag	UNP Q8DEM0
C	-21	HIS	-	expression tag	UNP Q8DEM0
C	-20	HIS	-	expression tag	UNP Q8DEM0
C	-19	HIS	-	expression tag	UNP Q8DEM0
C	-18	HIS	-	expression tag	UNP Q8DEM0
C	-17	SER	-	expression tag	UNP Q8DEM0
C	-16	SER	-	expression tag	UNP Q8DEM0
C	-15	GLY	-	expression tag	UNP Q8DEM0
C	-14	VAL	-	expression tag	UNP Q8DEM0
C	-13	ASP	-	expression tag	UNP Q8DEM0
C	-12	LEU	-	expression tag	UNP Q8DEM0
C	-11	GLY	-	expression tag	UNP Q8DEM0
C	-10	THR	-	expression tag	UNP Q8DEM0
C	-9	GLU	-	expression tag	UNP Q8DEM0
C	-8	ASN	-	expression tag	UNP Q8DEM0
C	-7	LEU	-	expression tag	UNP Q8DEM0
C	-6	TYR	-	expression tag	UNP Q8DEM0
C	-5	PHE	-	expression tag	UNP Q8DEM0
C	-4	GLN	-	expression tag	UNP Q8DEM0
C	-3	SER	-	expression tag	UNP Q8DEM0
C	-2	GLY	-	expression tag	UNP Q8DEM0
C	-1	SER	-	expression tag	UNP Q8DEM0
C	0	GLY	-	expression tag	UNP Q8DEM0
D	-24	MET	-	initiating methionine	UNP Q8DEM0
D	-23	HIS	-	expression tag	UNP Q8DEM0
D	-22	HIS	-	expression tag	UNP Q8DEM0
D	-21	HIS	-	expression tag	UNP Q8DEM0
D	-20	HIS	-	expression tag	UNP Q8DEM0
D	-19	HIS	-	expression tag	UNP Q8DEM0
D	-18	HIS	-	expression tag	UNP Q8DEM0
D	-17	SER	-	expression tag	UNP Q8DEM0
D	-16	SER	-	expression tag	UNP Q8DEM0
D	-15	GLY	-	expression tag	UNP Q8DEM0
D	-14	VAL	-	expression tag	UNP Q8DEM0
D	-13	ASP	-	expression tag	UNP Q8DEM0
D	-12	LEU	-	expression tag	UNP Q8DEM0
D	-11	GLY	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	THR	-	expression tag	UNP Q8DEM0
D	-9	GLU	-	expression tag	UNP Q8DEM0
D	-8	ASN	-	expression tag	UNP Q8DEM0
D	-7	LEU	-	expression tag	UNP Q8DEM0
D	-6	TYR	-	expression tag	UNP Q8DEM0
D	-5	PHE	-	expression tag	UNP Q8DEM0
D	-4	GLN	-	expression tag	UNP Q8DEM0
D	-3	SER	-	expression tag	UNP Q8DEM0
D	-2	GLY	-	expression tag	UNP Q8DEM0
D	-1	SER	-	expression tag	UNP Q8DEM0
D	0	GLY	-	expression tag	UNP Q8DEM0
E	-24	MET	-	initiating methionine	UNP Q8DEM0
E	-23	HIS	-	expression tag	UNP Q8DEM0
E	-22	HIS	-	expression tag	UNP Q8DEM0
E	-21	HIS	-	expression tag	UNP Q8DEM0
E	-20	HIS	-	expression tag	UNP Q8DEM0
E	-19	HIS	-	expression tag	UNP Q8DEM0
E	-18	HIS	-	expression tag	UNP Q8DEM0
E	-17	SER	-	expression tag	UNP Q8DEM0
E	-16	SER	-	expression tag	UNP Q8DEM0
E	-15	GLY	-	expression tag	UNP Q8DEM0
E	-14	VAL	-	expression tag	UNP Q8DEM0
E	-13	ASP	-	expression tag	UNP Q8DEM0
E	-12	LEU	-	expression tag	UNP Q8DEM0
E	-11	GLY	-	expression tag	UNP Q8DEM0
E	-10	THR	-	expression tag	UNP Q8DEM0
E	-9	GLU	-	expression tag	UNP Q8DEM0
E	-8	ASN	-	expression tag	UNP Q8DEM0
E	-7	LEU	-	expression tag	UNP Q8DEM0
E	-6	TYR	-	expression tag	UNP Q8DEM0
E	-5	PHE	-	expression tag	UNP Q8DEM0
E	-4	GLN	-	expression tag	UNP Q8DEM0
E	-3	SER	-	expression tag	UNP Q8DEM0
E	-2	GLY	-	expression tag	UNP Q8DEM0
E	-1	SER	-	expression tag	UNP Q8DEM0
E	0	GLY	-	expression tag	UNP Q8DEM0
F	-24	MET	-	initiating methionine	UNP Q8DEM0
F	-23	HIS	-	expression tag	UNP Q8DEM0
F	-22	HIS	-	expression tag	UNP Q8DEM0
F	-21	HIS	-	expression tag	UNP Q8DEM0
F	-20	HIS	-	expression tag	UNP Q8DEM0
F	-19	HIS	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	HIS	-	expression tag	UNP Q8DEM0
F	-17	SER	-	expression tag	UNP Q8DEM0
F	-16	SER	-	expression tag	UNP Q8DEM0
F	-15	GLY	-	expression tag	UNP Q8DEM0
F	-14	VAL	-	expression tag	UNP Q8DEM0
F	-13	ASP	-	expression tag	UNP Q8DEM0
F	-12	LEU	-	expression tag	UNP Q8DEM0
F	-11	GLY	-	expression tag	UNP Q8DEM0
F	-10	THR	-	expression tag	UNP Q8DEM0
F	-9	GLU	-	expression tag	UNP Q8DEM0
F	-8	ASN	-	expression tag	UNP Q8DEM0
F	-7	LEU	-	expression tag	UNP Q8DEM0
F	-6	TYR	-	expression tag	UNP Q8DEM0
F	-5	PHE	-	expression tag	UNP Q8DEM0
F	-4	GLN	-	expression tag	UNP Q8DEM0
F	-3	SER	-	expression tag	UNP Q8DEM0
F	-2	GLY	-	expression tag	UNP Q8DEM0
F	-1	SER	-	expression tag	UNP Q8DEM0
F	0	GLY	-	expression tag	UNP Q8DEM0
G	-24	MET	-	initiating methionine	UNP Q8DEM0
G	-23	HIS	-	expression tag	UNP Q8DEM0
G	-22	HIS	-	expression tag	UNP Q8DEM0
G	-21	HIS	-	expression tag	UNP Q8DEM0
G	-20	HIS	-	expression tag	UNP Q8DEM0
G	-19	HIS	-	expression tag	UNP Q8DEM0
G	-18	HIS	-	expression tag	UNP Q8DEM0
G	-17	SER	-	expression tag	UNP Q8DEM0
G	-16	SER	-	expression tag	UNP Q8DEM0
G	-15	GLY	-	expression tag	UNP Q8DEM0
G	-14	VAL	-	expression tag	UNP Q8DEM0
G	-13	ASP	-	expression tag	UNP Q8DEM0
G	-12	LEU	-	expression tag	UNP Q8DEM0
G	-11	GLY	-	expression tag	UNP Q8DEM0
G	-10	THR	-	expression tag	UNP Q8DEM0
G	-9	GLU	-	expression tag	UNP Q8DEM0
G	-8	ASN	-	expression tag	UNP Q8DEM0
G	-7	LEU	-	expression tag	UNP Q8DEM0
G	-6	TYR	-	expression tag	UNP Q8DEM0
G	-5	PHE	-	expression tag	UNP Q8DEM0
G	-4	GLN	-	expression tag	UNP Q8DEM0
G	-3	SER	-	expression tag	UNP Q8DEM0
G	-2	GLY	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	expression tag	UNP Q8DEM0
G	0	GLY	-	expression tag	UNP Q8DEM0
H	-24	MET	-	initiating methionine	UNP Q8DEM0
H	-23	HIS	-	expression tag	UNP Q8DEM0
H	-22	HIS	-	expression tag	UNP Q8DEM0
H	-21	HIS	-	expression tag	UNP Q8DEM0
H	-20	HIS	-	expression tag	UNP Q8DEM0
H	-19	HIS	-	expression tag	UNP Q8DEM0
H	-18	HIS	-	expression tag	UNP Q8DEM0
H	-17	SER	-	expression tag	UNP Q8DEM0
H	-16	SER	-	expression tag	UNP Q8DEM0
H	-15	GLY	-	expression tag	UNP Q8DEM0
H	-14	VAL	-	expression tag	UNP Q8DEM0
H	-13	ASP	-	expression tag	UNP Q8DEM0
H	-12	LEU	-	expression tag	UNP Q8DEM0
H	-11	GLY	-	expression tag	UNP Q8DEM0
H	-10	THR	-	expression tag	UNP Q8DEM0
H	-9	GLU	-	expression tag	UNP Q8DEM0
H	-8	ASN	-	expression tag	UNP Q8DEM0
H	-7	LEU	-	expression tag	UNP Q8DEM0
H	-6	TYR	-	expression tag	UNP Q8DEM0
H	-5	PHE	-	expression tag	UNP Q8DEM0
H	-4	GLN	-	expression tag	UNP Q8DEM0
H	-3	SER	-	expression tag	UNP Q8DEM0
H	-2	GLY	-	expression tag	UNP Q8DEM0
H	-1	SER	-	expression tag	UNP Q8DEM0
H	0	GLY	-	expression tag	UNP Q8DEM0
I	-24	MET	-	initiating methionine	UNP Q8DEM0
I	-23	HIS	-	expression tag	UNP Q8DEM0
I	-22	HIS	-	expression tag	UNP Q8DEM0
I	-21	HIS	-	expression tag	UNP Q8DEM0
I	-20	HIS	-	expression tag	UNP Q8DEM0
I	-19	HIS	-	expression tag	UNP Q8DEM0
I	-18	HIS	-	expression tag	UNP Q8DEM0
I	-17	SER	-	expression tag	UNP Q8DEM0
I	-16	SER	-	expression tag	UNP Q8DEM0
I	-15	GLY	-	expression tag	UNP Q8DEM0
I	-14	VAL	-	expression tag	UNP Q8DEM0
I	-13	ASP	-	expression tag	UNP Q8DEM0
I	-12	LEU	-	expression tag	UNP Q8DEM0
I	-11	GLY	-	expression tag	UNP Q8DEM0
I	-10	THR	-	expression tag	UNP Q8DEM0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-9	GLU	-	expression tag	UNP Q8DEM0
I	-8	ASN	-	expression tag	UNP Q8DEM0
I	-7	LEU	-	expression tag	UNP Q8DEM0
I	-6	TYR	-	expression tag	UNP Q8DEM0
I	-5	PHE	-	expression tag	UNP Q8DEM0
I	-4	GLN	-	expression tag	UNP Q8DEM0
I	-3	SER	-	expression tag	UNP Q8DEM0
I	-2	GLY	-	expression tag	UNP Q8DEM0
I	-1	SER	-	expression tag	UNP Q8DEM0
I	0	GLY	-	expression tag	UNP Q8DEM0
J	-24	MET	-	initiating methionine	UNP Q8DEM0
J	-23	HIS	-	expression tag	UNP Q8DEM0
J	-22	HIS	-	expression tag	UNP Q8DEM0
J	-21	HIS	-	expression tag	UNP Q8DEM0
J	-20	HIS	-	expression tag	UNP Q8DEM0
J	-19	HIS	-	expression tag	UNP Q8DEM0
J	-18	HIS	-	expression tag	UNP Q8DEM0
J	-17	SER	-	expression tag	UNP Q8DEM0
J	-16	SER	-	expression tag	UNP Q8DEM0
J	-15	GLY	-	expression tag	UNP Q8DEM0
J	-14	VAL	-	expression tag	UNP Q8DEM0
J	-13	ASP	-	expression tag	UNP Q8DEM0
J	-12	LEU	-	expression tag	UNP Q8DEM0
J	-11	GLY	-	expression tag	UNP Q8DEM0
J	-10	THR	-	expression tag	UNP Q8DEM0
J	-9	GLU	-	expression tag	UNP Q8DEM0
J	-8	ASN	-	expression tag	UNP Q8DEM0
J	-7	LEU	-	expression tag	UNP Q8DEM0
J	-6	TYR	-	expression tag	UNP Q8DEM0
J	-5	PHE	-	expression tag	UNP Q8DEM0
J	-4	GLN	-	expression tag	UNP Q8DEM0
J	-3	SER	-	expression tag	UNP Q8DEM0
J	-2	GLY	-	expression tag	UNP Q8DEM0
J	-1	SER	-	expression tag	UNP Q8DEM0
J	0	GLY	-	expression tag	UNP Q8DEM0
K	-24	MET	-	initiating methionine	UNP Q8DEM0
K	-23	HIS	-	expression tag	UNP Q8DEM0
K	-22	HIS	-	expression tag	UNP Q8DEM0
K	-21	HIS	-	expression tag	UNP Q8DEM0
K	-20	HIS	-	expression tag	UNP Q8DEM0
K	-19	HIS	-	expression tag	UNP Q8DEM0
K	-18	HIS	-	expression tag	UNP Q8DEM0

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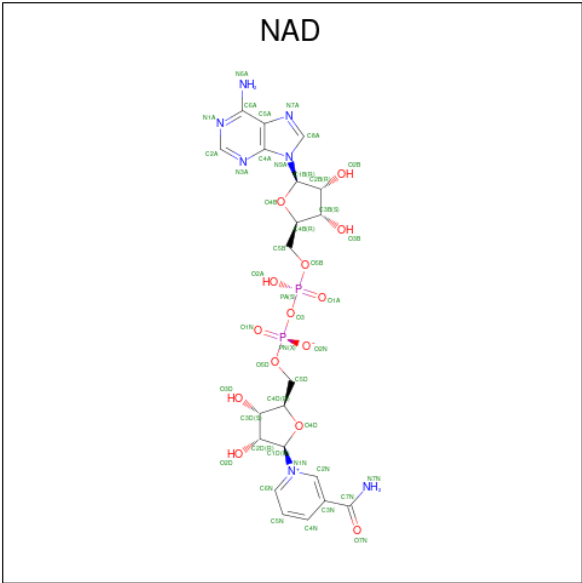
Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	SER	-	expression tag	UNP Q8DEM0
K	-16	SER	-	expression tag	UNP Q8DEM0
K	-15	GLY	-	expression tag	UNP Q8DEM0
K	-14	VAL	-	expression tag	UNP Q8DEM0
K	-13	ASP	-	expression tag	UNP Q8DEM0
K	-12	LEU	-	expression tag	UNP Q8DEM0
K	-11	GLY	-	expression tag	UNP Q8DEM0
K	-10	THR	-	expression tag	UNP Q8DEM0
K	-9	GLU	-	expression tag	UNP Q8DEM0
K	-8	ASN	-	expression tag	UNP Q8DEM0
K	-7	LEU	-	expression tag	UNP Q8DEM0
K	-6	TYR	-	expression tag	UNP Q8DEM0
K	-5	PHE	-	expression tag	UNP Q8DEM0
K	-4	GLN	-	expression tag	UNP Q8DEM0
K	-3	SER	-	expression tag	UNP Q8DEM0
K	-2	GLY	-	expression tag	UNP Q8DEM0
K	-1	SER	-	expression tag	UNP Q8DEM0
K	0	GLY	-	expression tag	UNP Q8DEM0
L	-24	MET	-	initiating methionine	UNP Q8DEM0
L	-23	HIS	-	expression tag	UNP Q8DEM0
L	-22	HIS	-	expression tag	UNP Q8DEM0
L	-21	HIS	-	expression tag	UNP Q8DEM0
L	-20	HIS	-	expression tag	UNP Q8DEM0
L	-19	HIS	-	expression tag	UNP Q8DEM0
L	-18	HIS	-	expression tag	UNP Q8DEM0
L	-17	SER	-	expression tag	UNP Q8DEM0
L	-16	SER	-	expression tag	UNP Q8DEM0
L	-15	GLY	-	expression tag	UNP Q8DEM0
L	-14	VAL	-	expression tag	UNP Q8DEM0
L	-13	ASP	-	expression tag	UNP Q8DEM0
L	-12	LEU	-	expression tag	UNP Q8DEM0
L	-11	GLY	-	expression tag	UNP Q8DEM0
L	-10	THR	-	expression tag	UNP Q8DEM0
L	-9	GLU	-	expression tag	UNP Q8DEM0
L	-8	ASN	-	expression tag	UNP Q8DEM0
L	-7	LEU	-	expression tag	UNP Q8DEM0
L	-6	TYR	-	expression tag	UNP Q8DEM0
L	-5	PHE	-	expression tag	UNP Q8DEM0
L	-4	GLN	-	expression tag	UNP Q8DEM0
L	-3	SER	-	expression tag	UNP Q8DEM0
L	-2	GLY	-	expression tag	UNP Q8DEM0
L	-1	SER	-	expression tag	UNP Q8DEM0

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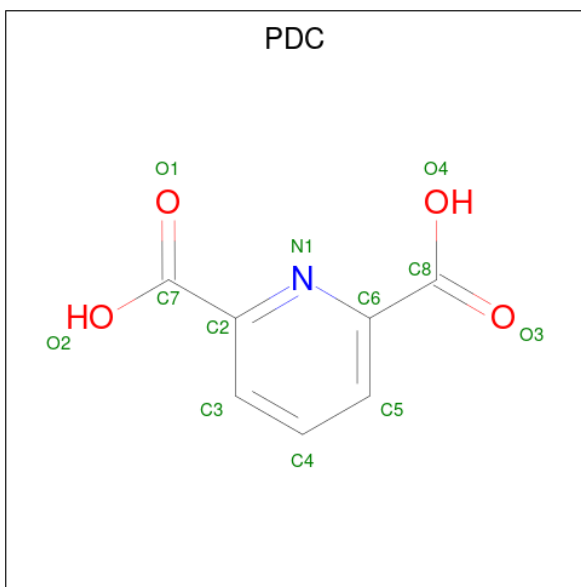
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	GLY	-	expression tag	UNP Q8DEM0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



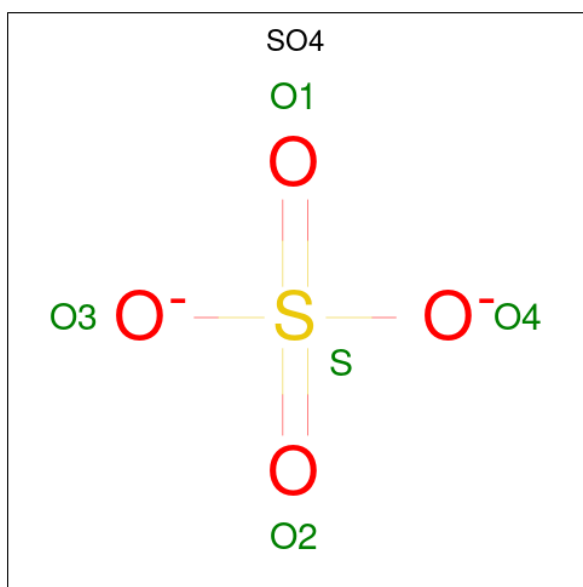
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I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

- Molecule 3 is PYRIDINE-2,6-DICARBOXYLIC ACID (CCD ID: PDC) (formula: C₇H₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		
3	C	1	Total	C	N	O	0	0
			12	7	1	4		
3	E	1	Total	C	N	O	0	0
			12	7	1	4		
3	F	1	Total	C	N	O	0	0
			12	7	1	4		
3	G	1	Total	C	N	O	0	0
			12	7	1	4		
3	I	1	Total	C	N	O	0	0
			12	7	1	4		
3	J	1	Total	C	N	O	0	0
			12	7	1	4		
3	K	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	7	Total O 7 7	0	0
5	C	13	Total O 13 13	0	0
5	D	22	Total O 22 22	0	0
5	E	21	Total O 21 21	0	0
5	F	14	Total O 14 14	0	0
5	G	18	Total O 18 18	0	0
5	H	10	Total O 10 10	0	0
5	I	19	Total O 19 19	0	0
5	J	12	Total O 12 12	0	0

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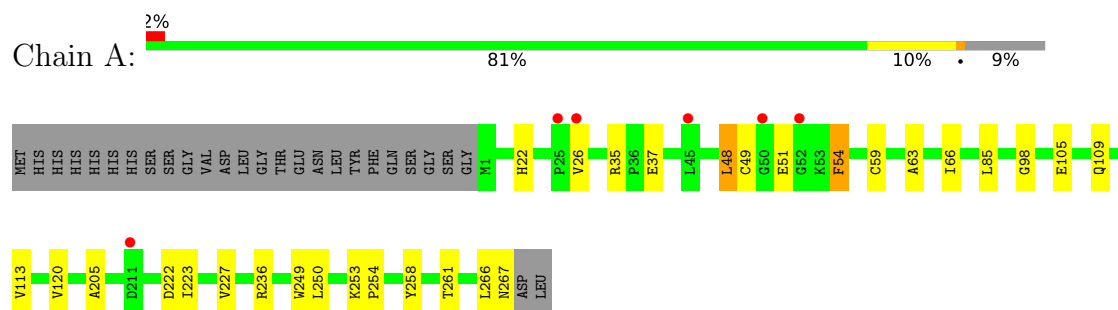
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	9	Total	O	0	0
			9	9		
5	L	9	Total	O	0	0
			9	9		

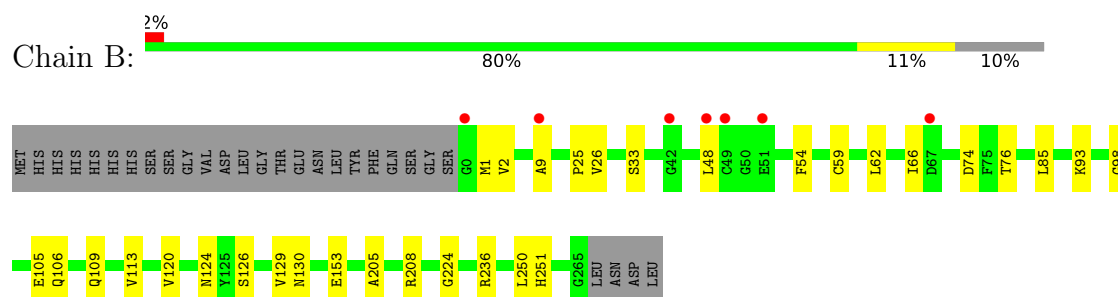
3 Residue-property plots [i](#)

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

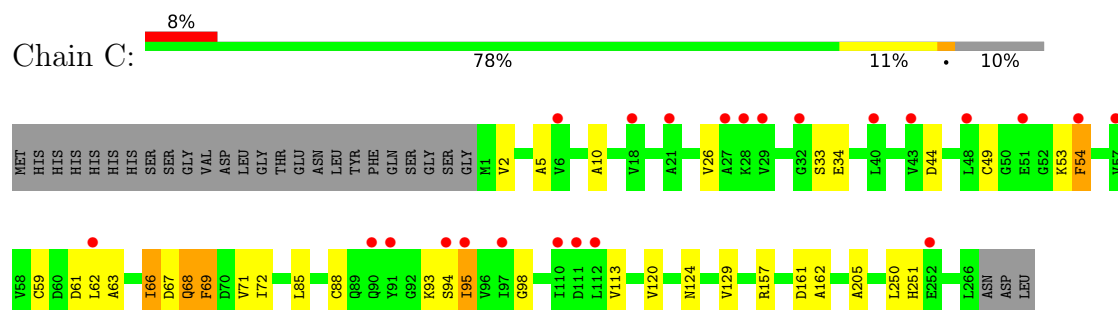
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



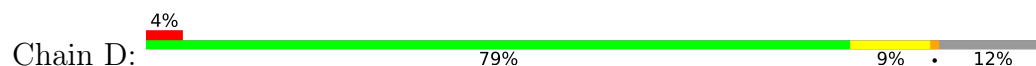
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

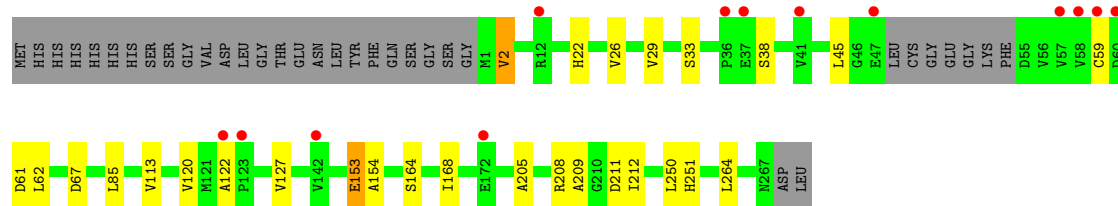


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

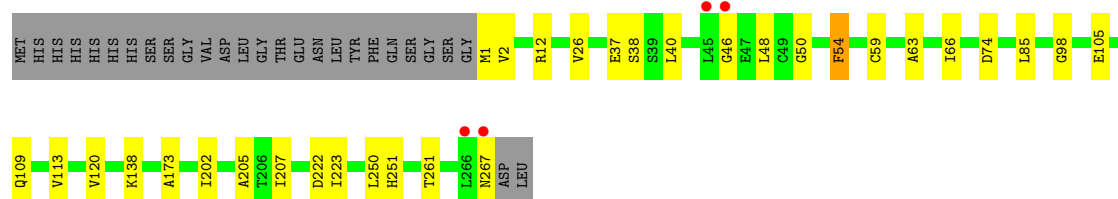
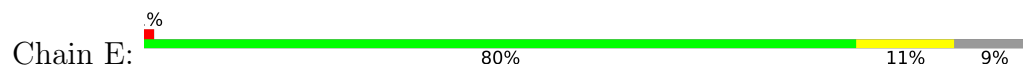


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase

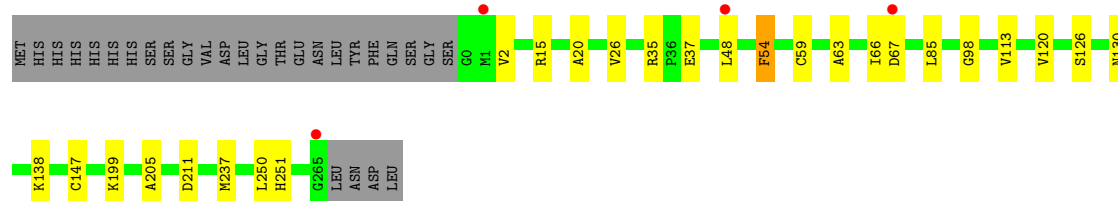
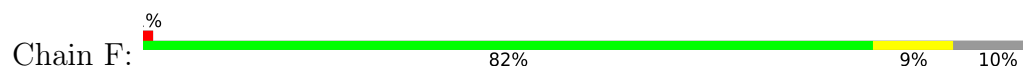




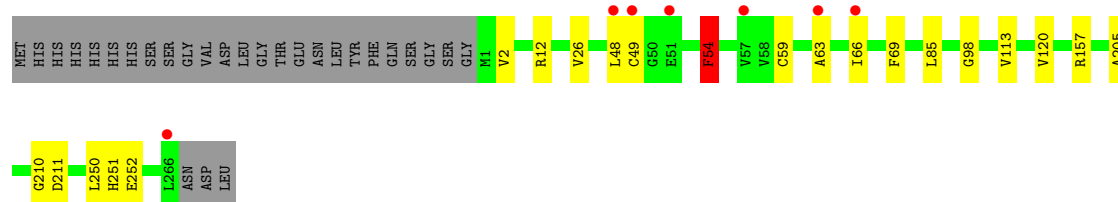
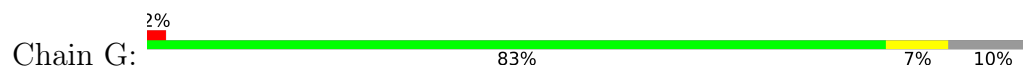
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



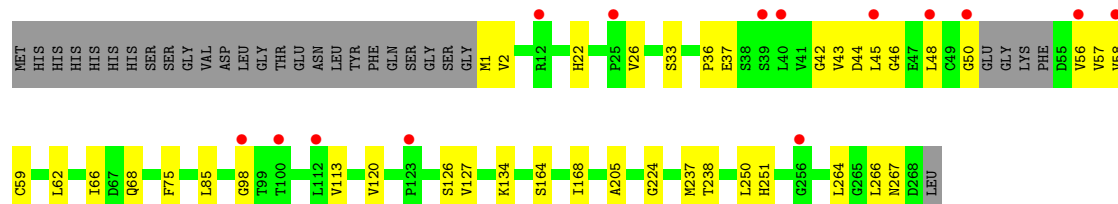
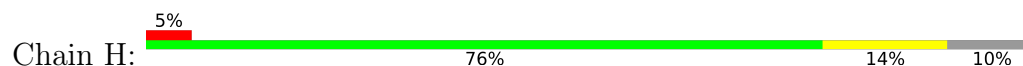
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



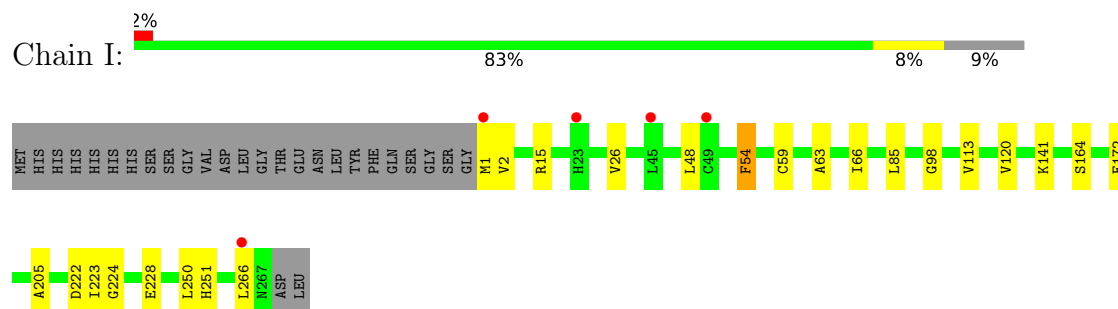
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



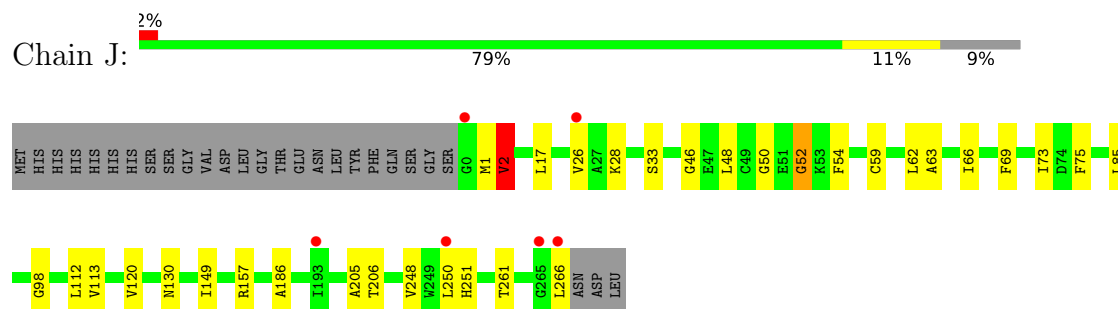
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



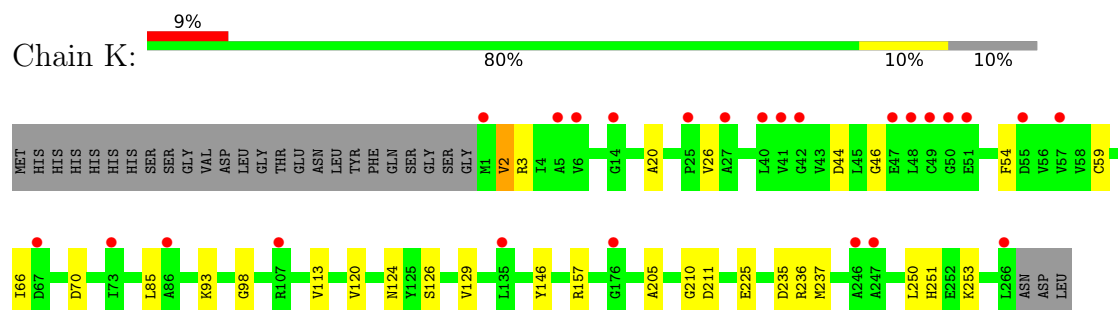
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



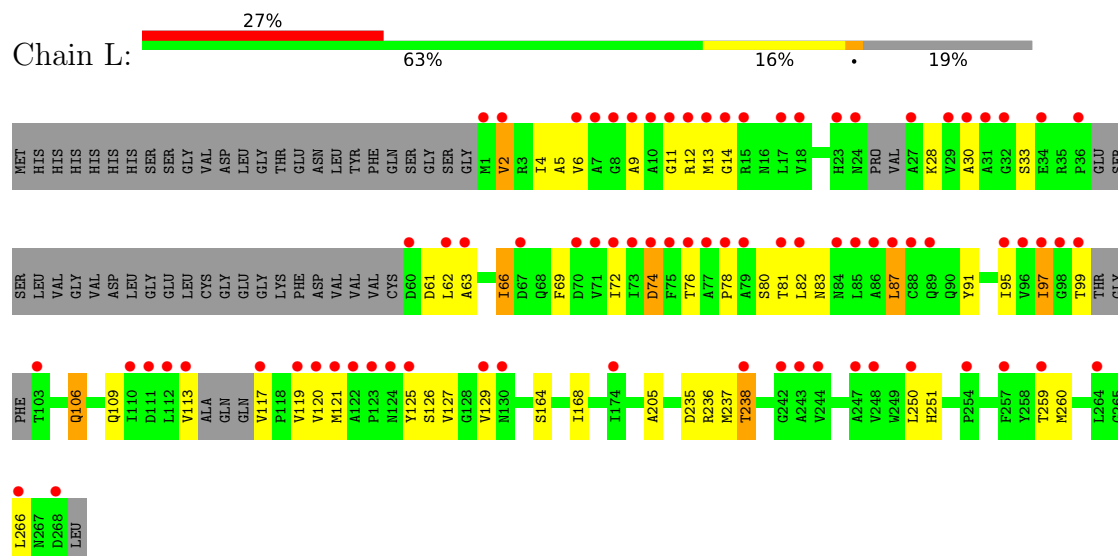
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate reductase



- 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	111.91Å 115.84Å 148.13Å 90.00° 96.10° 90.00°	Depositor
Resolution (Å)	40.00 – 2.61 40.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	92.7 (40.00-2.61) 92.9 (40.00-2.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.228 , 0.257 0.230 , 0.260	Depositor DCC
R_{free} test set	5512 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23790	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 76.21 % 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 1.0879e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PDC, SO4

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	1.18	1/1992 (0.1%)	1.08	2/2703 (0.1%)
1	B	1.12	0/1970	1.06	1/2674 (0.0%)
1	C	1.14	2/1957 (0.1%)	1.13	7/2658 (0.3%)
1	D	1.21	1/1904 (0.1%)	1.10	4/2589 (0.2%)
1	E	1.26	3/2000 (0.1%)	1.12	3/2711 (0.1%)
1	F	1.21	1/1986 (0.1%)	1.09	1/2692 (0.0%)
1	G	1.20	1/1977 (0.1%)	1.12	6/2683 (0.2%)
1	H	1.25	4/1928 (0.2%)	1.14	5/2620 (0.2%)
1	I	1.26	4/1992 (0.2%)	1.11	2/2703 (0.1%)
1	J	1.15	3/1988 (0.2%)	1.11	6/2695 (0.2%)
1	K	1.16	1/1966 (0.1%)	1.10	3/2670 (0.1%)
1	L	1.12	1/1698 (0.1%)	1.21	16/2306 (0.7%)
All	All	1.19	22/23358 (0.1%)	1.11	56/31704 (0.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	ASP	CA-C	6.54	1.60	1.52
1	H	267	ASN	CA-C	6.32	1.60	1.52
1	A	227	VAL	C-O	-5.90	1.17	1.24
1	C	162	ALA	C-O	-5.84	1.17	1.24
1	J	206	THR	N-CA	-5.70	1.39	1.46
1	I	141	LYS	C-O	-5.53	1.17	1.24
1	E	173	ALA	N-CA	-5.49	1.39	1.46
1	H	43	VAL	C-O	-5.43	1.18	1.24
1	H	42	GLY	C-O	-5.37	1.16	1.23
1	E	207	ILE	CA-CB	-5.32	1.48	1.54
1	J	186	ALA	C-O	-5.32	1.17	1.23
1	J	149	ILE	C-O	-5.30	1.18	1.24
1	L	87	LEU	C-O	-5.27	1.18	1.24
1	E	202	ILE	N-CA	-5.27	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	252	GLU	CA-CB	5.19	1.61	1.53
1	I	172	GLU	N-CA	5.16	1.52	1.46
1	K	157	ARG	NE-CZ	5.15	1.38	1.33
1	I	164	SER	N-CA	-5.14	1.39	1.45
1	D	122	ALA	C-O	5.14	1.30	1.24
1	H	126	SER	N-CA	-5.09	1.39	1.46
1	I	228	GLU	C-O	-5.05	1.18	1.24
1	F	147	CYS	C-O	-5.04	1.17	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	52	GLY	N-CA-C	-9.01	102.98	112.08
1	D	38	SER	N-CA-C	7.79	121.53	110.23
1	G	12	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	L	66	ILE	N-CA-C	7.29	121.23	111.17
1	I	266	LEU	N-CA-C	7.22	122.12	113.16
1	G	157	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	K	2	VAL	N-CA-C	7.20	118.29	109.30
1	L	33	SER	N-CA-C	7.03	120.96	109.85
1	L	119	VAL	N-CA-C	7.00	118.20	107.78
1	E	38	SER	N-CA-C	6.99	120.37	110.23
1	L	238	THR	N-CA-C	-6.99	102.88	111.33
1	C	68	GLN	N-CA-C	6.92	118.82	111.28
1	L	74	ASP	N-CA-C	6.84	120.09	107.99
1	C	95	ILE	N-CA-C	6.68	118.34	108.45
1	C	66	ILE	N-CA-C	6.54	117.29	110.62
1	H	22	HIS	CA-C-N	6.25	128.66	120.28
1	H	22	HIS	C-N-CA	6.25	128.66	120.28
1	H	68	GLN	N-CA-C	6.23	120.48	113.01
1	L	266	LEU	N-CA-C	6.20	119.01	111.82
1	L	11	GLY	N-CA-C	-6.18	102.47	110.69
1	E	12	ARG	NE-CZ-NH2	6.16	124.75	119.20
1	J	54	PHE	N-CA-C	-6.13	101.89	110.35
1	H	266	LEU	N-CA-C	5.90	119.66	112.23
1	K	157	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	C	54	PHE	N-CA-C	-5.83	100.49	109.52
1	L	117	VAL	CA-C-N	-5.81	113.80	119.90
1	L	117	VAL	C-N-CA	-5.81	113.80	119.90
1	D	2	VAL	N-CA-C	5.81	117.99	109.63
1	L	28	LYS	N-CA-C	-5.75	100.53	109.72
1	B	54	PHE	N-CA-C	-5.70	102.49	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	66	ILE	N-CA-C	5.70	118.17	111.05
1	L	2	VAL	CB-CA-C	-5.61	103.86	111.15
1	K	210	GLY	N-CA-C	5.58	121.49	111.34
1	L	82	LEU	N-CA-C	-5.50	105.28	111.28
1	D	22	HIS	CA-C-N	5.49	127.64	120.28
1	D	22	HIS	C-N-CA	5.49	127.64	120.28
1	J	2	VAL	N-CA-C	5.48	117.52	109.63
1	F	54	PHE	N-CA-C	-5.48	102.79	110.35
1	A	51	GLU	N-CA-C	5.47	117.83	109.62
1	G	12	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	G	210	GLY	N-CA-C	5.46	121.28	111.34
1	I	54	PHE	N-CA-C	-5.38	102.92	110.35
1	C	69	PHE	N-CA-C	5.36	117.83	109.52
1	J	48	LEU	N-CA-C	-5.29	105.52	111.28
1	C	157	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	C	49	CYS	N-CA-C	-5.25	106.14	112.54
1	J	157	ARG	N-CA-C	5.24	117.74	111.71
1	L	69	PHE	N-CA-C	5.23	117.14	109.24
1	E	74	ASP	N-CA-C	5.23	117.18	108.02
1	G	69	PHE	N-CA-C	5.22	117.12	109.24
1	L	119	VAL	CA-C-N	-5.09	115.80	122.37
1	L	119	VAL	C-N-CA	-5.09	115.80	122.37
1	J	69	PHE	N-CA-C	5.09	116.93	109.24
1	A	48	LEU	N-CA-C	-5.09	105.73	111.28
1	L	97	ILE	N-CA-C	5.02	115.33	107.99
1	G	54	PHE	N-CA-C	-5.02	103.42	110.35

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	1962	0	1925	25	0
1	B	1940	0	1896	26	0
1	C	1927	0	1881	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1876	0	1813	17	0
1	E	1970	0	1947	27	0
1	F	1956	0	1926	21	1
1	G	1947	0	1913	16	0
1	H	1900	0	1843	24	0
1	I	1962	0	1925	15	0
1	J	1958	0	1926	24	0
1	K	1936	0	1898	21	0
1	L	1676	0	1590	35	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	E	44	0	26	2	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	I	44	0	26	2	0
2	J	44	0	26	1	0
2	K	44	0	26	1	0
3	A	12	0	3	0	0
3	B	12	0	3	0	0
3	C	12	0	3	0	0
3	E	12	0	3	1	0
3	F	12	0	3	0	0
3	G	12	0	3	0	0
3	I	12	0	3	1	0
3	J	12	0	3	0	0
3	K	12	0	3	0	0
4	A	10	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	20	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	25	0	0	0	0
4	I	10	0	0	0	0
4	J	5	0	0	0	0
4	K	10	0	0	0	0
4	L	5	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
5	C	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	22	0	0	0	0
5	E	21	0	0	0	0
5	F	14	0	0	0	0
5	G	18	0	0	0	0
5	H	10	0	0	0	0
5	I	19	0	0	0	0
5	J	12	0	0	0	0
5	K	9	0	0	0	0
5	L	9	0	0	0	0
All	All	23790	0	22744	259	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (259) 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:J:1:MET:HE2	1:J:28:LYS:HG3	1.42	1.02
1:E:222:ASP:OD1	1:E:223:ILE:N	1.98	0.96
1:L:97:ILE:HG23	1:L:99:THR:HG22	1.51	0.92
1:B:2:VAL:HG22	1:B:251:HIS:CG	2.07	0.88
1:G:48:LEU:HD12	1:G:49:CYS:N	1.88	0.88
1:B:2:VAL:HG22	1:B:251:HIS:ND1	1.90	0.86
1:F:2:VAL:HG22	1:F:251:HIS:CG	2.11	0.86
1:F:15:ARG:HG2	1:F:48:LEU:HD21	1.58	0.85
1:L:106:GLN:N	1:L:106:GLN:OE1	2.09	0.84
1:J:98:GLY:O	2:J:1001:NAD:H2N	1.78	0.83
1:H:44:ASP:HA	1:H:56:VAL:O	1.80	0.80
1:F:2:VAL:HG22	1:F:251:HIS:ND1	1.99	0.77
1:H:46:GLY:O	1:H:50:GLY:N	2.19	0.75
1:E:98:GLY:O	2:E:1001:NAD:H2N	1.90	0.72
1:L:81:THR:HG21	1:L:99:THR:HG21	1.73	0.71
1:L:97:ILE:CG2	1:L:99:THR:HG22	2.20	0.71
1:E:46:GLY:O	1:E:50:GLY:N	2.22	0.71
1:A:48:LEU:HD12	1:A:49:CYS:N	2.05	0.71
1:A:98:GLY:O	2:A:1001:NAD:H2N	1.90	0.70
1:F:37:GLU:CD	1:F:37:GLU:H	1.98	0.70
1:F:37:GLU:N	1:F:37:GLU:OE2	2.25	0.69
1:J:130:ASN:HB3	1:J:266:LEU:CD1	2.23	0.69
1:E:223:ILE:HD12	1:G:211:ASP:HB3	1.77	0.67
1:L:126:SER:OG	1:L:129:VAL:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HG3	1:A:254:PRO:HD2	1.75	0.65
1:C:44:ASP:OD1	1:C:54:PHE:O	2.14	0.65
1:E:223:ILE:HG23	1:E:223:ILE:O	1.96	0.65
1:C:98:GLY:O	2:C:1001:NAD:H2N	1.97	0.65
1:F:98:GLY:O	2:F:1001:NAD:H2N	1.98	0.64
1:L:235:ASP:OD1	1:L:236:ARG:N	2.30	0.64
1:C:53:LYS:O	1:C:54:PHE:HD1	1.81	0.62
1:D:153:GLU:OE2	1:D:208:ARG:NH1	2.31	0.62
1:H:1:MET:HB2	1:H:26:VAL:O	1.99	0.62
1:I:98:GLY:O	2:I:302:NAD:H2N	1.99	0.62
1:L:109:GLN:O	1:L:113:VAL:HG23	1.99	0.62
1:A:223:ILE:O	1:A:223:ILE:HG23	1.99	0.61
1:L:80:SER:O	1:L:83:ASN:HB3	2.00	0.61
1:G:63:ALA:HA	1:G:66:ILE:HG23	1.82	0.61
1:H:2:VAL:HG22	1:H:251:HIS:CG	2.36	0.61
1:L:2:VAL:HG22	1:L:251:HIS:CG	2.36	0.61
1:E:261:THR:HG21	1:E:267:ASN:HB3	1.83	0.61
1:H:120:VAL:HG23	1:H:250:LEU:HD13	1.83	0.60
1:L:120:VAL:HG23	1:L:250:LEU:HD13	1.83	0.60
1:J:261:THR:HG23	1:J:266:LEU:HB2	1.84	0.60
1:J:46:GLY:O	1:J:50:GLY:N	2.34	0.60
1:C:88:CYS:HB3	1:C:93:LYS:O	2.01	0.59
1:D:120:VAL:HG23	1:D:250:LEU:HD13	1.84	0.59
1:G:48:LEU:HD12	1:G:48:LEU:C	2.27	0.59
1:B:153:GLU:OE1	1:B:208:ARG:NH1	2.23	0.59
1:J:130:ASN:HB3	1:J:266:LEU:HD11	1.83	0.59
1:L:121:MET:O	1:L:259:THR:HG22	2.02	0.59
1:C:2:VAL:HG22	1:C:251:HIS:ND1	2.17	0.59
1:D:2:VAL:HG22	1:D:251:HIS:CG	2.38	0.59
1:A:85:LEU:HG	1:A:113:VAL:HG11	1.86	0.58
1:F:15:ARG:HG2	1:F:48:LEU:CD2	2.32	0.58
1:B:85:LEU:HG	1:B:113:VAL:HG11	1.86	0.57
1:E:40:LEU:HD23	1:E:48:LEU:HD12	1.86	0.57
1:E:120:VAL:HG23	1:E:250:LEU:HD13	1.84	0.57
1:I:120:VAL:HG23	1:I:250:LEU:HD13	1.86	0.57
1:I:85:LEU:HG	1:I:113:VAL:HG11	1.86	0.57
1:C:85:LEU:HG	1:C:113:VAL:HG11	1.87	0.57
1:E:40:LEU:HD12	1:E:40:LEU:N	2.19	0.57
1:L:9:ALA:HA	1:L:14:GLY:HA3	1.85	0.57
1:K:120:VAL:HG23	1:K:250:LEU:HD13	1.87	0.57
1:F:85:LEU:HG	1:F:113:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:LEU:HG	1:E:113:VAL:HG11	1.86	0.56
1:G:120:VAL:HG23	1:G:250:LEU:HD13	1.87	0.56
1:B:126:SER:O	1:B:130:ASN:ND2	2.38	0.56
1:H:85:LEU:HG	1:H:113:VAL:HG11	1.87	0.56
1:A:120:VAL:HG23	1:A:250:LEU:HD13	1.87	0.56
1:L:2:VAL:HG22	1:L:251:HIS:ND1	2.21	0.56
1:A:35:ARG:NH1	1:A:37:GLU:HG2	2.21	0.56
1:H:164:SER:O	1:H:168:ILE:HG12	2.06	0.56
1:L:66:ILE:HD13	1:L:91:TYR:CD2	2.40	0.56
1:C:71:VAL:HG22	1:C:94:SER:OG	2.06	0.56
1:F:120:VAL:HG23	1:F:250:LEU:HD13	1.87	0.56
1:I:223:ILE:HD12	1:K:211:ASP:HB3	1.87	0.56
1:B:153:GLU:CD	1:B:208:ARG:HH22	2.14	0.56
1:L:78:PRO:HA	1:L:81:THR:HG22	1.88	0.55
1:G:85:LEU:HG	1:G:113:VAL:HG11	1.88	0.55
1:H:44:ASP:OD1	1:H:45:LEU:N	2.40	0.55
1:K:124:ASN:CG	1:K:129:VAL:HG21	2.31	0.55
1:D:85:LEU:HG	1:D:113:VAL:HG11	1.88	0.55
1:B:205:ALA:HB1	1:D:205:ALA:HB1	1.87	0.55
1:C:2:VAL:HG22	1:C:251:HIS:CG	2.40	0.55
1:C:10:ALA:HB3	1:C:34:GLU:OE2	2.07	0.55
1:B:124:ASN:CG	1:B:129:VAL:HG21	2.31	0.55
1:J:120:VAL:HG23	1:J:250:LEU:HD13	1.87	0.54
1:B:120:VAL:HG23	1:B:250:LEU:HD13	1.89	0.54
1:C:120:VAL:HG23	1:C:250:LEU:HD13	1.89	0.54
1:B:9:ALA:O	1:B:48:LEU:HD21	2.06	0.54
1:H:45:LEU:O	1:H:48:LEU:HB2	2.08	0.54
1:G:98:GLY:O	2:G:1001:NAD:H2N	2.08	0.54
1:I:63:ALA:HA	1:I:66:ILE:HG23	1.90	0.54
1:J:85:LEU:HG	1:J:113:VAL:HG11	1.89	0.54
1:I:223:ILE:HG23	1:I:223:ILE:O	2.08	0.54
1:A:22:HIS:CE1	1:J:112:LEU:HD11	2.43	0.53
1:B:1:MET:HE3	1:B:25:PRO:O	2.08	0.53
1:C:53:LYS:C	1:C:54:PHE:CD1	2.86	0.53
1:F:20:ALA:HB2	1:F:237:MET:HE1	1.89	0.53
1:B:2:VAL:HG21	1:B:251:HIS:HB2	1.91	0.53
1:K:85:LEU:HG	1:K:113:VAL:HG11	1.89	0.53
1:D:164:SER:O	1:D:168:ILE:HG12	2.09	0.53
1:E:223:ILE:O	1:E:223:ILE:CG2	2.57	0.53
1:C:66:ILE:HD12	1:C:67:ASP:OD1	2.08	0.53
1:F:2:VAL:HG22	1:F:251:HIS:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HG22	1:H:251:HIS:CB	2.39	0.53
1:C:124:ASN:CG	1:C:129:VAL:HG21	2.34	0.52
1:I:15:ARG:HG2	1:I:48:LEU:HD21	1.91	0.52
1:G:2:VAL:HG22	1:G:251:HIS:ND1	2.24	0.52
1:L:6:VAL:HG12	1:L:9:ALA:HB2	1.91	0.52
1:L:6:VAL:CG1	1:L:9:ALA:HB2	2.39	0.52
3:I:301:PDC:C5	2:I:302:NAD:C5N	2.89	0.51
1:C:5:ALA:HB2	1:C:69:PHE:CD2	2.46	0.51
1:B:2:VAL:CG2	1:B:251:HIS:CB	2.89	0.51
1:E:205:ALA:HB1	1:G:205:ALA:HB1	1.91	0.51
1:K:20:ALA:HB2	1:K:237:MET:HE1	1.93	0.51
1:D:153:GLU:OE2	1:D:208:ARG:NH2	2.44	0.51
1:D:209:ALA:O	1:D:212:ILE:HG13	2.10	0.51
1:E:63:ALA:HA	1:E:66:ILE:HG23	1.93	0.51
1:G:26:VAL:HG12	1:G:26:VAL:O	2.12	0.50
1:K:44:ASP:OD1	1:K:54:PHE:O	2.30	0.50
1:A:63:ALA:HA	1:A:66:ILE:HG23	1.93	0.50
1:D:67:ASP:OD1	1:D:67:ASP:O	2.29	0.50
1:L:125:TYR:CD1	1:L:260:MET:SD	3.04	0.50
1:F:26:VAL:HG12	1:F:26:VAL:O	2.12	0.50
1:K:250:LEU:O	1:K:253:LYS:HB2	2.12	0.50
1:G:2:VAL:HG22	1:G:251:HIS:CG	2.46	0.50
1:A:205:ALA:HB1	1:C:205:ALA:HB1	1.93	0.49
1:C:53:LYS:C	1:C:54:PHE:HD1	2.18	0.49
1:J:26:VAL:HG12	1:J:26:VAL:O	2.12	0.49
1:K:2:VAL:HG22	1:K:251:HIS:ND1	2.27	0.49
1:C:26:VAL:O	1:C:26:VAL:HG12	2.13	0.49
1:K:126:SER:OG	1:K:129:VAL:HG23	2.12	0.49
1:L:237:MET:O	1:L:238:THR:C	2.54	0.49
1:A:254:PRO:O	1:A:258:TYR:OH	2.20	0.49
1:B:26:VAL:HG12	1:B:26:VAL:O	2.12	0.49
1:H:56:VAL:HG12	1:H:57:VAL:N	2.27	0.49
1:B:2:VAL:HG22	1:B:251:HIS:CB	2.42	0.49
1:I:2:VAL:HG22	1:I:251:HIS:CG	2.48	0.49
1:B:66:ILE:CD1	1:B:93:LYS:HE3	2.43	0.49
1:D:26:VAL:HG12	1:D:26:VAL:O	2.13	0.49
1:E:1:MET:HB2	1:E:26:VAL:O	2.12	0.49
1:J:63:ALA:HA	1:J:66:ILE:HG23	1.94	0.49
1:A:249:TRP:CZ2	1:A:253:LYS:HE2	2.48	0.48
1:I:2:VAL:HG22	1:I:251:HIS:ND1	2.28	0.48
1:K:66:ILE:CD1	1:K:93:LYS:HE3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:ALA:HB1	1:L:62:LEU:HD11	1.94	0.48
1:B:98:GLY:O	2:B:1001:NAD:H2N	2.12	0.48
1:I:1:MET:HB2	1:I:26:VAL:O	2.12	0.48
1:K:26:VAL:HG12	1:K:26:VAL:O	2.14	0.48
1:H:237:MET:O	1:H:238:THR:C	2.55	0.48
1:E:26:VAL:O	1:E:26:VAL:HG12	2.13	0.48
1:F:126:SER:O	1:F:130:ASN:ND2	2.47	0.48
1:I:26:VAL:O	1:I:26:VAL:HG12	2.13	0.48
1:J:46:GLY:HA3	1:J:52:GLY:O	2.13	0.48
1:C:69:PHE:CD1	1:C:69:PHE:C	2.91	0.48
1:D:59:CYS:SG	1:D:61:ASP:O	2.56	0.48
1:F:63:ALA:HA	1:F:66:ILE:HG23	1.94	0.48
1:C:66:ILE:CD1	1:C:67:ASP:OD1	2.62	0.48
1:E:223:ILE:CD1	1:G:211:ASP:HB3	2.42	0.48
1:L:5:ALA:HA	1:L:30:ALA:HB3	1.96	0.48
1:A:26:VAL:HG12	1:A:26:VAL:O	2.13	0.47
1:B:2:VAL:CG2	1:B:251:HIS:HB2	2.44	0.47
1:G:63:ALA:HA	1:G:66:ILE:CG2	2.44	0.47
1:H:26:VAL:O	1:H:26:VAL:HG12	2.14	0.47
1:K:225:GLU:CD	1:L:238:THR:OG1	2.56	0.47
1:H:57:VAL:O	1:H:58:VAL:C	2.57	0.47
1:C:124:ASN:ND2	1:C:129:VAL:HG21	2.29	0.47
1:A:236:ARG:NH1	4:A:1003:SO4:O3	2.47	0.47
1:L:12:ARG:HG3	1:L:13:MET:N	2.29	0.47
1:L:12:ARG:CG	1:L:13:MET:H	2.27	0.47
1:L:72:ILE:HB	1:L:95:ILE:HG13	1.96	0.47
1:J:130:ASN:CB	1:J:266:LEU:HD11	2.44	0.47
1:K:146:TYR:OH	1:L:127:VAL:HG11	2.14	0.47
1:C:88:CYS:CB	1:C:93:LYS:O	2.63	0.47
1:A:223:ILE:O	1:A:223:ILE:CG2	2.61	0.47
1:F:211:ASP:OD2	1:H:224:GLY:N	2.47	0.46
1:C:63:ALA:HA	1:C:66:ILE:HG23	1.96	0.46
1:F:205:ALA:HB1	1:H:205:ALA:HB1	1.95	0.46
1:G:63:ALA:O	1:G:66:ILE:HG23	2.15	0.46
1:H:2:VAL:HG22	1:H:251:HIS:HB2	1.97	0.46
1:F:2:VAL:CG2	1:F:251:HIS:CB	2.93	0.46
1:K:46:GLY:N	1:K:54:PHE:HD2	2.13	0.46
1:K:98:GLY:O	2:K:1001:NAD:H2N	2.15	0.46
1:I:15:ARG:HG2	1:I:48:LEU:CD2	2.44	0.46
1:F:2:VAL:CG2	1:F:251:HIS:HB2	2.45	0.45
1:D:2:VAL:HG22	1:D:251:HIS:ND1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:O	1:B:109:GLN:HG2	2.16	0.45
1:B:124:ASN:ND2	1:B:129:VAL:HG21	2.31	0.45
1:J:1:MET:CE	1:J:28:LYS:HG3	2.31	0.45
1:A:48:LEU:HD12	1:A:48:LEU:C	2.42	0.45
1:K:250:LEU:HA	1:K:253:LYS:HG3	1.99	0.45
1:L:2:VAL:HG22	1:L:251:HIS:CB	2.47	0.45
1:I:205:ALA:HB1	1:K:205:ALA:HB1	1.98	0.44
1:J:205:ALA:HB1	1:L:205:ALA:HB1	1.99	0.44
1:L:4:ILE:O	1:L:30:ALA:N	2.49	0.44
1:B:2:VAL:CG2	1:B:251:HIS:CG	2.93	0.44
1:A:222:ASP:CG	1:A:223:ILE:H	2.25	0.44
1:C:59:CYS:SG	1:C:61:ASP:O	2.59	0.44
1:E:223:ILE:HD12	1:G:211:ASP:CB	2.47	0.44
1:J:2:VAL:HG21	1:J:248:VAL:HA	1.99	0.44
1:B:74:ASP:OD1	1:B:76:THR:OG1	2.29	0.44
1:C:88:CYS:SG	1:C:93:LYS:O	2.75	0.44
1:E:40:LEU:HD23	1:E:48:LEU:CD1	2.48	0.44
1:E:40:LEU:HD12	1:E:40:LEU:H	1.80	0.44
1:K:3:ARG:NH1	1:K:70:ASP:OD1	2.44	0.44
1:A:250:LEU:O	1:A:253:LYS:HB2	2.18	0.44
1:J:130:ASN:HB3	1:J:266:LEU:HD12	2.00	0.44
1:E:261:THR:CG2	1:E:267:ASN:HB3	2.48	0.44
1:E:2:VAL:HG22	1:E:251:HIS:ND1	2.32	0.43
1:F:2:VAL:CG2	1:F:251:HIS:ND1	2.77	0.43
1:L:164:SER:O	1:L:168:ILE:HG12	2.17	0.43
1:H:75:PHE:CZ	1:H:98:GLY:HA3	2.52	0.43
1:D:127:VAL:HG22	1:D:264:LEU:HD21	1.99	0.43
1:H:134:LYS:HA	1:H:134:LYS:HD3	1.90	0.43
1:I:222:ASP:CG	1:I:223:ILE:H	2.26	0.43
1:L:125:TYR:HD1	1:L:260:MET:SD	2.41	0.43
1:A:54:PHE:CD1	1:A:54:PHE:N	2.87	0.43
1:E:54:PHE:CD1	1:E:54:PHE:N	2.86	0.43
1:H:127:VAL:HG22	1:H:264:LEU:HD21	2.00	0.43
1:J:33:SER:HB3	1:J:62:LEU:HG	2.00	0.43
1:H:2:VAL:CG2	1:H:251:HIS:HB2	2.49	0.43
1:B:33:SER:HB3	1:B:62:LEU:HG	2.01	0.43
1:L:87:LEU:HD23	1:L:87:LEU:HA	1.70	0.43
1:K:235:ASP:OD1	1:K:236:ARG:N	2.52	0.43
1:A:261:THR:HG22	1:A:267:ASN:ND2	2.34	0.42
1:E:37:GLU:H	1:E:37:GLU:CD	2.26	0.42
1:A:35:ARG:CZ	1:A:35:ARG:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:O	1:B:109:GLN:HB2	2.19	0.42
1:L:63:ALA:O	1:L:66:ILE:HG13	2.19	0.42
1:B:224:GLY:N	1:D:211:ASP:OD2	2.53	0.42
1:G:54:PHE:CD1	1:G:54:PHE:N	2.88	0.41
2:E:1001:NAD:C5N	3:E:1002:PDC:C3	2.98	0.41
1:B:236:ARG:NH2	4:B:1003:SO4:O3	2.53	0.41
1:J:2:VAL:HG22	1:J:251:HIS:ND1	2.36	0.41
1:L:12:ARG:CG	1:L:13:MET:N	2.83	0.41
1:C:33:SER:HB3	1:C:62:LEU:HG	2.02	0.41
1:D:33:SER:HB3	1:D:62:LEU:HG	2.03	0.41
1:H:36:PRO:O	1:H:37:GLU:CB	2.68	0.41
1:K:124:ASN:ND2	1:K:129:VAL:HG21	2.35	0.41
1:A:249:TRP:O	1:A:253:LYS:HD3	2.20	0.41
1:E:138:LYS:HB2	1:F:138:LYS:HZ2	1.85	0.41
1:H:33:SER:HB3	1:H:62:LEU:HG	2.03	0.41
1:E:105:GLU:OE1	1:J:1:MET:HG2	2.20	0.41
1:I:224:GLY:N	1:K:211:ASP:OD2	2.44	0.41
1:D:153:GLU:HG2	1:D:154:ALA:N	2.35	0.41
1:E:105:GLU:CD	1:J:1:MET:HG2	2.46	0.41
1:D:29:VAL:CG1	1:D:45:LEU:HD13	2.51	0.41
1:J:75:PHE:CZ	1:J:98:GLY:HA3	2.55	0.41
1:A:35:ARG:HH11	1:A:37:GLU:HG2	1.86	0.40
1:H:75:PHE:CE1	1:H:98:GLY:HA3	2.56	0.40
1:C:72:ILE:O	1:C:95:ILE:HG13	2.21	0.40
1:E:109:GLN:CD	1:J:1:MET:HE1	2.46	0.40
1:A:105:GLU:O	1:A:109:GLN:HG2	2.21	0.40
1:F:35:ARG:NH2	1:F:37:GLU:OE1	2.52	0.40
1:J:17:LEU:HD22	1:J:73:ILE:HG21	2.03	0.40
1:L:237:MET:HE3	1:L:237:MET:HB3	1.86	0.40
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ASP:OD1	1:F:199:LYS:NZ[2_556]	2.12	0.08

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	265/294 (90%)	260 (98%)	5 (2%)	0	100	100
1	B	264/294 (90%)	260 (98%)	4 (2%)	0	100	100
1	C	264/294 (90%)	260 (98%)	4 (2%)	0	100	100
1	D	256/294 (87%)	253 (99%)	3 (1%)	0	100	100
1	E	265/294 (90%)	262 (99%)	3 (1%)	0	100	100
1	F	264/294 (90%)	259 (98%)	5 (2%)	0	100	100
1	G	264/294 (90%)	261 (99%)	3 (1%)	0	100	100
1	H	260/294 (88%)	256 (98%)	4 (2%)	0	100	100
1	I	265/294 (90%)	261 (98%)	4 (2%)	0	100	100
1	J	265/294 (90%)	261 (98%)	4 (2%)	0	100	100
1	K	264/294 (90%)	260 (98%)	4 (2%)	0	100	100
1	L	227/294 (77%)	221 (97%)	5 (2%)	1 (0%)	30	49
All	All	3123/3528 (88%)	3074 (98%)	48 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	76	THR

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	198/228 (87%)	196 (99%)	2 (1%)	68	85
1	B	194/228 (85%)	193 (100%)	1 (0%)	81	91
1	C	190/228 (83%)	189 (100%)	1 (0%)	81	91
1	D	185/228 (81%)	184 (100%)	1 (0%)	81	91
1	E	200/228 (88%)	198 (99%)	2 (1%)	68	85
1	F	197/228 (86%)	195 (99%)	2 (1%)	68	85
1	G	195/228 (86%)	193 (99%)	2 (1%)	68	85
1	H	187/228 (82%)	186 (100%)	1 (0%)	81	91
1	I	198/228 (87%)	196 (99%)	2 (1%)	68	85
1	J	196/228 (86%)	194 (99%)	2 (1%)	68	85
1	K	192/228 (84%)	191 (100%)	1 (0%)	81	91
1	L	155/228 (68%)	152 (98%)	3 (2%)	50	74
All	All	2287/2736 (84%)	2267 (99%)	20 (1%)	70	86

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	PHE
1	A	59	CYS
1	B	59	CYS
1	C	68	GLN
1	D	153	GLU
1	E	54	PHE
1	E	59	CYS
1	F	54	PHE
1	F	59	CYS
1	G	54	PHE
1	G	59	CYS
1	H	59	CYS
1	I	54	PHE
1	I	59	CYS
1	J	2	VAL
1	J	59	CYS
1	K	59	CYS
1	L	61	ASP
1	L	74	ASP
1	L	106	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	267	ASN
1	B	22	HIS
1	B	83	ASN
1	B	241	ASN
1	C	22	HIS
1	C	241	ASN
1	D	16	ASN
1	D	65	GLN
1	D	68	GLN
1	D	267	ASN
1	E	65	GLN
1	E	68	GLN
1	E	241	ASN
1	F	115	GLN
1	G	241	ASN
1	H	16	ASN
1	H	241	ASN
1	I	241	ASN
1	J	89	GLN
1	J	109	GLN
1	J	115	GLN
1	J	124	ASN
1	J	241	ASN
1	K	23	HIS
1	K	241	ASN
1	L	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

41 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$
3	PDC	F	1002	-	12,12,12	1.26	2 (16%)	16,16,16	2.38	6 (37%)
4	SO4	D	303	-	4,4,4	0.52	0	6,6,6	0.09	0
4	SO4	F	1003	-	4,4,4	0.52	0	6,6,6	0.38	0
3	PDC	E	1002	-	12,12,12	1.02	1 (8%)	16,16,16	2.24	7 (43%)
2	NAD	A	1001	-	46,48,48	1.44	7 (15%)	64,73,73	1.89	13 (20%)
4	SO4	K	1003	-	4,4,4	0.47	0	6,6,6	0.18	0
3	PDC	G	1002	-	12,12,12	1.21	1 (8%)	16,16,16	1.74	4 (25%)
4	SO4	I	303	-	4,4,4	0.61	0	6,6,6	0.66	0
4	SO4	A	1004	-	4,4,4	0.49	0	6,6,6	0.37	0
3	PDC	I	301	-	12,12,12	1.13	0	16,16,16	1.62	3 (18%)
3	PDC	J	1002	-	12,12,12	0.85	0	16,16,16	2.08	6 (37%)
4	SO4	H	301	-	4,4,4	0.47	0	6,6,6	0.13	0
4	SO4	J	1003	-	4,4,4	0.49	0	6,6,6	0.41	0
2	NAD	B	1001	-	46,48,48	1.29	5 (10%)	64,73,73	1.93	15 (23%)
4	SO4	C	1003	-	4,4,4	0.52	0	6,6,6	0.31	0
4	SO4	H	304	-	4,4,4	0.53	0	6,6,6	0.14	0
4	SO4	H	305	-	4,4,4	0.47	0	6,6,6	0.26	0
2	NAD	E	1001	-	46,48,48	1.27	7 (15%)	64,73,73	1.92	13 (20%)
2	NAD	K	1001	-	46,48,48	1.33	7 (15%)	64,73,73	1.86	14 (21%)
3	PDC	K	1002	-	12,12,12	1.05	0	16,16,16	1.62	5 (31%)
4	SO4	D	301	-	4,4,4	0.50	0	6,6,6	0.28	0
4	SO4	A	1003	-	4,4,4	0.57	0	6,6,6	0.25	0
4	SO4	H	302	-	4,4,4	0.53	0	6,6,6	0.48	0
2	NAD	C	1001	-	46,48,48	1.56	7 (15%)	64,73,73	1.87	15 (23%)
4	SO4	K	1004	-	4,4,4	0.45	0	6,6,6	0.07	0
4	SO4	L	301	-	4,4,4	0.54	0	6,6,6	0.20	0
4	SO4	D	302	-	4,4,4	0.56	0	6,6,6	0.26	0
2	NAD	F	1001	-	46,48,48	1.15	5 (10%)	64,73,73	1.78	13 (20%)
3	PDC	C	1002	-	12,12,12	0.97	1 (8%)	16,16,16	1.64	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PDC	A	1002	-	12,12,12	1.36	2 (16%)	16,16,16	1.58	2 (12%)
3	PDC	B	1002	-	12,12,12	1.48	2 (16%)	16,16,16	2.73	8 (50%)
4	SO4	E	1004	-	4,4,4	0.47	0	6,6,6	0.13	0
2	NAD	J	1001	-	46,48,48	1.31	7 (15%)	64,73,73	1.98	16 (25%)
4	SO4	H	303	-	4,4,4	0.56	0	6,6,6	0.32	0
4	SO4	B	1003	-	4,4,4	0.54	0	6,6,6	0.33	0
4	SO4	I	304	-	4,4,4	0.55	0	6,6,6	0.14	0
2	NAD	I	302	-	46,48,48	1.45	9 (19%)	64,73,73	2.00	19 (29%)
4	SO4	D	304	-	4,4,4	0.39	0	6,6,6	0.08	0
4	SO4	G	1003	-	4,4,4	0.50	0	6,6,6	0.20	0
4	SO4	E	1003	-	4,4,4	0.53	0	6,6,6	0.31	0
2	NAD	G	1001	-	46,48,48	1.25	6 (13%)	64,73,73	1.80	11 (17%)

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
3	PDC	F	1002	-	-	0/8/8/8	0/1/1/1
3	PDC	E	1002	-	-	2/8/8/8	0/1/1/1
2	NAD	E	1001	-	-	6/30/62/62	0/5/5/5
2	NAD	A	1001	-	-	5/30/62/62	0/5/5/5
2	NAD	K	1001	-	-	5/30/62/62	0/5/5/5
2	NAD	I	302	-	-	5/30/62/62	0/5/5/5
3	PDC	J	1002	-	-	0/8/8/8	0/1/1/1
3	PDC	G	1002	-	-	0/8/8/8	0/1/1/1
2	NAD	C	1001	-	-	8/30/62/62	0/5/5/5
3	PDC	K	1002	-	-	0/8/8/8	0/1/1/1
2	NAD	B	1001	-	-	4/30/62/62	0/5/5/5
2	NAD	F	1001	-	-	7/30/62/62	0/5/5/5
3	PDC	C	1002	-	-	0/8/8/8	0/1/1/1
3	PDC	A	1002	-	-	0/8/8/8	0/1/1/1
3	PDC	B	1002	-	-	0/8/8/8	0/1/1/1
2	NAD	G	1001	-	-	6/30/62/62	0/5/5/5
3	PDC	I	301	-	-	4/8/8/8	0/1/1/1
2	NAD	J	1001	-	-	11/30/62/62	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NAD	C5A-C4A	5.42	1.48	1.39
2	C	1001	NAD	PN-O3	5.18	1.65	1.59
2	B	1001	NAD	C5A-C4A	4.96	1.47	1.39
2	K	1001	NAD	C5A-C4A	4.76	1.47	1.39
2	I	302	NAD	C5A-C4A	4.63	1.47	1.39
2	A	1001	NAD	C5A-C4A	4.54	1.47	1.39
2	J	1001	NAD	PN-O3	4.45	1.64	1.59
2	E	1001	NAD	C5A-C4A	4.15	1.46	1.39
2	G	1001	NAD	C5A-C4A	3.83	1.45	1.39
2	A	1001	NAD	PN-O3	3.75	1.63	1.59
2	F	1001	NAD	C5A-C4A	3.53	1.45	1.39
2	K	1001	NAD	PA-O3	3.44	1.63	1.59
3	B	1002	PDC	C6-N1	3.34	1.39	1.34
2	G	1001	NAD	C5A-N7A	-3.16	1.33	1.39
2	A	1001	NAD	O4D-C1D	3.09	1.44	1.40
2	I	302	NAD	PA-O3	3.07	1.62	1.59
2	J	1001	NAD	C5A-N7A	-3.05	1.33	1.39
2	F	1001	NAD	C4A-N9A	-3.05	1.31	1.37
2	C	1001	NAD	C5A-C6A	3.03	1.49	1.41
2	I	302	NAD	C8A-N7A	3.01	1.37	1.31
2	F	1001	NAD	C5A-N7A	-2.99	1.33	1.39
2	J	1001	NAD	C5A-C4A	2.94	1.44	1.39
2	I	302	NAD	C2N-N1N	-2.89	1.31	1.35
2	A	1001	NAD	C5A-C6A	2.86	1.49	1.41
3	F	1002	PDC	O4-C8	-2.84	1.22	1.30
2	B	1001	NAD	C5A-C6A	2.72	1.48	1.41
2	C	1001	NAD	C5A-N7A	-2.69	1.34	1.39
2	A	1001	NAD	C4A-N9A	-2.67	1.32	1.37
2	G	1001	NAD	C8A-N9A	-2.65	1.33	1.37
2	C	1001	NAD	PA-O3	2.64	1.62	1.59
2	K	1001	NAD	C5A-C6A	2.63	1.48	1.41
2	K	1001	NAD	C5A-N7A	-2.61	1.34	1.39
2	A	1001	NAD	PA-O3	2.60	1.62	1.59
2	I	302	NAD	C5A-C6A	2.59	1.48	1.41
2	J	1001	NAD	PA-O3	2.58	1.62	1.59
2	F	1001	NAD	C5A-C6A	2.58	1.48	1.41
2	G	1001	NAD	C4A-N9A	-2.54	1.32	1.37
2	G	1001	NAD	C5A-C6A	2.53	1.48	1.41
2	B	1001	NAD	C4A-N9A	-2.50	1.32	1.37
2	A	1001	NAD	C8A-N7A	2.40	1.36	1.31
3	B	1002	PDC	C2-N1	2.35	1.38	1.34
3	E	1002	PDC	C2-C7	-2.34	1.46	1.50
2	J	1001	NAD	O4D-C1D	2.33	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1001	NAD	C8A-N7A	2.32	1.36	1.31
2	E	1001	NAD	C5A-C6A	2.31	1.47	1.41
2	I	302	NAD	C4N-C3N	-2.31	1.35	1.39
2	C	1001	NAD	C8A-N7A	2.30	1.36	1.31
2	F	1001	NAD	C8A-N9A	-2.30	1.33	1.37
2	J	1001	NAD	C8A-N9A	-2.28	1.33	1.37
2	B	1001	NAD	O4B-C1B	2.26	1.47	1.42
2	E	1001	NAD	C4A-N9A	-2.25	1.33	1.37
2	I	302	NAD	C4A-N9A	-2.24	1.33	1.37
2	B	1001	NAD	C5A-N7A	-2.23	1.35	1.39
2	K	1001	NAD	O4D-C1D	2.23	1.43	1.40
3	A	1002	PDC	O3-C8	2.22	1.29	1.22
2	E	1001	NAD	PN-O3	2.20	1.61	1.59
3	F	1002	PDC	O1-C7	2.19	1.29	1.22
3	A	1002	PDC	O1-C7	2.18	1.29	1.22
2	G	1001	NAD	O4D-C1D	2.17	1.43	1.40
2	K	1001	NAD	C4A-N9A	-2.16	1.33	1.37
3	G	1002	PDC	C6-C8	-2.15	1.46	1.50
2	E	1001	NAD	C5A-N7A	-2.13	1.35	1.39
2	I	302	NAD	C5A-N7A	-2.12	1.35	1.39
2	E	1001	NAD	C8A-N9A	-2.11	1.34	1.37
3	C	1002	PDC	O3-C8	2.10	1.28	1.22
2	E	1001	NAD	C3N-C7N	-2.07	1.47	1.50
2	C	1001	NAD	C4A-N3A	2.07	1.38	1.34
2	I	302	NAD	C8A-N9A	-2.03	1.34	1.37
2	J	1001	NAD	C4A-N9A	-2.02	1.33	1.37

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1001	NAD	C5A-C4A-N3A	-6.39	117.92	126.72
2	J	1001	NAD	C5A-C4A-N3A	-6.19	118.19	126.72
2	B	1001	NAD	C5A-C4A-N3A	-5.84	118.67	126.72
2	A	1001	NAD	C5A-C4A-N3A	-5.81	118.71	126.72
2	C	1001	NAD	C5A-C4A-N3A	-5.80	118.72	126.72
2	K	1001	NAD	C5A-C4A-N3A	-5.77	118.78	126.72
2	E	1001	NAD	N3A-C4A-N9A	5.75	136.95	127.17
2	F	1001	NAD	C5A-C4A-N3A	-5.75	118.80	126.72
2	G	1001	NAD	C5A-C4A-N3A	-5.65	118.94	126.72
3	B	1002	PDC	C7-C2-N1	5.65	124.90	116.46
2	I	302	NAD	C5A-C4A-N3A	-5.50	119.14	126.72
2	G	1001	NAD	O4B-C1B-N9A	5.45	118.56	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1001	NAD	N3A-C4A-N9A	5.42	136.38	127.17
2	B	1001	NAD	N3A-C4A-N9A	5.34	136.24	127.17
2	F	1001	NAD	N3A-C4A-N9A	5.07	135.79	127.17
2	K	1001	NAD	N3A-C4A-N9A	4.95	135.58	127.17
2	C	1001	NAD	N3A-C4A-N9A	4.92	135.53	127.17
2	G	1001	NAD	N3A-C4A-N9A	4.77	135.28	127.17
2	A	1001	NAD	N3A-C4A-N9A	4.71	135.18	127.17
3	F	1002	PDC	C6-N1-C2	4.70	123.35	117.54
3	F	1002	PDC	C5-C6-N1	-4.69	117.45	122.92
2	E	1001	NAD	C2A-N3A-C4A	4.69	123.28	111.83
2	K	1001	NAD	O4B-C1B-N9A	4.65	117.01	108.09
2	I	302	NAD	N3A-C4A-N9A	4.54	134.88	127.17
2	E	1001	NAD	N3A-C2A-N1A	-4.52	121.74	128.58
3	J	1002	PDC	C8-C6-N1	4.48	123.15	116.46
2	J	1001	NAD	O2N-PN-O3	4.44	119.26	107.27
3	F	1002	PDC	C8-C6-N1	4.31	122.90	116.46
2	I	302	NAD	C6N-N1N-C2N	-4.29	118.22	121.88
2	J	1001	NAD	C2A-N3A-C4A	4.25	122.21	111.83
2	F	1001	NAD	C2A-N3A-C4A	4.17	122.03	111.83
3	B	1002	PDC	C3-C2-N1	-4.14	118.09	122.92
2	J	1001	NAD	C4D-O4D-C1D	4.10	113.68	109.92
2	A	1001	NAD	C2A-N3A-C4A	4.10	121.83	111.83
2	A	1001	NAD	C3N-C7N-N7N	4.09	122.78	117.74
2	J	1001	NAD	N3A-C2A-N1A	-4.02	122.49	128.58
2	F	1001	NAD	N3A-C2A-N1A	-4.00	122.53	128.58
2	I	302	NAD	C5N-C4N-C3N	-3.96	116.47	120.36
2	K	1001	NAD	C2A-N3A-C4A	3.89	121.33	111.83
3	E	1002	PDC	C5-C6-N1	-3.88	118.39	122.92
3	A	1002	PDC	C6-N1-C2	3.86	122.31	117.54
3	B	1002	PDC	C8-C6-N1	3.86	122.23	116.46
2	J	1001	NAD	O4B-C1B-N9A	3.84	115.47	108.09
2	B	1001	NAD	C2A-N3A-C4A	3.82	121.17	111.83
3	I	301	PDC	C6-N1-C2	3.78	122.21	117.54
2	A	1001	NAD	N3A-C2A-N1A	-3.77	122.88	128.58
2	K	1001	NAD	N3A-C2A-N1A	-3.74	122.92	128.58
2	I	302	NAD	C2A-N3A-C4A	3.72	120.92	111.83
2	C	1001	NAD	N3A-C2A-N1A	-3.72	122.96	128.58
2	B	1001	NAD	C4A-N9A-C8A	3.70	109.63	105.74
3	E	1002	PDC	O4-C8-C6	3.69	123.46	114.71
2	C	1001	NAD	O4B-C1B-N9A	3.65	115.10	108.09
2	C	1001	NAD	C6N-N1N-C2N	-3.65	118.77	121.88
3	E	1002	PDC	C6-N1-C2	3.65	122.05	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	PDC	C5-C6-N1	-3.64	118.68	122.92
2	C	1001	NAD	C2A-N3A-C4A	3.62	120.68	111.83
2	G	1001	NAD	C2A-N3A-C4A	3.61	120.65	111.83
2	I	302	NAD	C4A-N9A-C8A	3.60	109.51	105.74
2	C	1001	NAD	C3N-C7N-N7N	3.58	122.16	117.74
2	A	1001	NAD	C4A-N9A-C8A	3.51	109.42	105.74
3	I	301	PDC	C3-C2-N1	-3.49	118.85	122.92
2	E	1001	NAD	C4A-N9A-C8A	3.46	109.37	105.74
2	I	302	NAD	O4B-C1B-N9A	3.44	114.70	108.09
2	B	1001	NAD	O3-PN-O1N	-3.43	100.39	110.70
3	E	1002	PDC	O1-C7-C2	-3.42	114.41	121.30
3	B	1002	PDC	C6-N1-C2	3.36	121.70	117.54
2	F	1001	NAD	C4A-N9A-C8A	3.34	109.25	105.74
3	G	1002	PDC	C6-N1-C2	3.33	121.65	117.54
2	G	1001	NAD	N3A-C2A-N1A	-3.31	123.56	128.58
2	B	1001	NAD	C3N-C7N-N7N	3.31	121.82	117.74
2	C	1001	NAD	C4A-C5A-N7A	-3.29	106.83	110.58
2	B	1001	NAD	O2A-PA-O3	3.26	116.08	107.27
2	I	302	NAD	N3A-C2A-N1A	-3.24	123.68	128.58
3	J	1002	PDC	C5-C6-N1	-3.23	119.15	122.92
2	B	1001	NAD	N3A-C2A-N1A	-3.22	123.70	128.58
2	A	1001	NAD	C4A-C5A-N7A	-3.21	106.91	110.58
2	A	1001	NAD	O7N-C7N-N7N	-3.17	118.03	122.62
3	C	1002	PDC	C5-C6-N1	-3.13	119.26	122.92
2	I	302	NAD	C4A-C5A-N7A	-3.13	107.01	110.58
3	B	1002	PDC	O2-C7-C2	3.12	122.12	114.71
3	C	1002	PDC	C6-N1-C2	3.12	121.39	117.54
2	J	1001	NAD	C6N-N1N-C2N	-3.07	119.27	121.88
2	C	1001	NAD	C5N-C4N-C3N	-3.06	117.36	120.36
2	G	1001	NAD	C4A-C5A-N7A	-3.06	107.08	110.58
3	K	1002	PDC	C3-C2-N1	-3.05	119.36	122.92
2	E	1001	NAD	C4B-O4B-C1B	-3.01	102.82	109.47
2	E	1001	NAD	C3N-C7N-N7N	2.97	121.39	117.74
3	J	1002	PDC	C7-C2-N1	2.96	120.88	116.46
2	F	1001	NAD	C4A-C5A-N7A	-2.95	107.20	110.58
2	B	1001	NAD	C4B-O4B-C1B	-2.95	102.96	109.47
2	I	302	NAD	C6A-C5A-N7A	2.94	137.76	132.09
3	G	1002	PDC	O2-C7-C2	2.93	121.68	114.71
3	K	1002	PDC	C6-N1-C2	2.90	121.13	117.54
2	K	1001	NAD	C3N-C7N-N7N	2.89	121.30	117.74
3	F	1002	PDC	C7-C2-N1	2.88	120.76	116.46
2	E	1001	NAD	O2A-PA-O3	2.82	114.90	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	302	NAD	C3N-C7N-N7N	2.81	121.19	117.74
2	J	1001	NAD	C4A-N9A-C8A	2.80	108.68	105.74
2	A	1001	NAD	O2A-PA-O3	2.80	114.84	107.27
2	I	302	NAD	C6N-N1N-C1D	2.79	125.21	119.73
3	J	1002	PDC	C6-N1-C2	2.79	120.99	117.54
2	I	302	NAD	C4A-N9A-C1B	-2.78	120.14	126.63
2	A	1001	NAD	C6A-C5A-N7A	2.77	137.43	132.09
2	A	1001	NAD	C6N-N1N-C2N	-2.77	119.52	121.88
2	K	1001	NAD	O3-PA-O1A	-2.75	102.43	110.70
2	K	1001	NAD	C4A-N9A-C8A	2.73	108.61	105.74
2	I	302	NAD	O3-PA-O1A	-2.71	102.56	110.70
2	B	1001	NAD	C4A-C5A-N7A	-2.68	107.52	110.58
2	B	1001	NAD	O7N-C7N-N7N	-2.67	118.75	122.62
2	E	1001	NAD	O4B-C1B-N9A	2.66	113.20	108.09
2	I	302	NAD	O7N-C7N-C3N	-2.66	116.34	119.60
2	G	1001	NAD	C6N-N1N-C2N	-2.66	119.62	121.88
2	G	1001	NAD	C4A-N9A-C8A	2.64	108.51	105.74
2	J	1001	NAD	O7N-C7N-N7N	-2.63	118.81	122.62
2	F	1001	NAD	O7N-C7N-N7N	-2.60	118.86	122.62
2	C	1001	NAD	O2A-PA-O3	2.57	114.22	107.27
2	F	1001	NAD	C6A-C5A-N7A	2.56	137.02	132.09
3	F	1002	PDC	O4-C8-O3	-2.55	117.87	123.35
2	K	1001	NAD	C4A-C5A-N7A	-2.54	107.67	110.58
2	C	1001	NAD	C2A-N1A-C6A	2.54	122.90	118.73
2	C	1001	NAD	C4A-N9A-C8A	2.53	108.39	105.74
3	C	1002	PDC	C8-C6-N1	2.53	120.24	116.46
2	K	1001	NAD	O2A-PA-O3	2.50	114.03	107.27
2	J	1001	NAD	O2A-PA-O1A	2.49	124.05	112.44
2	E	1001	NAD	C6A-C5A-N7A	2.49	136.89	132.09
2	C	1001	NAD	C5A-N7A-C8A	2.48	107.35	103.45
3	J	1002	PDC	O3-C8-C6	-2.47	116.33	121.30
2	J	1001	NAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	B	1001	NAD	O5D-C5D-C4D	2.42	117.24	108.99
2	J	1001	NAD	O3-PN-O1N	-2.41	103.44	110.70
3	B	1002	PDC	O4-C8-C6	2.41	120.44	114.71
2	I	302	NAD	O2A-PA-O1A	2.41	123.65	112.44
2	G	1001	NAD	C5N-C4N-C3N	-2.38	118.03	120.36
3	B	1002	PDC	C5-C6-C8	-2.37	116.19	120.32
2	B	1001	NAD	O5D-PN-O1N	2.37	118.31	108.94
2	E	1001	NAD	C4A-C5A-N7A	-2.36	107.89	110.58
3	B	1002	PDC	O2-C7-O1	-2.34	118.32	123.35
2	B	1001	NAD	C4D-O4D-C1D	-2.33	107.79	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1002	PDC	O3-C8-C6	-2.32	116.62	121.30
2	F	1001	NAD	C5A-N7A-C8A	2.32	107.09	103.45
2	I	302	NAD	O2A-PA-O3	2.31	113.52	107.27
2	A	1001	NAD	N9A-C8A-N7A	-2.30	110.68	113.94
2	J	1001	NAD	C5A-N7A-C8A	2.29	107.05	103.45
3	E	1002	PDC	C4-C3-C2	-2.29	115.89	118.63
3	F	1002	PDC	C3-C2-N1	-2.28	120.26	122.92
2	K	1001	NAD	O7N-C7N-N7N	-2.27	119.33	122.62
2	G	1001	NAD	O3D-C3D-C4D	-2.25	104.61	111.08
3	G	1002	PDC	C5-C6-N1	-2.25	120.30	122.92
2	I	302	NAD	N9A-C8A-N7A	-2.24	110.75	113.94
3	K	1002	PDC	O1-C7-C2	-2.23	116.80	121.30
3	E	1002	PDC	O2-C7-O1	2.21	128.12	123.35
3	J	1002	PDC	O4-C8-C6	2.21	119.95	114.71
2	K	1001	NAD	O3D-C3D-C4D	-2.20	104.77	111.08
2	F	1001	NAD	O3-PN-O1N	-2.20	104.09	110.70
2	E	1001	NAD	C5A-C6A-N6A	-2.20	117.85	123.29
3	E	1002	PDC	O3-C8-C6	-2.20	116.88	121.30
2	G	1001	NAD	C5A-N7A-C8A	2.19	106.89	103.45
2	A	1001	NAD	C5A-N7A-C8A	2.18	106.87	103.45
3	G	1002	PDC	C3-C2-N1	-2.16	120.39	122.92
2	F	1001	NAD	C6N-N1N-C2N	-2.16	120.04	121.88
2	J	1001	NAD	C5A-C6A-N6A	-2.15	117.95	123.29
2	F	1001	NAD	C4B-O4B-C1B	-2.15	104.72	109.47
2	C	1001	NAD	O7N-C7N-N7N	-2.13	119.53	122.62
3	K	1002	PDC	O2-C7-C2	2.13	119.77	114.71
2	C	1001	NAD	O3-PN-O1N	2.11	117.06	110.70
2	B	1001	NAD	C6A-C5A-N7A	2.11	136.16	132.09
2	I	302	NAD	C5A-N7A-C8A	2.11	106.76	103.45
2	E	1001	NAD	O3-PA-O1A	-2.10	104.39	110.70
3	I	301	PDC	C3-C2-C7	2.07	123.92	120.32
3	C	1002	PDC	O1-C7-C2	-2.06	117.16	121.30
3	C	1002	PDC	O2-C7-C2	2.04	119.56	114.71
2	K	1001	NAD	O4B-C4B-C3B	2.04	109.20	105.15
2	K	1001	NAD	C5N-C4N-C3N	-2.03	118.37	120.36
2	F	1001	NAD	N9A-C8A-N7A	-2.03	111.06	113.94
2	J	1001	NAD	N9A-C8A-N7A	-2.03	111.06	113.94

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAD	O4D-C1D-N1N-C2N
2	A	1001	NAD	O4D-C1D-N1N-C6N
2	A	1001	NAD	C2D-C1D-N1N-C2N
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	C	1001	NAD	C5D-O5D-PN-O1N
2	C	1001	NAD	C5D-O5D-PN-O2N
2	C	1001	NAD	O4D-C1D-N1N-C2N
2	C	1001	NAD	O4D-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	C5D-O5D-PN-O2N
2	F	1001	NAD	O4D-C1D-N1N-C6N
2	G	1001	NAD	C5D-O5D-PN-O3
2	G	1001	NAD	O4D-C1D-N1N-C2N
2	G	1001	NAD	O4D-C1D-N1N-C6N
2	I	302	NAD	O4D-C1D-N1N-C2N
2	I	302	NAD	O4D-C1D-N1N-C6N
2	I	302	NAD	C2D-C1D-N1N-C2N
2	I	302	NAD	C2D-C1D-N1N-C6N
2	J	1001	NAD	C5B-O5B-PA-O2A
2	J	1001	NAD	C5B-O5B-PA-O3
2	J	1001	NAD	PN-O3-PA-O5B
2	J	1001	NAD	O4D-C1D-N1N-C2N
2	J	1001	NAD	O4D-C1D-N1N-C6N
2	J	1001	NAD	C2D-C1D-N1N-C2N
2	K	1001	NAD	C5D-O5D-PN-O3
2	K	1001	NAD	O4D-C1D-N1N-C2N
2	K	1001	NAD	O4D-C1D-N1N-C6N
2	F	1001	NAD	O4D-C4D-C5D-O5D
2	J	1001	NAD	O4B-C4B-C5B-O5B
2	E	1001	NAD	PN-O3-PA-O1A
3	I	301	PDC	N1-C2-C7-O1
2	C	1001	NAD	C5D-O5D-PN-O3
2	F	1001	NAD	C5D-O5D-PN-O3
2	F	1001	NAD	C5D-O5D-PN-O1N
2	G	1001	NAD	C5D-O5D-PN-O1N
2	J	1001	NAD	C5B-O5B-PA-O1A
3	I	301	PDC	C3-C2-C7-O1
2	E	1001	NAD	PN-O3-PA-O2A
2	J	1001	NAD	PA-O3-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	A	1001	NAD	C2D-C1D-N1N-C6N
2	B	1001	NAD	C2D-C1D-N1N-C6N
2	C	1001	NAD	C2D-C1D-N1N-C2N
2	E	1001	NAD	C2D-C1D-N1N-C6N
2	G	1001	NAD	C2D-C1D-N1N-C2N
2	J	1001	NAD	C2D-C1D-N1N-C6N
2	K	1001	NAD	C2D-C1D-N1N-C2N
3	I	301	PDC	N1-C2-C7-O2
2	J	1001	NAD	C3B-C4B-C5B-O5B
3	I	301	PDC	C3-C2-C7-O2
2	C	1001	NAD	O4D-C4D-C5D-O5D
2	F	1001	NAD	C3D-C4D-C5D-O5D
2	F	1001	NAD	O4D-C1D-N1N-C2N
3	E	1002	PDC	N1-C6-C8-O4
2	A	1001	NAD	PN-O3-PA-O2A
2	G	1001	NAD	PN-O3-PA-O2A
3	E	1002	PDC	C5-C6-C8-O4
2	K	1001	NAD	O4B-C4B-C5B-O5B
2	C	1001	NAD	PN-O3-PA-O2A
2	I	302	NAD	O4B-C4B-C5B-O5B

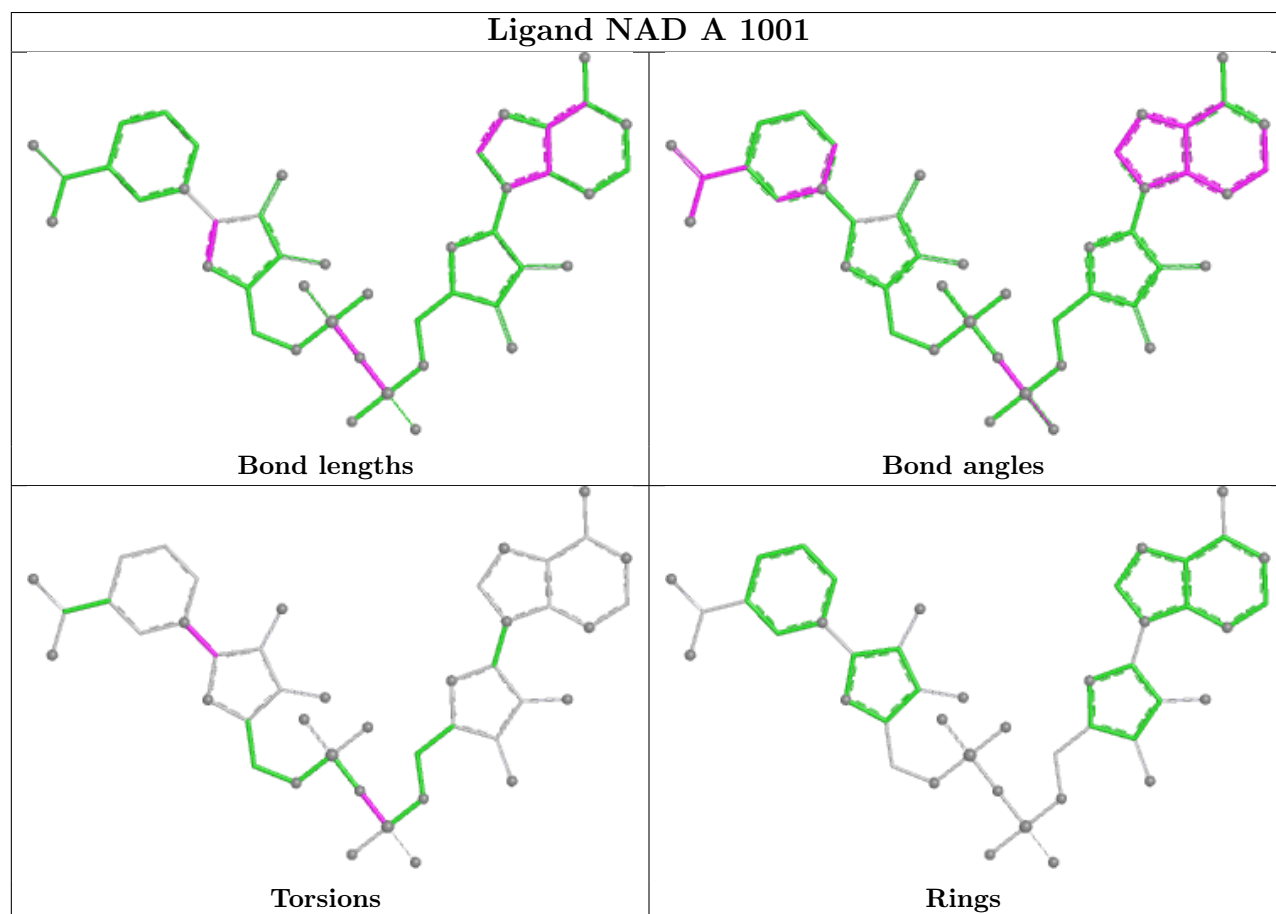
There are no ring outliers.

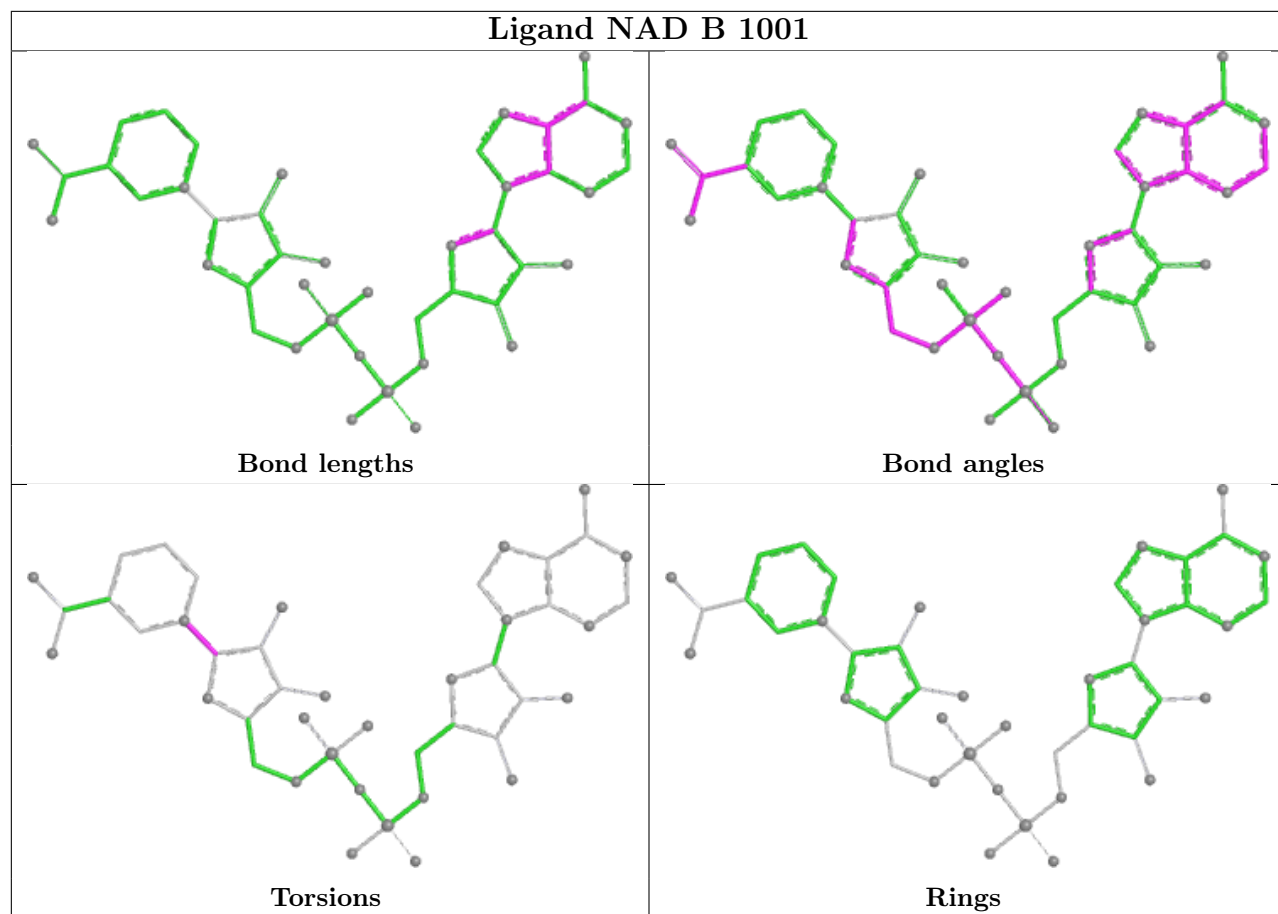
13 monomers are involved in 13 short contacts:

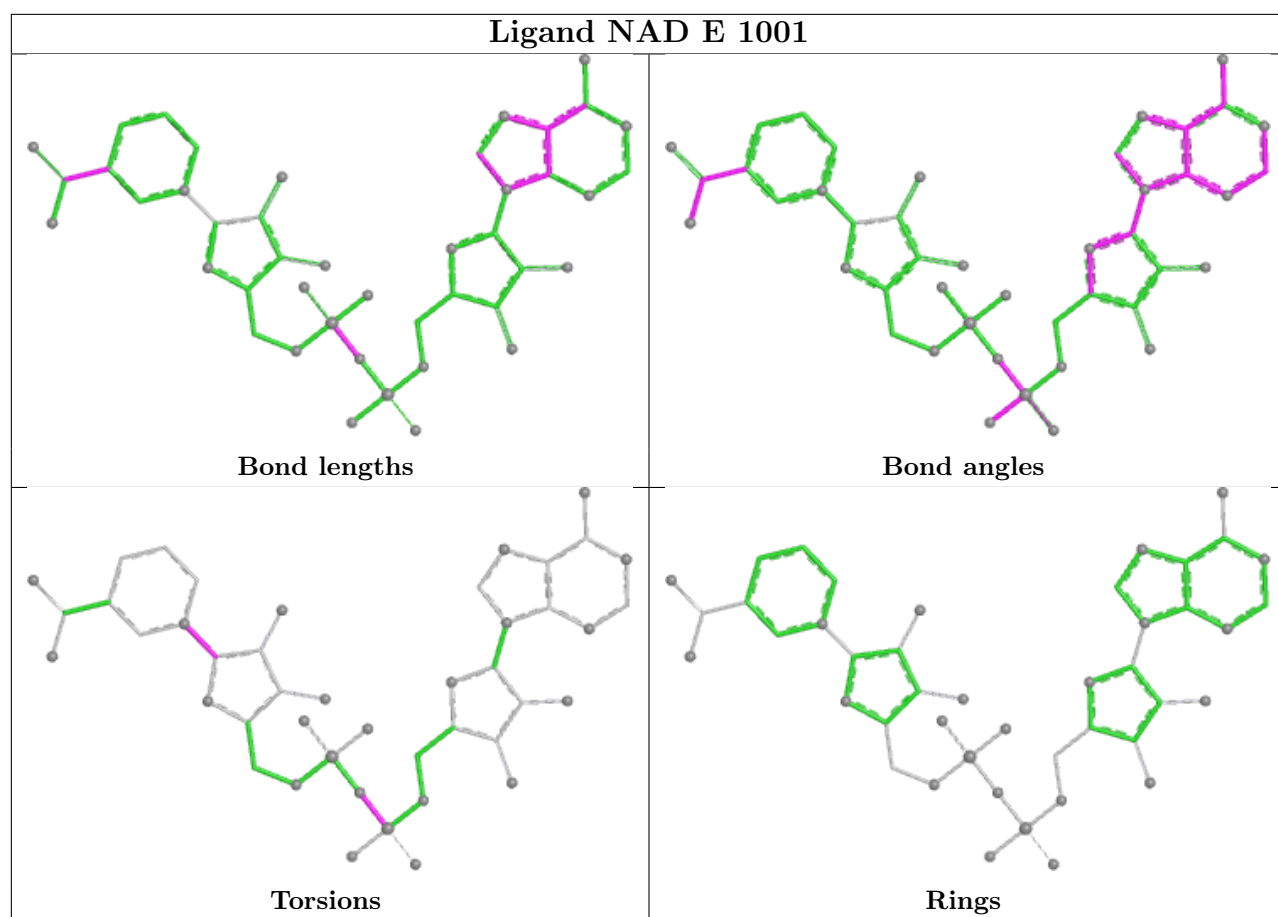
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1002	PDC	1	0
2	A	1001	NAD	1	0
3	I	301	PDC	1	0
2	B	1001	NAD	1	0
2	E	1001	NAD	2	0
2	K	1001	NAD	1	0
4	A	1003	SO4	1	0
2	C	1001	NAD	1	0
2	F	1001	NAD	1	0
2	J	1001	NAD	1	0
4	B	1003	SO4	1	0
2	I	302	NAD	2	0
2	G	1001	NAD	1	0

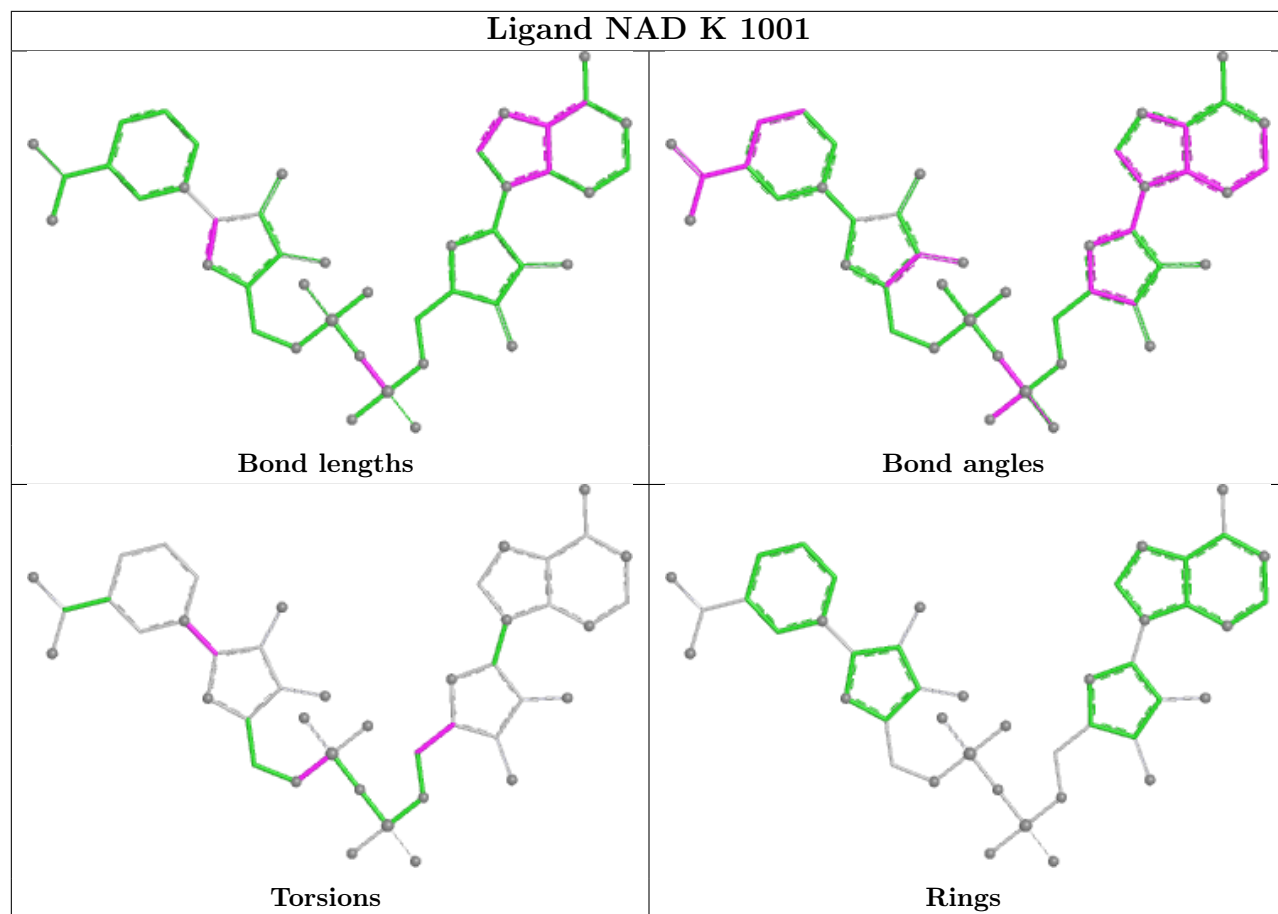
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

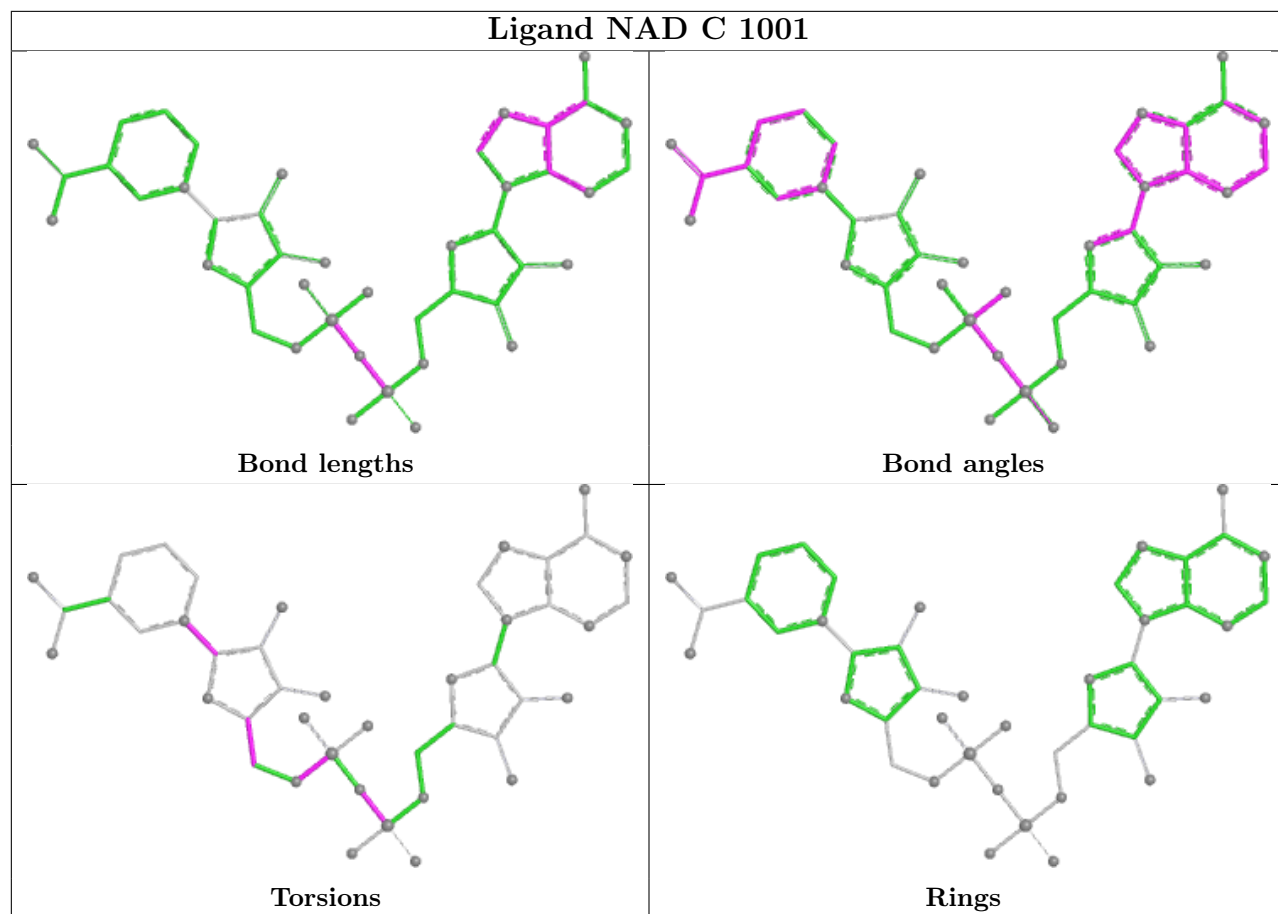
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

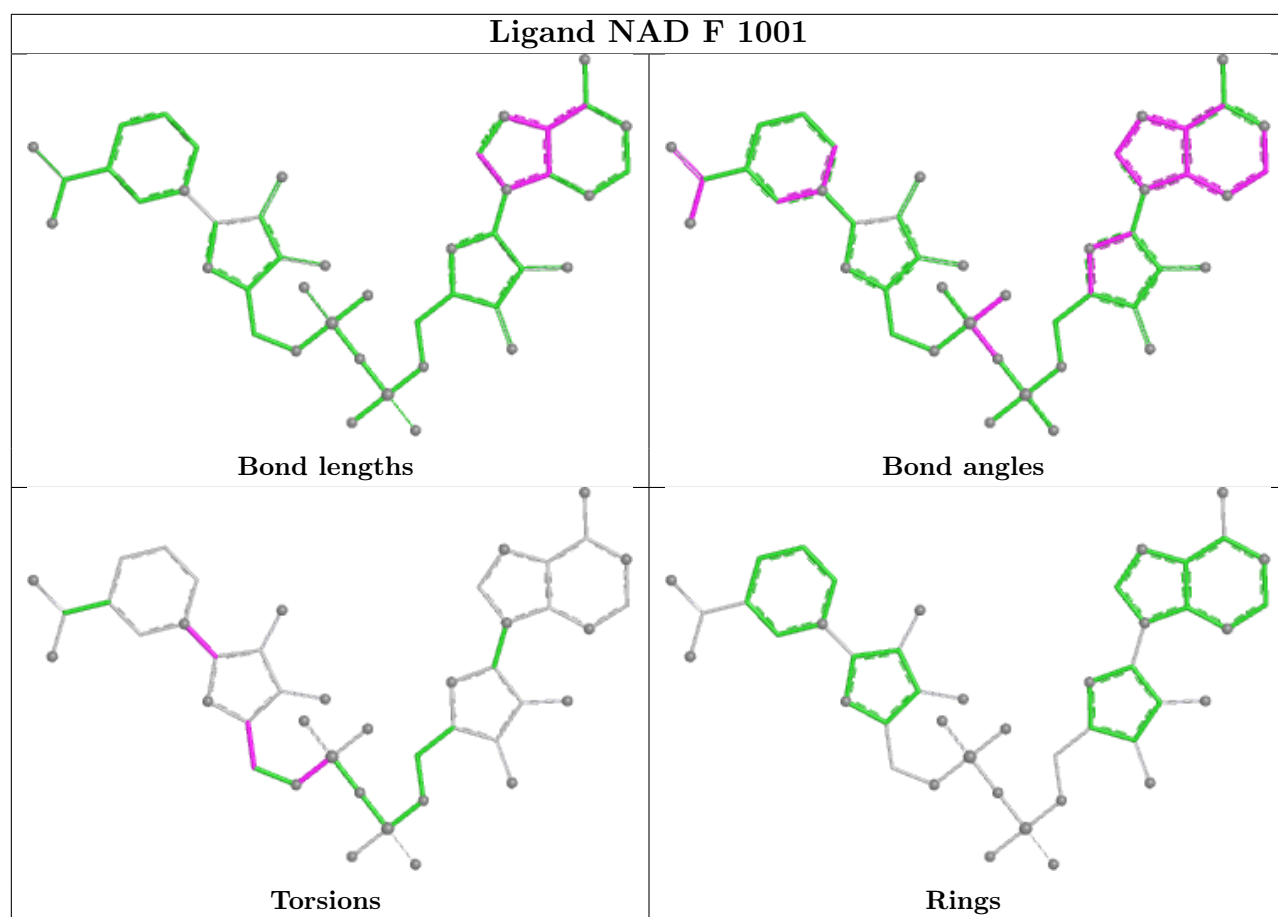


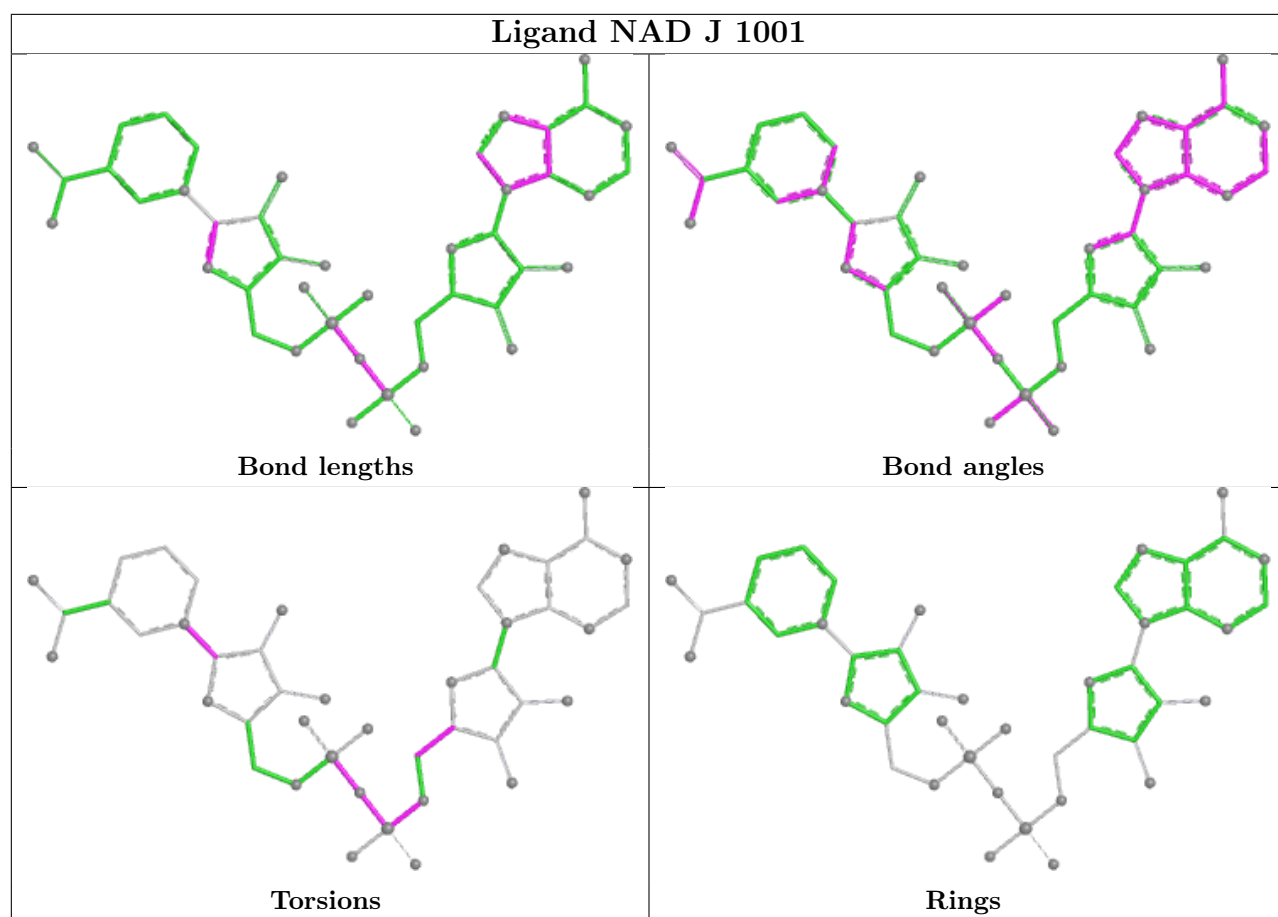


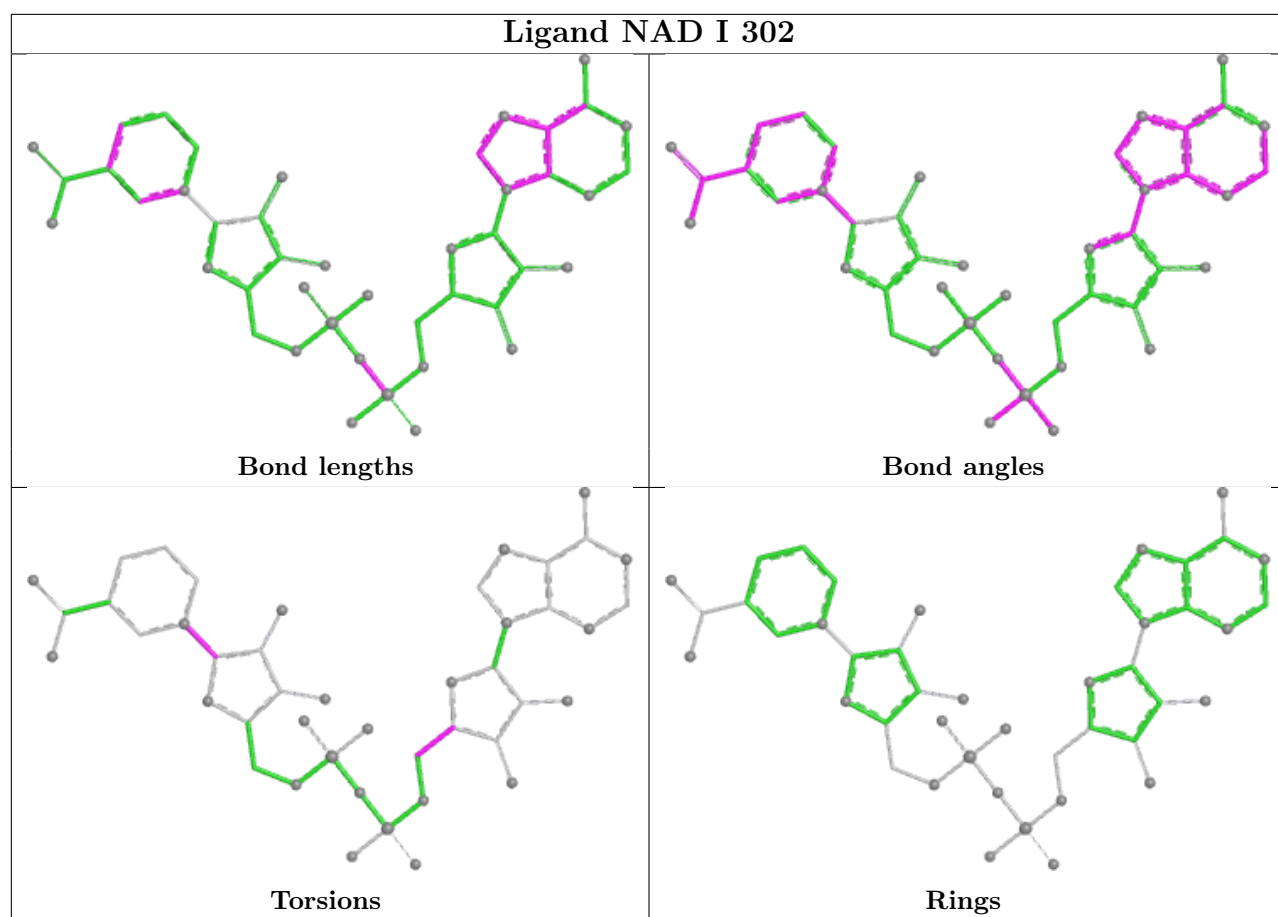


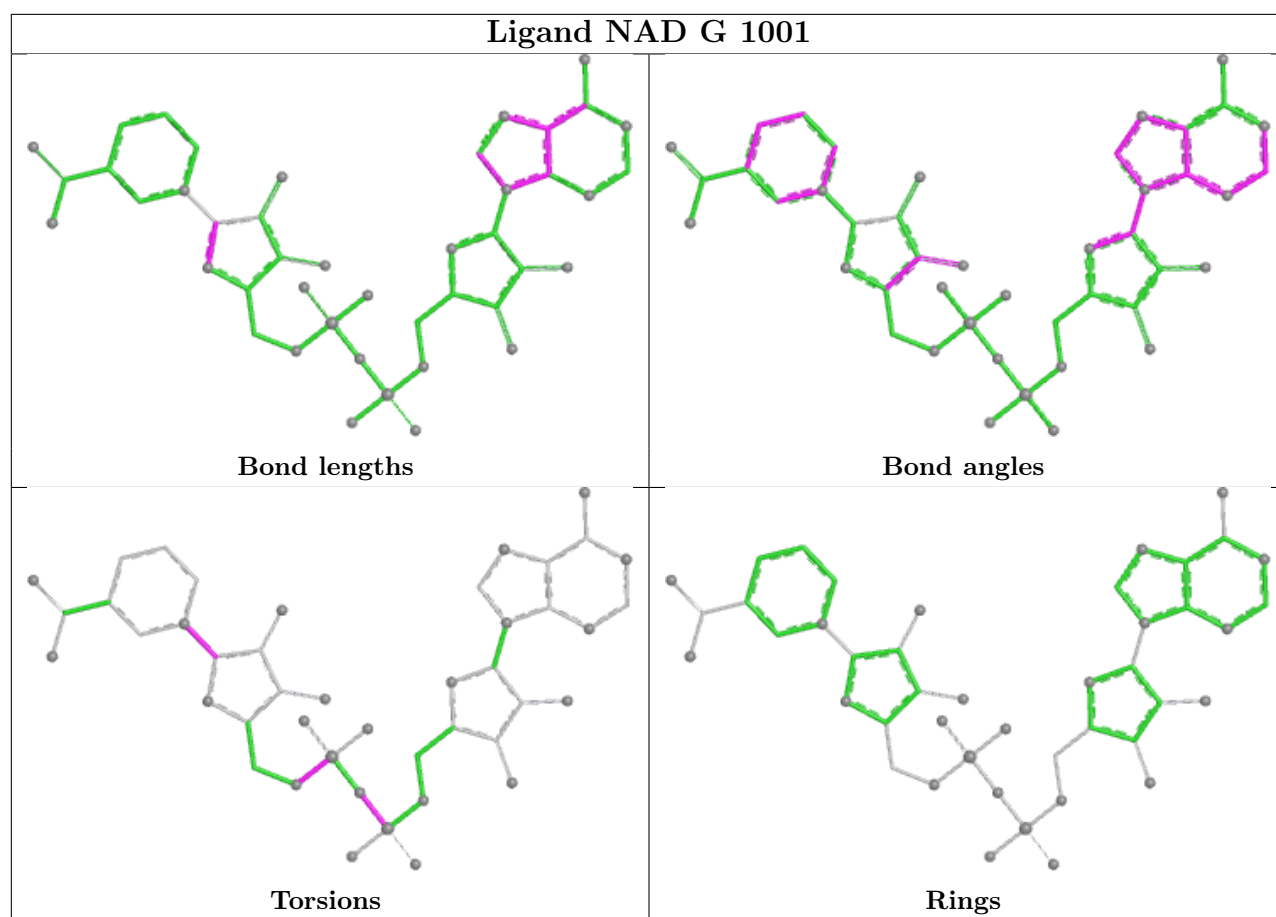












5.7 Other polymers [i](#)

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	267/294 (90%)	0.22	6 (2%) 62 57	40, 62, 109, 161	0
1	B	266/294 (90%)	0.42	7 (2%) 57 52	42, 62, 103, 142	0
1	C	266/294 (90%)	0.65	23 (8%) 16 13	39, 73, 135, 182	0
1	D	260/294 (88%)	0.49	13 (5%) 34 29	43, 66, 125, 163	0
1	E	267/294 (90%)	-0.03	4 (1%) 72 68	29, 49, 89, 149	0
1	F	266/294 (90%)	-0.05	4 (1%) 72 68	33, 52, 90, 138	0
1	G	266/294 (90%)	-0.03	7 (2%) 57 52	29, 54, 101, 145	0
1	H	264/294 (89%)	0.36	14 (5%) 32 27	38, 64, 147, 182	0
1	I	267/294 (90%)	0.09	5 (1%) 66 62	33, 52, 106, 151	0
1	J	267/294 (90%)	0.37	6 (2%) 62 57	36, 60, 108, 154	0
1	K	266/294 (90%)	0.63	25 (9%) 14 11	38, 69, 123, 155	0
1	L	237/294 (80%)	1.58	79 (33%) 1 1	46, 83, 128, 173	0
All	All	3159/3528 (89%)	0.38	193 (6%) 27 22	29, 62, 120, 182	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	81	THR	9.1
1	L	17	LEU	6.1
1	L	96	VAL	5.9
1	L	27	ALA	5.6
1	L	14	GLY	5.6
1	L	77	ALA	5.4
1	L	244	VAL	4.8
1	L	250	LEU	4.7
1	L	31	ALA	4.6
1	L	36	PRO	4.6
1	L	85	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	9	ALA	4.2
1	L	120	VAL	4.2
1	C	94	SER	4.2
1	L	73	ILE	4.1
1	L	76	THR	4.1
1	L	13	MET	4.0
1	L	243	ALA	4.0
1	L	242	GLY	4.0
1	L	30	ALA	4.0
1	L	86	ALA	4.0
1	K	57	VAL	3.8
1	L	18	VAL	3.8
1	K	48	LEU	3.8
1	C	6	VAL	3.7
1	H	48	LEU	3.7
1	L	87	LEU	3.7
1	K	86	ALA	3.6
1	I	266	LEU	3.6
1	L	82	LEU	3.6
1	D	58	VAL	3.5
1	L	99	THR	3.5
1	L	29	VAL	3.5
1	C	40	LEU	3.5
1	L	122	ALA	3.4
1	L	78	PRO	3.3
1	J	193	ILE	3.3
1	B	51	GLU	3.3
1	H	40	LEU	3.3
1	L	125	TYR	3.3
1	K	247	ALA	3.2
1	L	111	ASP	3.2
1	L	62	LEU	3.2
1	D	123	PRO	3.2
1	L	70	ASP	3.1
1	B	48	LEU	3.1
1	F	265	GLY	3.1
1	L	113	VAL	3.1
1	G	49	CYS	3.1
1	L	10	ALA	3.1
1	L	119	VAL	3.1
1	L	12	ARG	3.1
1	C	29	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	75	PHE	3.1
1	A	45	LEU	3.0
1	L	123	PRO	3.0
1	L	72	ILE	3.0
1	L	6	VAL	3.0
1	D	122	ALA	3.0
1	L	15	ARG	3.0
1	H	50	GLY	3.0
1	K	266	LEU	2.9
1	L	11	GLY	2.9
1	H	25	PRO	2.9
1	L	63	ALA	2.9
1	L	103	THR	2.9
1	B	9	ALA	2.9
1	G	48	LEU	2.9
1	G	57	VAL	2.9
1	G	266	LEU	2.9
1	E	267	ASN	2.8
1	L	112	LEU	2.8
1	L	124	ASN	2.8
1	L	247	ALA	2.8
1	D	47	GLU	2.8
1	L	121	MET	2.8
1	C	62	LEU	2.8
1	L	23	HIS	2.8
1	L	2	VAL	2.8
1	C	27	ALA	2.7
1	L	71	VAL	2.7
1	L	257	PHE	2.7
1	I	49	CYS	2.7
1	K	73	ILE	2.7
1	E	46	GLY	2.7
1	L	84	ASN	2.7
1	L	60	ASP	2.7
1	K	1	MET	2.7
1	K	42	GLY	2.7
1	C	18	VAL	2.7
1	H	45	LEU	2.7
1	L	32	GLY	2.7
1	H	39	SER	2.7
1	K	6	VAL	2.7
1	K	67	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	2.6
1	C	54	PHE	2.6
1	H	56	VAL	2.6
1	L	7	ALA	2.6
1	L	110	ILE	2.6
1	K	5	ALA	2.6
1	L	264	LEU	2.6
1	K	50	GLY	2.6
1	K	25	PRO	2.6
1	B	67	ASP	2.5
1	D	60	ASP	2.5
1	J	266	LEU	2.5
1	C	28	LYS	2.5
1	C	90	GLN	2.5
1	K	49	CYS	2.5
1	K	246	ALA	2.5
1	K	41	VAL	2.5
1	D	12	ARG	2.5
1	C	110	ILE	2.5
1	E	266	LEU	2.5
1	L	254	PRO	2.5
1	L	238	THR	2.4
1	C	97	ILE	2.4
1	H	123	PRO	2.4
1	L	98	GLY	2.4
1	D	41	VAL	2.4
1	L	97	ILE	2.4
1	C	252	GLU	2.4
1	D	57	VAL	2.4
1	L	259	THR	2.4
1	D	37	GLU	2.4
1	F	1	MET	2.4
1	J	26	VAL	2.4
1	L	117	VAL	2.4
1	E	45	LEU	2.4
1	I	23	HIS	2.4
1	K	51	GLU	2.4
1	A	50	GLY	2.4
1	J	0	GLY	2.4
1	L	95	ILE	2.3
1	L	24	ASN	2.3
1	A	25	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	256	GLY	2.3
1	C	57	VAL	2.3
1	G	66	ILE	2.3
1	K	14	GLY	2.3
1	G	63	ALA	2.3
1	L	266	LEU	2.3
1	L	129	VAL	2.3
1	L	248	VAL	2.3
1	L	130	ASN	2.3
1	A	211	ASP	2.3
1	H	112	LEU	2.3
1	C	95	ILE	2.2
1	H	100	THR	2.2
1	J	265	GLY	2.2
1	D	142	VAL	2.2
1	K	27	ALA	2.2
1	F	67	ASP	2.2
1	H	58	VAL	2.2
1	D	59	CYS	2.2
1	L	88	CYS	2.2
1	D	36	PRO	2.2
1	B	0	GLY	2.2
1	L	74	ASP	2.2
1	C	43	VAL	2.2
1	L	174	ILE	2.2
1	K	107	ARG	2.2
1	C	21	ALA	2.1
1	D	172	GLU	2.1
1	L	89	GLN	2.1
1	F	48	LEU	2.1
1	I	1	MET	2.1
1	K	135	LEU	2.1
1	C	111	ASP	2.1
1	C	48	LEU	2.1
1	I	45	LEU	2.1
1	L	268	ASP	2.1
1	C	51	GLU	2.1
1	J	250	LEU	2.1
1	C	91	TYR	2.1
1	A	26	VAL	2.1
1	K	40	LEU	2.1
1	L	8	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	1	MET	2.0
1	A	52	GLY	2.0
1	C	32	GLY	2.0
1	K	176	GLY	2.0
1	B	49	CYS	2.0
1	H	12	ARG	2.0
1	G	51	GLU	2.0
1	K	47	GLU	2.0
1	K	55	ASP	2.0
1	L	34	GLU	2.0
1	L	67	ASP	2.0
1	L	79	ALA	2.0
1	B	42	GLY	2.0
1	H	98	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
4	SO4	A	1004	5/5	0.38	0.13	148,156,164,164	0
4	SO4	H	301	5/5	0.51	0.10	155,157,164,169	0
4	SO4	H	304	5/5	0.51	0.12	153,153,169,169	0
4	SO4	K	1004	5/5	0.51	0.13	182,184,186,191	0
4	SO4	D	304	5/5	0.58	0.49	49,49,49,49	0
4	SO4	D	303	5/5	0.60	0.10	146,149,159,161	0
4	SO4	I	304	5/5	0.63	0.10	118,126,131,135	0
4	SO4	L	301	5/5	0.64	0.13	126,130,146,155	0
4	SO4	C	1003	5/5	0.66	0.13	117,129,132,135	0

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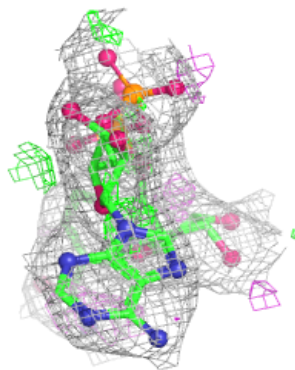
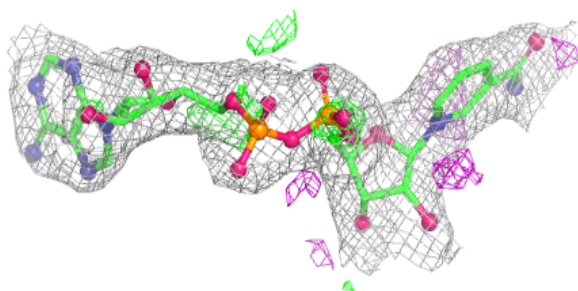
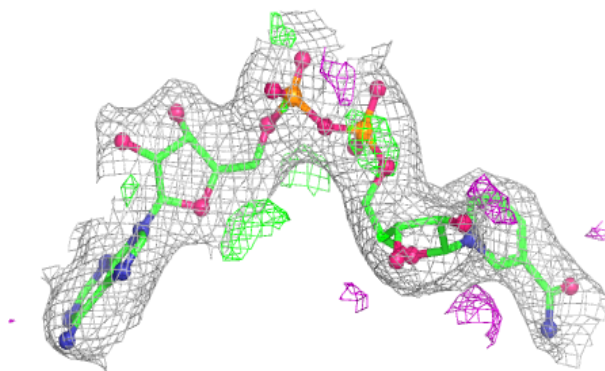
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	K	1003	5/5	0.66	0.12	131,133,141,148	0
4	SO4	E	1004	5/5	0.68	0.09	132,135,141,141	0
4	SO4	D	302	5/5	0.69	0.16	138,140,150,155	0
4	SO4	J	1003	5/5	0.70	0.12	120,121,131,137	0
4	SO4	A	1003	5/5	0.72	0.13	113,134,136,144	0
4	SO4	B	1003	5/5	0.75	0.12	97,106,125,135	0
4	SO4	H	305	5/5	0.77	0.09	144,147,152,159	0
4	SO4	I	303	5/5	0.79	0.10	101,106,111,112	0
4	SO4	E	1003	5/5	0.80	0.11	102,108,115,130	0
4	SO4	D	301	5/5	0.81	0.10	100,103,109,110	0
4	SO4	H	303	5/5	0.81	0.15	130,132,150,155	0
4	SO4	G	1003	5/5	0.82	0.10	115,115,119,135	0
4	SO4	F	1003	5/5	0.83	0.11	100,106,111,117	0
4	SO4	H	302	5/5	0.84	0.10	92,96,111,114	0
3	PDC	J	1002	12/12	0.87	0.16	66,70,73,77	0
3	PDC	A	1002	12/12	0.92	0.12	57,61,65,69	0
3	PDC	K	1002	12/12	0.93	0.12	54,59,64,68	0
2	NAD	B	1001	44/44	0.93	0.11	60,70,85,90	0
3	PDC	B	1002	12/12	0.93	0.14	57,63,70,70	0
2	NAD	K	1001	44/44	0.93	0.11	64,73,92,95	0
2	NAD	C	1001	44/44	0.94	0.10	65,76,102,107	0
2	NAD	J	1001	44/44	0.94	0.10	61,71,82,91	0
3	PDC	F	1002	12/12	0.95	0.15	49,54,60,63	0
3	PDC	G	1002	12/12	0.95	0.10	43,49,59,60	0
3	PDC	I	301	12/12	0.95	0.11	54,57,62,65	0
2	NAD	F	1001	44/44	0.95	0.11	54,65,73,79	0
2	NAD	G	1001	44/44	0.95	0.11	52,62,74,75	0
2	NAD	A	1001	44/44	0.95	0.11	56,68,77,79	0
3	PDC	C	1002	12/12	0.95	0.12	66,69,76,79	0
2	NAD	E	1001	44/44	0.96	0.11	49,55,63,66	0
3	PDC	E	1002	12/12	0.96	0.12	48,49,54,59	0
2	NAD	I	302	44/44	0.96	0.10	54,59,64,68	0

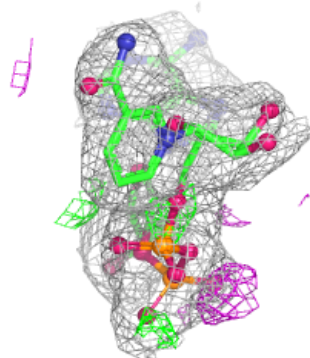
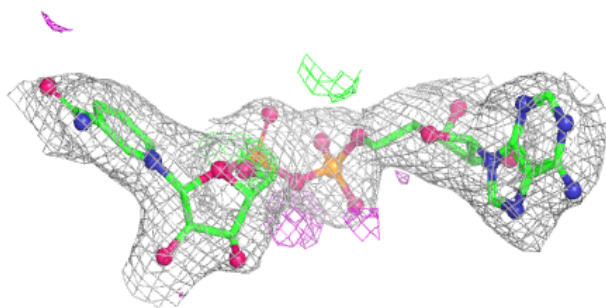
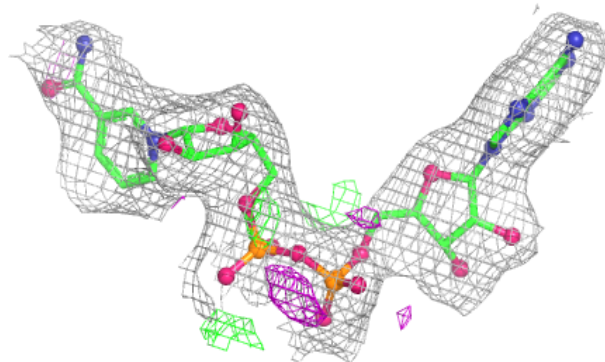
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 1001:

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

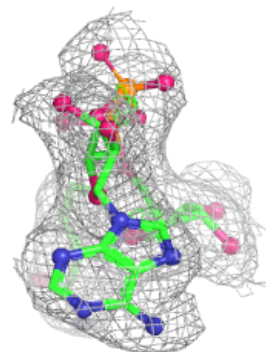
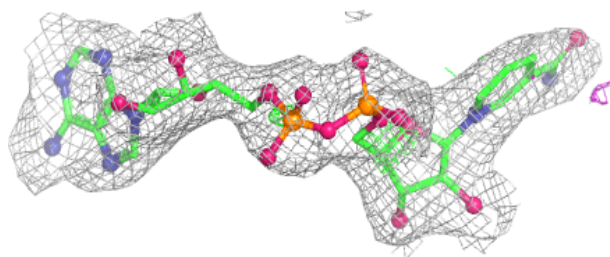
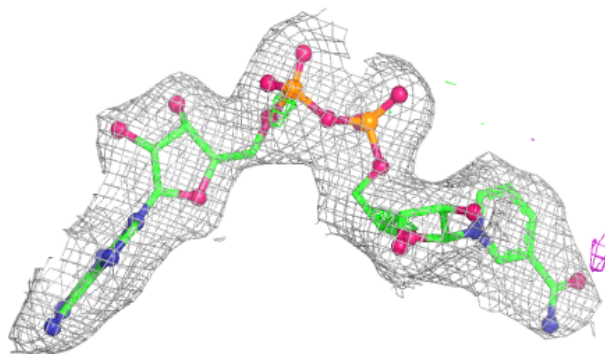
**Electron density around NAD K 1001:**

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

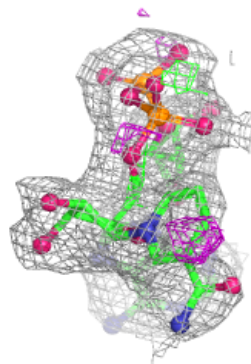
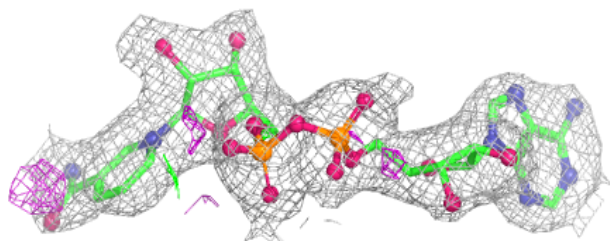
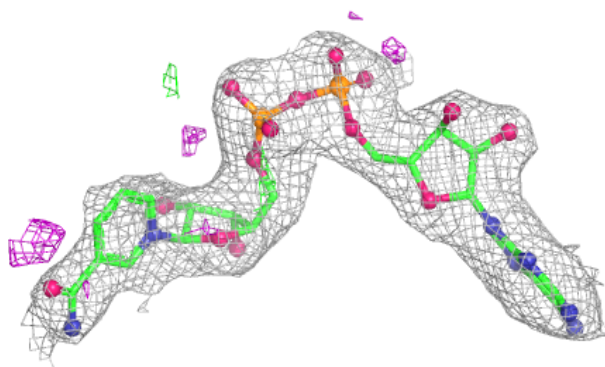


Electron density around NAD C 1001:

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

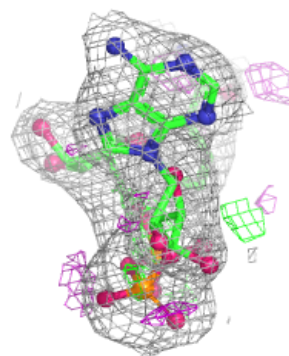
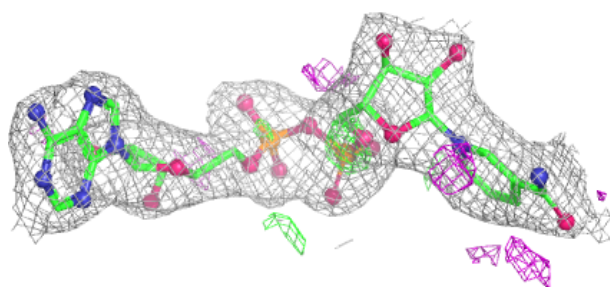
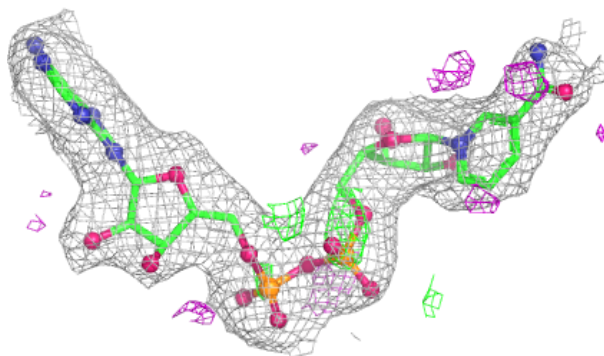
**Electron density around NAD J 1001:**

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

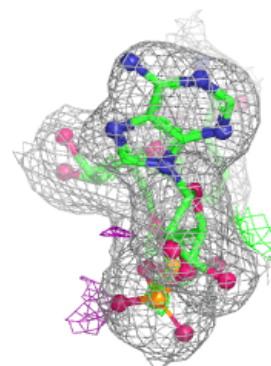
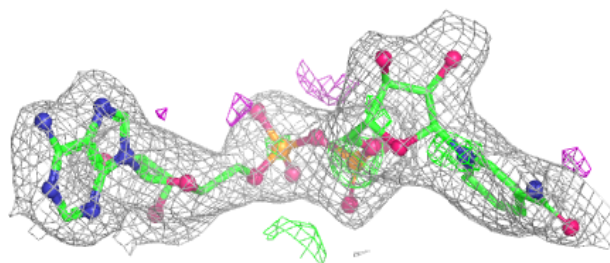
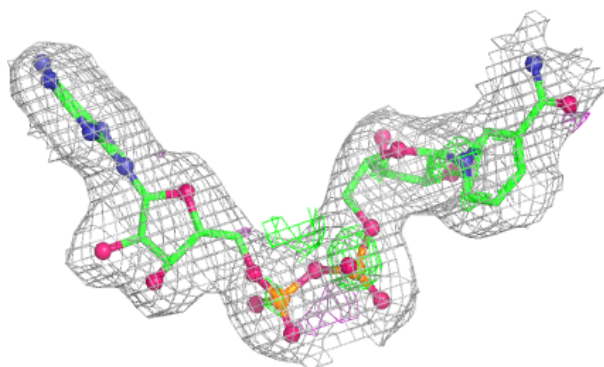


Electron density around NAD F 1001:

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

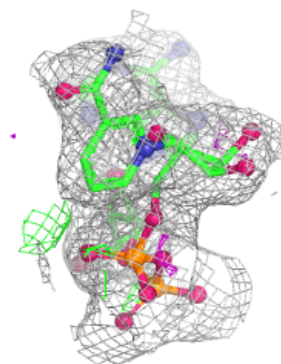
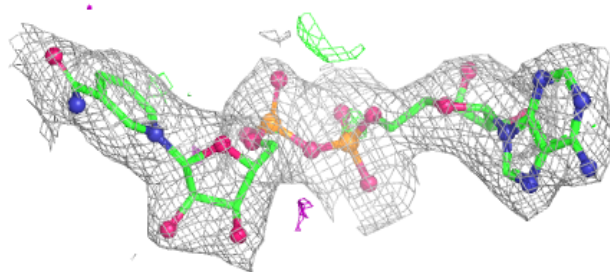
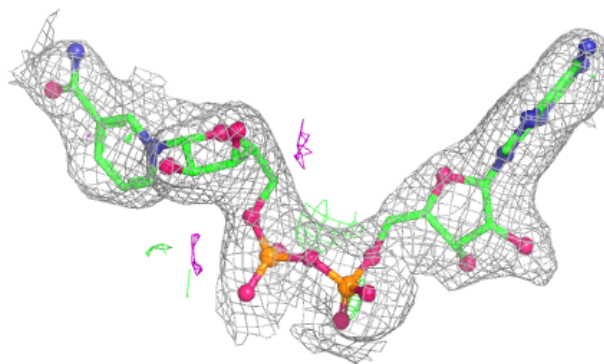
**Electron density around NAD G 1001:**

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

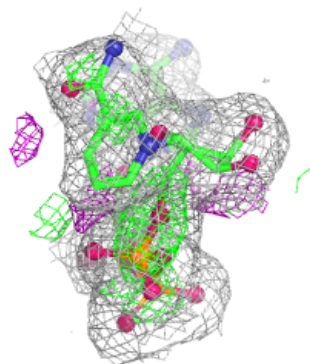
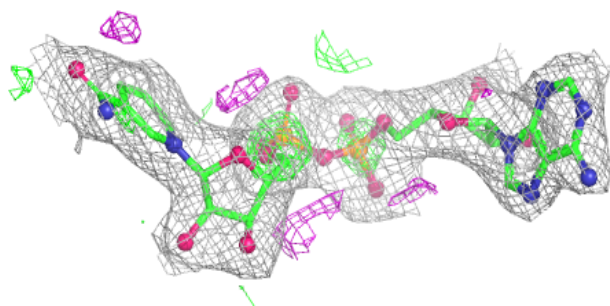
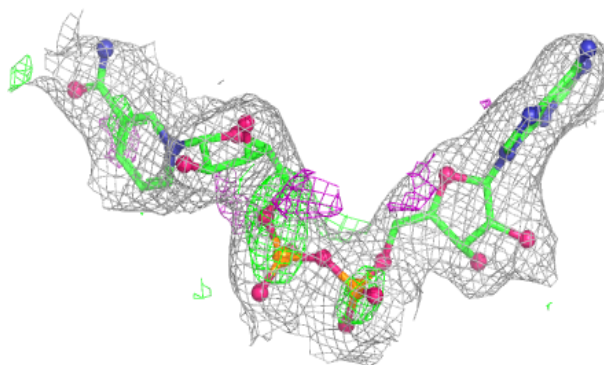


Electron density around NAD A 1001:

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and green (positive)

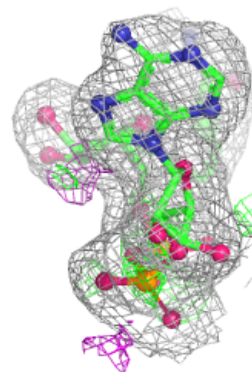
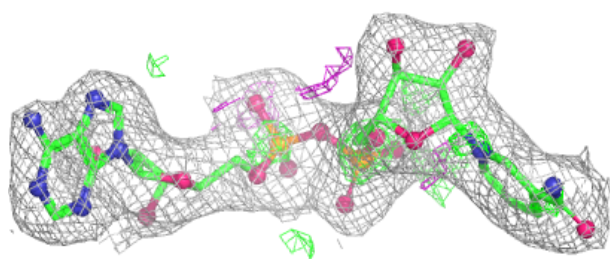
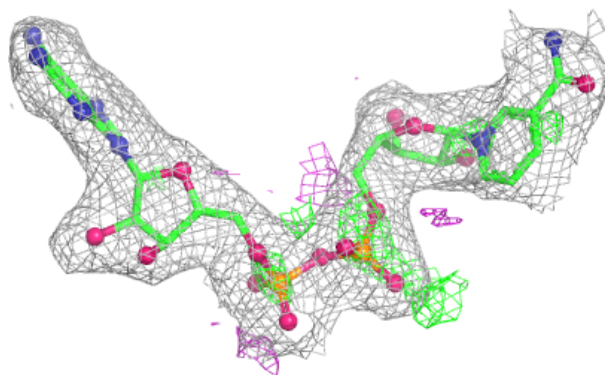
**Electron density around NAD E 1001:**

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



Electron density around NAD I 302:

$2mF_o-DF_c$ (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.