



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 02:40 AM UTC

PDB ID : 6TOE / pdb_00006toe
Title : Imine Reductase from Myxococcus stipitatus V8 variant in complex with NAD+
Authors : Sharma, M.; Nestl, B.; Grogan, G.
Deposited on : 2019-12-11
Resolution : 2.78 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)
Xtrriage (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

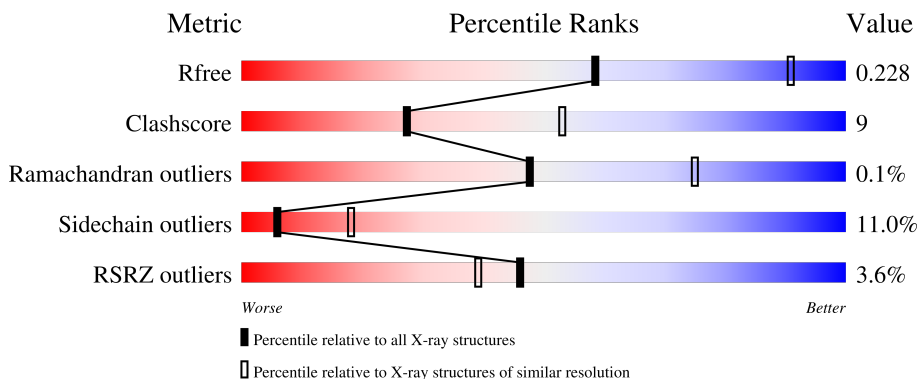
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	311	
1	B	311	
1	C	311	
1	D	311	
1	E	311	

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Mol	Chain	Length	Quality of chain
1	F	311	 <p>%</p> <p>71% 18% 5% 6%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13254 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 Coenzyme F420-dependent NADP oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	Total 2174	C 1373	N 380	O 414	S 7	0	0	0
1	B	293	Total 2182	C 1378	N 384	O 413	S 7	0	0	0
1	C	292	Total 2129	C 1344	N 371	O 408	S 6	0	0	0
1	D	286	Total 2019	C 1279	N 348	O 385	S 7	0	0	0
1	E	289	Total 2137	C 1352	N 371	O 407	S 7	0	0	0
1	F	291	Total 2203	C 1394	N 388	O 414	S 7	0	3	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP L7U9F5
A	-18	GLY	-	expression tag	UNP L7U9F5
A	-17	SER	-	expression tag	UNP L7U9F5
A	-16	SER	-	expression tag	UNP L7U9F5
A	-15	HIS	-	expression tag	UNP L7U9F5
A	-14	HIS	-	expression tag	UNP L7U9F5
A	-13	HIS	-	expression tag	UNP L7U9F5
A	-12	HIS	-	expression tag	UNP L7U9F5
A	-11	HIS	-	expression tag	UNP L7U9F5
A	-10	HIS	-	expression tag	UNP L7U9F5
A	-9	SER	-	expression tag	UNP L7U9F5
A	-8	SER	-	expression tag	UNP L7U9F5
A	-7	GLY	-	expression tag	UNP L7U9F5
A	-6	LEU	-	expression tag	UNP L7U9F5
A	-5	VAL	-	expression tag	UNP L7U9F5
A	-4	PRO	-	expression tag	UNP L7U9F5
A	-3	ARG	-	expression tag	UNP L7U9F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP L7U9F5
A	-1	SER	-	expression tag	UNP L7U9F5
A	0	HIS	-	expression tag	UNP L7U9F5
A	32	GLU	ASN	conflict	UNP L7U9F5
A	33	TYR	ARG	conflict	UNP L7U9F5
A	34	GLU	THR	conflict	UNP L7U9F5
A	37	ARG	LYS	conflict	UNP L7U9F5
A	67	ILE	LEU	conflict	UNP L7U9F5
A	71	VAL	THR	conflict	UNP L7U9F5
B	-19	MET	-	initiating methionine	UNP L7U9F5
B	-18	GLY	-	expression tag	UNP L7U9F5
B	-17	SER	-	expression tag	UNP L7U9F5
B	-16	SER	-	expression tag	UNP L7U9F5
B	-15	HIS	-	expression tag	UNP L7U9F5
B	-14	HIS	-	expression tag	UNP L7U9F5
B	-13	HIS	-	expression tag	UNP L7U9F5
B	-12	HIS	-	expression tag	UNP L7U9F5
B	-11	HIS	-	expression tag	UNP L7U9F5
B	-10	HIS	-	expression tag	UNP L7U9F5
B	-9	SER	-	expression tag	UNP L7U9F5
B	-8	SER	-	expression tag	UNP L7U9F5
B	-7	GLY	-	expression tag	UNP L7U9F5
B	-6	LEU	-	expression tag	UNP L7U9F5
B	-5	VAL	-	expression tag	UNP L7U9F5
B	-4	PRO	-	expression tag	UNP L7U9F5
B	-3	ARG	-	expression tag	UNP L7U9F5
B	-2	GLY	-	expression tag	UNP L7U9F5
B	-1	SER	-	expression tag	UNP L7U9F5
B	0	HIS	-	expression tag	UNP L7U9F5
B	32	GLU	ASN	conflict	UNP L7U9F5
B	33	TYR	ARG	conflict	UNP L7U9F5
B	34	GLU	THR	conflict	UNP L7U9F5
B	37	ARG	LYS	conflict	UNP L7U9F5
B	67	ILE	LEU	conflict	UNP L7U9F5
B	71	VAL	THR	conflict	UNP L7U9F5
C	-19	MET	-	initiating methionine	UNP L7U9F5
C	-18	GLY	-	expression tag	UNP L7U9F5
C	-17	SER	-	expression tag	UNP L7U9F5
C	-16	SER	-	expression tag	UNP L7U9F5
C	-15	HIS	-	expression tag	UNP L7U9F5
C	-14	HIS	-	expression tag	UNP L7U9F5
C	-13	HIS	-	expression tag	UNP L7U9F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP L7U9F5
C	-11	HIS	-	expression tag	UNP L7U9F5
C	-10	HIS	-	expression tag	UNP L7U9F5
C	-9	SER	-	expression tag	UNP L7U9F5
C	-8	SER	-	expression tag	UNP L7U9F5
C	-7	GLY	-	expression tag	UNP L7U9F5
C	-6	LEU	-	expression tag	UNP L7U9F5
C	-5	VAL	-	expression tag	UNP L7U9F5
C	-4	PRO	-	expression tag	UNP L7U9F5
C	-3	ARG	-	expression tag	UNP L7U9F5
C	-2	GLY	-	expression tag	UNP L7U9F5
C	-1	SER	-	expression tag	UNP L7U9F5
C	0	HIS	-	expression tag	UNP L7U9F5
C	32	GLU	ASN	conflict	UNP L7U9F5
C	33	TYR	ARG	conflict	UNP L7U9F5
C	34	GLU	THR	conflict	UNP L7U9F5
C	37	ARG	LYS	conflict	UNP L7U9F5
C	67	ILE	LEU	conflict	UNP L7U9F5
C	71	VAL	THR	conflict	UNP L7U9F5
D	-19	MET	-	initiating methionine	UNP L7U9F5
D	-18	GLY	-	expression tag	UNP L7U9F5
D	-17	SER	-	expression tag	UNP L7U9F5
D	-16	SER	-	expression tag	UNP L7U9F5
D	-15	HIS	-	expression tag	UNP L7U9F5
D	-14	HIS	-	expression tag	UNP L7U9F5
D	-13	HIS	-	expression tag	UNP L7U9F5
D	-12	HIS	-	expression tag	UNP L7U9F5
D	-11	HIS	-	expression tag	UNP L7U9F5
D	-10	HIS	-	expression tag	UNP L7U9F5
D	-9	SER	-	expression tag	UNP L7U9F5
D	-8	SER	-	expression tag	UNP L7U9F5
D	-7	GLY	-	expression tag	UNP L7U9F5
D	-6	LEU	-	expression tag	UNP L7U9F5
D	-5	VAL	-	expression tag	UNP L7U9F5
D	-4	PRO	-	expression tag	UNP L7U9F5
D	-3	ARG	-	expression tag	UNP L7U9F5
D	-2	GLY	-	expression tag	UNP L7U9F5
D	-1	SER	-	expression tag	UNP L7U9F5
D	0	HIS	-	expression tag	UNP L7U9F5
D	32	GLU	ASN	conflict	UNP L7U9F5
D	33	TYR	ARG	conflict	UNP L7U9F5
D	34	GLU	THR	conflict	UNP L7U9F5

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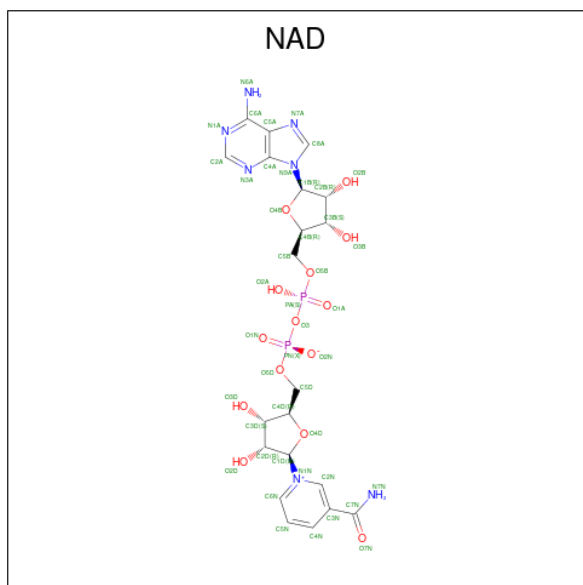
Chain	Residue	Modelled	Actual	Comment	Reference
D	37	ARG	LYS	conflict	UNP L7U9F5
D	67	ILE	LEU	conflict	UNP L7U9F5
D	71	VAL	THR	conflict	UNP L7U9F5
E	-19	MET	-	initiating methionine	UNP L7U9F5
E	-18	GLY	-	expression tag	UNP L7U9F5
E	-17	SER	-	expression tag	UNP L7U9F5
E	-16	SER	-	expression tag	UNP L7U9F5
E	-15	HIS	-	expression tag	UNP L7U9F5
E	-14	HIS	-	expression tag	UNP L7U9F5
E	-13	HIS	-	expression tag	UNP L7U9F5
E	-12	HIS	-	expression tag	UNP L7U9F5
E	-11	HIS	-	expression tag	UNP L7U9F5
E	-10	HIS	-	expression tag	UNP L7U9F5
E	-9	SER	-	expression tag	UNP L7U9F5
E	-8	SER	-	expression tag	UNP L7U9F5
E	-7	GLY	-	expression tag	UNP L7U9F5
E	-6	LEU	-	expression tag	UNP L7U9F5
E	-5	VAL	-	expression tag	UNP L7U9F5
E	-4	PRO	-	expression tag	UNP L7U9F5
E	-3	ARG	-	expression tag	UNP L7U9F5
E	-2	GLY	-	expression tag	UNP L7U9F5
E	-1	SER	-	expression tag	UNP L7U9F5
E	0	HIS	-	expression tag	UNP L7U9F5
E	32	GLU	ASN	conflict	UNP L7U9F5
E	33	TYR	ARG	conflict	UNP L7U9F5
E	34	GLU	THR	conflict	UNP L7U9F5
E	37	ARG	LYS	conflict	UNP L7U9F5
E	67	ILE	LEU	conflict	UNP L7U9F5
E	71	VAL	THR	conflict	UNP L7U9F5
F	-19	MET	-	initiating methionine	UNP L7U9F5
F	-18	GLY	-	expression tag	UNP L7U9F5
F	-17	SER	-	expression tag	UNP L7U9F5
F	-16	SER	-	expression tag	UNP L7U9F5
F	-15	HIS	-	expression tag	UNP L7U9F5
F	-14	HIS	-	expression tag	UNP L7U9F5
F	-13	HIS	-	expression tag	UNP L7U9F5
F	-12	HIS	-	expression tag	UNP L7U9F5
F	-11	HIS	-	expression tag	UNP L7U9F5
F	-10	HIS	-	expression tag	UNP L7U9F5
F	-9	SER	-	expression tag	UNP L7U9F5
F	-8	SER	-	expression tag	UNP L7U9F5
F	-7	GLY	-	expression tag	UNP L7U9F5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	LEU	-	expression tag	UNP L7U9F5
F	-5	VAL	-	expression tag	UNP L7U9F5
F	-4	PRO	-	expression tag	UNP L7U9F5
F	-3	ARG	-	expression tag	UNP L7U9F5
F	-2	GLY	-	expression tag	UNP L7U9F5
F	-1	SER	-	expression tag	UNP L7U9F5
F	0	HIS	-	expression tag	UNP L7U9F5
F	32	GLU	ASN	conflict	UNP L7U9F5
F	33	TYR	ARG	conflict	UNP L7U9F5
F	34	GLU	THR	conflict	UNP L7U9F5
F	37	ARG	LYS	conflict	UNP L7U9F5
F	67	ILE	LEU	conflict	UNP L7U9F5
F	71	VAL	THR	conflict	UNP L7U9F5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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	F	1	Total	C	N	O	P	0	0
			26	11	2	11	2		

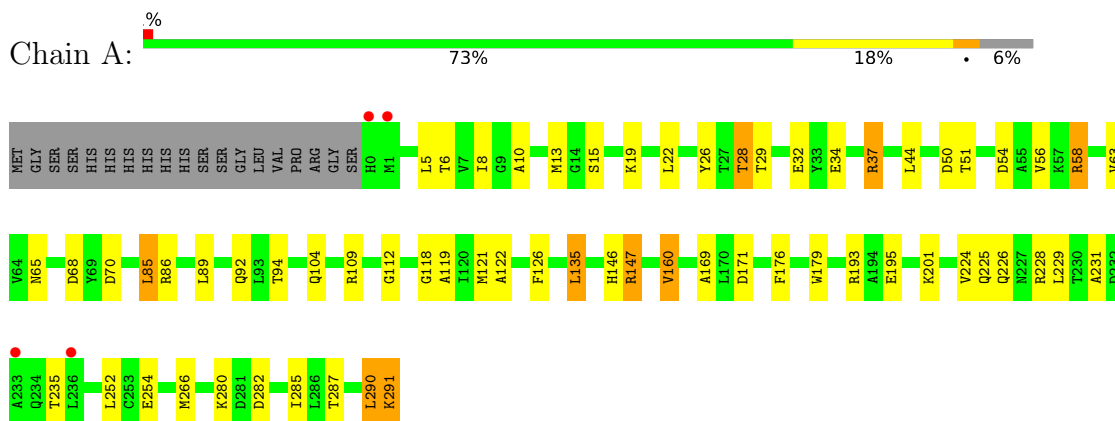
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	34	Total O 34 34	0	0
3	C	36	Total O 36 36	0	0
3	D	33	Total O 33 33	0	0
3	E	52	Total O 52 52	0	0
3	F	59	Total O 59 59	0	0

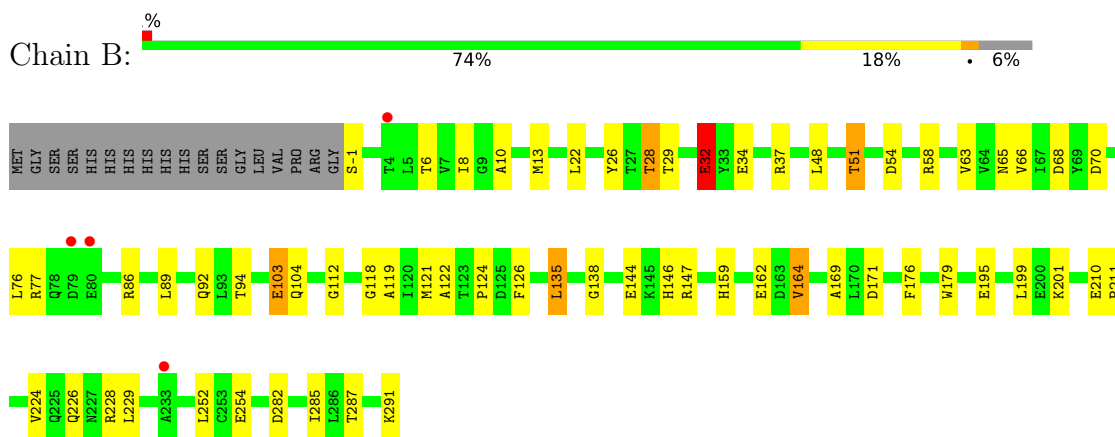
3 Residue-property plots [i](#)

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.

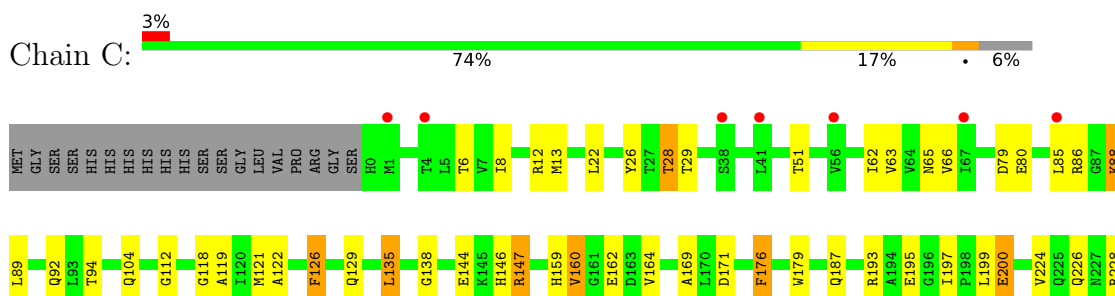
- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase

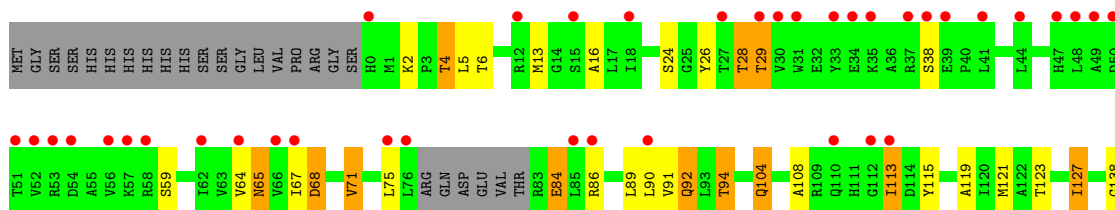
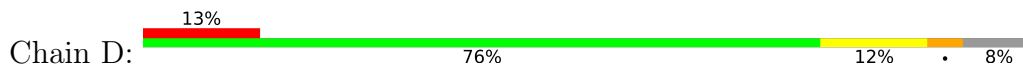


- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase

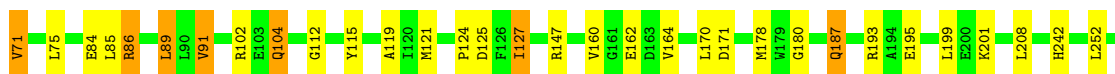
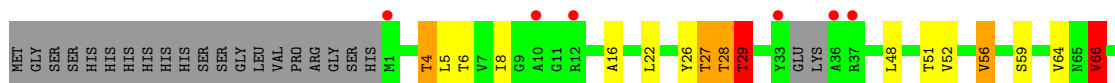
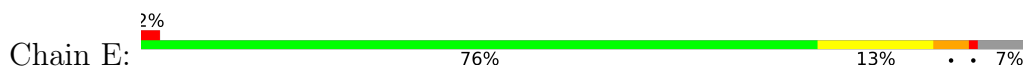




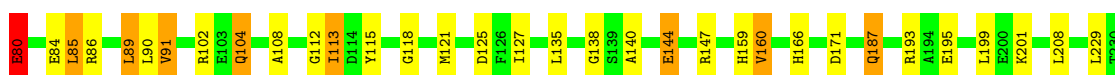
- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	199.41 Å 199.41 Å 97.94 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.94 – 2.78 47.94 – 2.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.94-2.78) 100.0 (47.94-2.78)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.77 Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.228 0.195 , 0.228	Depositor DCC
R_{free} test set	2844 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13254	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	1.04	0/2209	1.49	4/3004 (0.1%)
1	B	1.06	0/2218	1.49	1/3016 (0.0%)
1	C	1.05	0/2164	1.51	3/2949 (0.1%)
1	D	1.05	0/2049	1.50	2/2794 (0.1%)
1	E	1.08	0/2170	1.52	5/2951 (0.2%)
1	F	1.05	0/2247	1.51	4/3050 (0.1%)
All	All	1.05	0/13057	1.50	19/17764 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	29	THR	CB-CA-C	7.22	121.70	109.50
1	F	4	THR	CB-CA-C	6.84	120.98	109.48
1	E	66	VAL	N-CA-CB	-6.40	104.34	112.60
1	F	27	THR	CB-CA-C	6.10	119.95	110.67
1	C	160	VAL	N-CA-CB	-5.85	105.78	112.21
1	E	27	THR	CB-CA-C	5.70	119.33	110.67
1	A	235	THR	CA-C-N	5.34	127.70	120.44
1	A	235	THR	C-N-CA	5.34	127.70	120.44
1	D	4	THR	CB-CA-C	5.32	118.41	109.48
1	B	32	GLU	CB-CG-CD	5.30	121.61	112.60
1	E	86	ARG	CB-CG-CD	5.28	123.44	111.30
1	F	80	GLU	CB-CA-C	5.27	119.54	110.79
1	F	160	VAL	N-CA-CB	-5.20	106.14	112.33
1	E	4	THR	CB-CA-C	5.18	118.08	109.53
1	A	160	VAL	N-CA-CB	-5.16	106.19	112.33
1	D	68	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	291	LYS	CB-CA-C	-5.02	100.56	110.10
1	C	126	PHE	CA-CB-CG	5.01	118.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	PHE	CA-CB-CG	-5.00	108.80	113.80

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	2174	0	2146	45	0
1	B	2182	0	2151	44	0
1	C	2129	0	2049	45	0
1	D	2019	0	1923	45	0
1	E	2137	0	2111	38	0
1	F	2203	0	2202	43	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	0	0
2	F	26	0	14	2	0
3	A	38	0	0	0	0
3	B	34	0	0	1	0
3	C	36	0	0	1	0
3	D	33	0	0	0	0
3	E	52	0	0	1	0
3	F	59	0	0	0	0
All	All	13254	0	12674	233	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 9.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ALA:O	1:D:127:ILE:HD11	1.68	0.94
1:F:90:LEU:HB2	1:F:113:ILE:HD11	1.53	0.91
1:D:16:ALA:C	1:D:127:ILE:HD11	1.97	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:GLN:HE21	1:D:92:GLN:HA	1.38	0.85
1:F:4:THR:HG23	1:F:59:SER:HA	1.66	0.78
1:C:119:ALA:HB1	1:C:121:MET:CE	2.17	0.75
1:D:92:GLN:HA	1:D:92:GLN:NE2	2.01	0.75
1:D:4:THR:HG23	1:D:59:SER:HA	1.68	0.75
1:F:56:VAL:CG2	1:F:84:GLU:HB3	2.15	0.75
1:F:140:ALA:O	1:F:144:GLU:HG2	1.88	0.74
1:E:127:ILE:O	1:E:127:ILE:HD12	1.88	0.73
1:D:16:ALA:O	1:D:127:ILE:CD1	2.36	0.73
1:B:119:ALA:HB1	1:B:121:MET:CE	2.19	0.72
1:B:169:ALA:CB	1:F:195:GLU:HG2	2.19	0.72
1:A:54:ASP:O	1:A:58:ARG:HG3	1.88	0.71
1:F:52:VAL:O	1:F:56:VAL:HG13	1.89	0.71
1:A:119:ALA:HB1	1:A:121:MET:CE	2.20	0.71
1:B:68:ASP:OD1	1:B:70:ASP:HB2	1.91	0.71
1:B:179:TRP:HE1	1:F:242:HIS:HD2	1.37	0.71
1:D:16:ALA:C	1:D:127:ILE:CD1	2.64	0.70
1:C:92:GLN:HE21	1:C:94:THR:H	1.39	0.69
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.59	0.68
1:A:92:GLN:HE21	1:A:94:THR:H	1.41	0.68
1:E:16:ALA:HB1	1:E:127:ILE:CG1	2.23	0.68
1:E:52:VAL:O	1:E:56:VAL:HG13	1.94	0.67
1:D:65:ASN:CG	1:D:65:ASN:O	2.37	0.67
1:F:68:ASP:OD1	1:F:70:ASP:HB2	1.94	0.67
1:B:92:GLN:HE21	1:B:94:THR:H	1.40	0.66
1:D:147:ARG:HH11	1:D:147:ARG:HG2	1.60	0.66
1:D:92:GLN:HE21	1:D:92:GLN:CA	2.09	0.66
1:B:119:ALA:HB1	1:B:121:MET:HE1	1.79	0.64
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.63	0.63
1:C:119:ALA:HB1	1:C:121:MET:HE1	1.80	0.63
1:B:77:ARG:NH2	1:B:103:GLU:OE2	2.32	0.62
1:E:4:THR:HG23	1:E:59:SER:HA	1.81	0.62
1:B:169:ALA:HB1	1:F:195:GLU:HG2	1.81	0.61
1:D:16:ALA:HB1	1:D:127:ILE:HG12	1.81	0.61
1:A:119:ALA:HB1	1:A:121:MET:HE1	1.81	0.61
1:A:56:VAL:HG11	1:A:85:LEU:HD13	1.82	0.61
1:D:90:LEU:HB2	1:D:113:ILE:HD11	1.81	0.61
1:C:200:GLU:CD	1:C:200:GLU:H	2.09	0.60
1:C:179:TRP:HE1	1:D:242:HIS:HD2	1.49	0.60
1:E:56:VAL:CG2	1:E:84:GLU:HB3	2.32	0.59
1:C:252:LEU:HD23	1:C:252:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:MET:HB3	1:B:65:ASN:HD21	1.68	0.59
1:A:68:ASP:HB3	1:A:70:ASP:OD1	2.03	0.59
1:A:252:LEU:C	1:A:252:LEU:HD23	2.28	0.59
1:C:226:GLN:OE1	1:C:228:ARG:NH2	2.35	0.58
1:D:16:ALA:HB1	1:D:127:ILE:CG1	2.33	0.58
1:A:13:MET:HB3	1:A:65:ASN:HD21	1.68	0.58
1:A:56:VAL:CG1	1:A:85:LEU:HD13	2.34	0.57
1:B:252:LEU:C	1:B:252:LEU:HD23	2.28	0.57
1:E:89:LEU:HD13	1:E:91:VAL:HG12	1.86	0.57
1:F:53:ARG:HG3	1:F:80:GLU:HG3	1.86	0.57
1:E:147:ARG:HG2	1:E:147:ARG:HH11	1.69	0.57
1:A:224:VAL:HG21	1:A:287:THR:HG21	1.86	0.57
1:A:22:LEU:HD23	1:A:28:THR:HG23	1.87	0.57
1:C:169:ALA:HB2	1:D:195:GLU:HG2	1.86	0.57
1:A:226:GLN:OE1	1:A:228:ARG:NH2	2.36	0.57
1:A:179:TRP:HE1	1:E:242:HIS:HD2	1.51	0.57
1:D:147:ARG:HG2	1:D:147:ARG:NH1	2.20	0.57
1:A:121:MET:HE1	1:A:171:ASP:OD1	2.05	0.56
1:D:138:GLY:O	1:D:159:HIS:HE1	1.88	0.56
1:B:124:PRO:HD3	2:B:301:NAD:N7N	2.20	0.56
1:C:26:TYR:O	1:C:28:THR:HG22	2.06	0.56
1:C:176:PHE:CE1	1:D:187:GLN:HG3	2.41	0.56
1:C:13:MET:HB3	1:C:65:ASN:HD21	1.69	0.56
1:A:26:TYR:O	1:A:28:THR:HG22	2.05	0.56
1:D:26:TYR:O	1:D:28:THR:HG22	2.06	0.56
1:B:147:ARG:HH11	1:B:147:ARG:HG2	1.70	0.56
1:C:252:LEU:HD23	1:C:252:LEU:C	2.31	0.55
1:B:10:ALA:HB3	1:B:32:GLU:HG2	1.88	0.55
1:F:56:VAL:HG23	1:F:84:GLU:HB3	1.88	0.55
1:A:252:LEU:HD23	1:A:252:LEU:O	2.07	0.55
1:B:226:GLN:OE1	1:B:228:ARG:NH2	2.40	0.55
1:B:121:MET:HE1	1:B:171:ASP:OD1	2.07	0.55
1:C:138:GLY:O	1:C:159:HIS:HE1	1.90	0.55
1:E:195:GLU:OE1	1:E:252:LEU:HD11	2.06	0.55
1:B:138:GLY:O	1:B:159:HIS:HE1	1.89	0.54
1:D:2:LYS:NZ	1:D:24:SER:O	2.40	0.54
1:B:169:ALA:HB2	1:F:195:GLU:HG2	1.88	0.54
1:C:169:ALA:CB	1:D:195:GLU:HG2	2.37	0.54
1:D:65:ASN:O	1:D:65:ASN:OD1	2.26	0.54
1:F:26:TYR:O	1:F:28:THR:HG22	2.08	0.54
1:D:68:ASP:HB2	1:D:71:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:GLY:O	1:F:159:HIS:HE1	1.90	0.54
1:C:121:MET:HE1	1:C:171:ASP:OD1	2.08	0.53
1:E:16:ALA:HB1	1:E:127:ILE:HD11	1.90	0.53
1:A:15:SER:O	1:A:19:LYS:HG3	2.09	0.53
1:B:26:TYR:O	1:B:28:THR:HG22	2.08	0.53
1:F:85:LEU:HG	1:F:113:ILE:HD12	1.89	0.53
1:B:195:GLU:HG3	1:F:102:ARG:HH22	1.74	0.52
1:A:10:ALA:HB3	1:A:32:GLU:HG2	1.91	0.52
1:C:197:ILE:HD12	1:C:197:ILE:N	2.24	0.52
1:E:26:TYR:O	1:E:28:THR:HG22	2.10	0.52
1:E:22:LEU:HD23	1:E:28:THR:HG23	1.91	0.52
1:C:119:ALA:CB	1:C:121:MET:CE	2.88	0.52
1:A:176:PHE:CE1	1:E:187:GLN:HG3	2.44	0.52
1:F:22:LEU:HD23	1:F:28:THR:HG23	1.91	0.52
1:F:85:LEU:HG	1:F:113:ILE:CD1	2.39	0.52
1:A:224:VAL:CG2	1:A:287:THR:HG21	2.40	0.51
1:F:195:GLU:OE1	1:F:252:LEU:HD11	2.09	0.51
1:A:290:LEU:O	1:A:291:LYS:OXT	2.27	0.51
1:F:65:ASN:OD1	2:F:301:NAD:H51N	2.10	0.51
1:B:179:TRP:HE1	1:F:242:HIS:CD2	2.23	0.51
1:D:121:MET:HE1	1:D:171:ASP:CB	2.40	0.51
1:B:119:ALA:CB	1:B:121:MET:CE	2.89	0.51
1:C:147:ARG:HH11	1:C:147:ARG:CG	2.24	0.51
1:E:124:PRO:O	1:E:127:ILE:HG13	2.11	0.50
1:B:176:PHE:CD1	1:F:187:GLN:HB2	2.46	0.50
1:B:176:PHE:CE1	1:F:187:GLN:HG3	2.46	0.50
1:E:104:GLN:HG2	1:E:115:TYR:CE1	2.46	0.50
1:E:22:LEU:CD2	1:E:28:THR:HG23	2.42	0.49
1:A:176:PHE:CD1	1:E:187:GLN:HB2	2.47	0.49
1:B:122:ALA:HB1	1:B:126:PHE:HB2	1.95	0.49
1:F:89:LEU:HD13	1:F:91:VAL:HG12	1.93	0.49
1:A:119:ALA:CB	1:A:121:MET:CE	2.91	0.48
1:E:16:ALA:HB1	1:E:127:ILE:HG12	1.94	0.48
1:E:121:MET:HE1	1:E:171:ASP:OD1	2.13	0.48
1:F:22:LEU:CD2	1:F:28:THR:HG23	2.43	0.48
1:D:13:MET:HE1	1:D:127:ILE:HG21	1.95	0.48
1:E:119:ALA:HB1	1:E:121:MET:CE	2.44	0.48
1:E:127:ILE:O	1:E:127:ILE:CD1	2.58	0.48
1:B:22:LEU:HD23	1:B:28:THR:HG23	1.97	0.47
1:B:124:PRO:HD3	2:B:301:NAD:H72N	1.79	0.47
1:C:176:PHE:CD1	1:D:187:GLN:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ALA:HB1	1:E:127:ILE:CD1	2.44	0.47
1:C:89:LEU:HD22	1:C:146:HIS:CD2	2.50	0.47
1:D:121:MET:HE1	1:D:171:ASP:CG	2.38	0.47
1:B:22:LEU:CD2	1:B:28:THR:HG23	2.45	0.47
1:B:195:GLU:O	1:F:166:HIS:NE2	2.47	0.47
1:F:13:MET:HE1	1:F:127:ILE:HD13	1.96	0.47
1:C:119:ALA:CB	1:C:121:MET:HE3	2.45	0.47
1:D:84:GLU:N	1:D:84:GLU:CD	2.73	0.47
1:C:236:LEU:HB3	1:D:123:THR:HG21	1.97	0.46
1:B:252:LEU:HD23	1:B:252:LEU:O	2.14	0.46
1:C:119:ALA:HB1	1:C:121:MET:HE3	1.96	0.46
1:C:122:ALA:HB1	1:C:126:PHE:HB2	1.97	0.46
1:A:290:LEU:O	1:A:291:LYS:C	2.59	0.46
1:C:179:TRP:HE1	1:D:242:HIS:CD2	2.32	0.46
1:A:225:GLN:CB	3:E:342:HOH:O	2.63	0.46
1:C:282:ASP:O	1:C:285:ILE:HG22	2.16	0.46
1:E:119:ALA:HB1	1:E:121:MET:HE1	1.97	0.46
1:B:89:LEU:HD22	1:B:146:HIS:CD2	2.51	0.46
1:C:22:LEU:CD2	1:C:28:THR:HG23	2.46	0.46
1:C:22:LEU:HD23	1:C:28:THR:HG23	1.98	0.46
1:A:147:ARG:HH11	1:A:147:ARG:CG	2.28	0.45
1:A:122:ALA:HB1	1:A:126:PHE:HB2	1.99	0.45
1:B:282:ASP:O	1:B:285:ILE:HG22	2.17	0.45
1:D:119:ALA:HB1	1:D:121:MET:CE	2.47	0.45
1:F:12[A]:ARG:HG3	2:F:301:NAD:O2N	2.17	0.45
1:C:129:GLN:OE1	1:F:86[A]:ARG:NH1	2.45	0.45
1:D:16:ALA:HB1	1:D:127:ILE:CD1	2.47	0.45
1:B:32:GLU:OE1	1:B:37:ARG:HD3	2.17	0.45
1:E:66:VAL:HG13	1:E:71:VAL:HG22	1.99	0.45
1:F:1:MET:O	1:F:1:MET:HG3	2.15	0.45
1:D:16:ALA:HB1	1:D:127:ILE:HD11	1.98	0.45
1:B:32:GLU:HA	1:B:32:GLU:OE2	2.17	0.45
1:C:195:GLU:HB3	1:C:197:ILE:CD1	2.47	0.45
1:A:89:LEU:HD22	1:A:146:HIS:CD2	2.52	0.44
1:D:104:GLN:HG2	1:D:115:TYR:CE1	2.51	0.44
1:A:119:ALA:HB1	1:A:121:MET:HE3	1.98	0.44
1:D:108:ALA:HA	1:D:113:ILE:HG23	1.99	0.44
1:E:121:MET:HE1	1:E:171:ASP:CG	2.42	0.44
1:A:118:GLY:HA2	1:A:135:LEU:O	2.18	0.44
1:E:86:ARG:O	1:E:112:GLY:O	2.36	0.44
1:F:118:GLY:HA2	1:F:135:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ALA:CB	1:A:121:MET:HE3	2.48	0.44
1:D:121:MET:HE1	1:D:171:ASP:OD1	2.17	0.44
1:A:282:ASP:O	1:A:285:ILE:HG22	2.18	0.44
1:C:118:GLY:HA2	1:C:135:LEU:O	2.17	0.44
1:D:68:ASP:HB2	1:D:71:VAL:CG1	2.48	0.44
1:F:282:ASP:O	1:F:285:ILE:HG22	2.18	0.44
1:A:10:ALA:O	1:A:37:ARG:HG2	2.18	0.43
1:C:12:ARG:NH2	3:C:402:HOH:O	2.51	0.43
1:E:282:ASP:O	1:E:285:ILE:HG22	2.18	0.43
1:D:282:ASP:O	1:D:285:ILE:HG22	2.18	0.43
1:C:187:GLN:HB3	1:D:176:PHE:CD1	2.54	0.43
1:F:231:ALA:HB2	1:F:280:LYS:O	2.18	0.43
1:B:86:ARG:O	1:B:112:GLY:O	2.37	0.43
1:B:119:ALA:CB	1:B:121:MET:HE3	2.48	0.43
1:F:108:ALA:HA	1:F:113:ILE:HG23	2.00	0.43
1:A:252:LEU:C	1:A:252:LEU:CD2	2.92	0.43
1:A:266:MET:HE1	1:E:180:GLY:HA2	2.00	0.43
1:A:231:ALA:HB2	1:A:280:LYS:O	2.19	0.43
1:A:86:ARG:O	1:A:112:GLY:O	2.37	0.43
1:E:102:ARG:HA	1:E:164:VAL:CG1	2.49	0.43
1:C:144:GLU:OE1	1:C:147:ARG:HD2	2.20	0.42
1:D:256:ARG:HA	1:D:256:ARG:HD3	1.85	0.42
1:E:66:VAL:CG1	1:E:71:VAL:HG22	2.49	0.42
1:C:135:LEU:N	1:C:135:LEU:CD1	2.82	0.42
1:C:252:LEU:C	1:C:252:LEU:CD2	2.91	0.42
1:C:85:LEU:O	1:C:88:LYS:HG2	2.20	0.42
1:F:121:MET:SD	1:F:171:ASP:OD1	2.78	0.42
1:C:195:GLU:HG2	1:D:169:ALA:HB2	2.02	0.41
1:C:256:ARG:HA	1:C:256:ARG:HD3	1.90	0.41
1:B:6:THR:HA	1:B:29:THR:O	2.20	0.41
1:A:6:THR:HA	1:A:29:THR:O	2.21	0.41
1:F:147:ARG:HG2	1:F:147:ARG:HH11	1.85	0.41
1:A:290:LEU:O	1:E:259:HIS:HB2	2.20	0.41
1:B:118:GLY:HA2	1:B:135:LEU:O	2.20	0.41
1:B:224:VAL:HG21	1:B:287:THR:HG21	2.02	0.41
1:C:176:PHE:CZ	1:D:187:GLN:HG3	2.55	0.41
1:C:224:VAL:HG21	1:C:287:THR:HG21	2.02	0.41
1:C:231:ALA:HB2	1:C:280:LYS:O	2.20	0.41
1:F:5:LEU:O	1:F:28:THR:HA	2.21	0.41
1:A:32:GLU:OE2	2:A:301:NAD:O3B	2.24	0.41
1:B:144:GLU:OE1	1:B:147:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:O	1:C:112:GLY:O	2.38	0.41
1:B:210:GLU:HB3	1:B:211:PRO:HD3	2.03	0.41
1:C:6:THR:HA	1:C:29:THR:O	2.21	0.41
1:D:5:LEU:O	1:D:28:THR:HA	2.21	0.41
1:D:6:THR:HA	1:D:29:THR:O	2.21	0.41
1:D:92:GLN:NE2	1:D:94:THR:OG1	2.53	0.41
1:E:6:THR:HA	1:E:29:THR:O	2.20	0.41
1:E:147:ARG:HH11	1:E:147:ARG:CG	2.34	0.41
1:A:22:LEU:CD2	1:A:28:THR:HG23	2.51	0.41
1:E:5:LEU:O	1:E:28:THR:HA	2.21	0.41
1:B:252:LEU:C	1:B:252:LEU:CD2	2.93	0.40
1:F:67:ILE:CG2	1:F:71:VAL:HG11	2.51	0.40
1:B:51:THR:HG23	1:B:54:ASP:CB	2.51	0.40
1:B:119:ALA:HB1	1:B:121:MET:HE3	2.01	0.40
1:B:164:VAL:HG22	3:B:416:HOH:O	2.20	0.40
1:F:6:THR:HA	1:F:29:THR:O	2.21	0.40
1:F:67:ILE:HG22	1:F:71:VAL:HG11	2.03	0.40
1:A:5:LEU:O	1:A:28:THR:HA	2.21	0.40
1:A:169:ALA:CB	1:E:195:GLU:HG2	2.51	0.40
1:A:195:GLU:HG3	1:E:102:ARG:HH22	1.86	0.40
1:E:160:VAL:HG11	1:E:170:LEU:HD23	2.03	0.40
1:F:256:ARG:HA	1:F:256:ARG:HD3	1.87	0.40
1:E:178:MET:HE2	1:E:178:MET:HB3	2.00	0.40
1:F:104:GLN:HG2	1:F:115:TYR:CE1	2.56	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	290/311 (93%)	287 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/311 (94%)	285 (98%)	6 (2%)	0	100	100
1	C	290/311 (93%)	286 (99%)	4 (1%)	0	100	100
1	D	282/311 (91%)	274 (97%)	7 (2%)	1 (0%)	30	57
1	E	285/311 (92%)	282 (99%)	3 (1%)	0	100	100
1	F	292/311 (94%)	288 (99%)	4 (1%)	0	100	100
All	All	1730/1866 (93%)	1702 (98%)	27 (2%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	86	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/247 (88%)	197 (91%)	20 (9%)	8	25
1	B	217/247 (88%)	196 (90%)	21 (10%)	8	23
1	C	204/247 (83%)	183 (90%)	21 (10%)	7	20
1	D	186/247 (75%)	164 (88%)	22 (12%)	5	15
1	E	213/247 (86%)	189 (89%)	24 (11%)	5	17
1	F	221/247 (90%)	190 (86%)	31 (14%)	3	10
All	All	1258/1482 (85%)	1119 (89%)	139 (11%)	6	18

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	28	THR
1	A	34	GLU
1	A	37	ARG
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	50	ASP
1	A	51	THR
1	A	58	ARG
1	A	63	VAL
1	A	85	LEU
1	A	104	GLN
1	A	109	ARG
1	A	135	LEU
1	A	147	ARG
1	A	160	VAL
1	A	193	ARG
1	A	201	LYS
1	A	229	LEU
1	A	254	GLU
1	A	290	LEU
1	B	-1	SER
1	B	8	ILE
1	B	28	THR
1	B	32	GLU
1	B	34	GLU
1	B	48	LEU
1	B	51	THR
1	B	58	ARG
1	B	63	VAL
1	B	66	VAL
1	B	76	LEU
1	B	103	GLU
1	B	104	GLN
1	B	135	LEU
1	B	162	GLU
1	B	164	VAL
1	B	199	LEU
1	B	201	LYS
1	B	229	LEU
1	B	254	GLU
1	B	291	LYS
1	C	8	ILE
1	C	28	THR
1	C	51	THR
1	C	62	ILE
1	C	63	VAL
1	C	66	VAL

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Mol	Chain	Res	Type
1	C	79	ASP
1	C	80	GLU
1	C	88	LYS
1	C	104	GLN
1	C	135	LEU
1	C	147	ARG
1	C	160	VAL
1	C	162	GLU
1	C	164	VAL
1	C	193	ARG
1	C	199	LEU
1	C	200	GLU
1	C	229	LEU
1	C	254	GLU
1	C	291	LYS
1	D	28	THR
1	D	29	THR
1	D	38	SER
1	D	64	VAL
1	D	65	ASN
1	D	67	ILE
1	D	71	VAL
1	D	75	LEU
1	D	84	GLU
1	D	89	LEU
1	D	91	VAL
1	D	92	GLN
1	D	94	THR
1	D	104	GLN
1	D	113	ILE
1	D	127	ILE
1	D	139	SER
1	D	147	ARG
1	D	162	GLU
1	D	199	LEU
1	D	208	LEU
1	D	280	LYS
1	E	8	ILE
1	E	27	THR
1	E	28	THR
1	E	29	THR
1	E	48	LEU

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Mol	Chain	Res	Type
1	E	51	THR
1	E	56	VAL
1	E	64	VAL
1	E	66	VAL
1	E	71	VAL
1	E	75	LEU
1	E	85	LEU
1	E	89	LEU
1	E	91	VAL
1	E	104	GLN
1	E	125	ASP
1	E	127	ILE
1	E	162	GLU
1	E	187	GLN
1	E	193	ARG
1	E	199	LEU
1	E	201	LYS
1	E	208	LEU
1	E	272	GLU
1	F	8	ILE
1	F	12[A]	ARG
1	F	12[B]	ARG
1	F	27	THR
1	F	28	THR
1	F	35	LYS
1	F	51	THR
1	F	56	VAL
1	F	64	VAL
1	F	66	VAL
1	F	71	VAL
1	F	75	LEU
1	F	76	LEU
1	F	80	GLU
1	F	85	LEU
1	F	89	LEU
1	F	91	VAL
1	F	104	GLN
1	F	113	ILE
1	F	125	ASP
1	F	144	GLU
1	F	160	VAL
1	F	187	GLN

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Mol	Chain	Res	Type
1	F	193	ARG
1	F	199	LEU
1	F	201	LYS
1	F	208	LEU
1	F	229	LEU
1	F	254	GLU
1	F	271	ARG
1	F	275	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	92	GLN
1	A	104	GLN
1	A	129	GLN
1	A	146	HIS
1	A	166	HIS
1	A	248	HIS
1	A	278	HIS
1	B	65	ASN
1	B	92	GLN
1	B	104	GLN
1	B	110	GLN
1	B	129	GLN
1	B	146	HIS
1	B	159	HIS
1	B	177	GLN
1	B	278	HIS
1	C	65	ASN
1	C	92	GLN
1	C	104	GLN
1	C	146	HIS
1	C	159	HIS
1	C	177	GLN
1	C	278	HIS
1	D	92	GLN
1	D	159	HIS
1	D	177	GLN
1	D	234	GLN
1	D	242	HIS
1	D	278	HIS

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Mol	Chain	Res	Type
1	E	159	HIS
1	E	177	GLN
1	E	187	GLN
1	E	234	GLN
1	E	242	HIS
1	E	247	GLN
1	E	278	HIS
1	F	23	GLN
1	F	159	HIS
1	F	177	GLN
1	F	187	GLN
1	F	242	HIS
1	F	247	GLN
1	F	278	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	301	-	46,48,48	0.72	1 (2%)	64,73,73	0.83	2 (3%)
2	NAD	A	301	-	46,48,48	0.76	1 (2%)	64,73,73	0.82	2 (3%)
2	NAD	F	301	-	24,27,48	1.40	3 (12%)	33,41,73	1.14	3 (9%)
2	NAD	B	301	-	46,48,48	0.61	1 (2%)	64,73,73	0.75	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	301	-	-	11/30/62/62	0/5/5/5
2	NAD	A	301	-	-	5/30/62/62	0/5/5/5
2	NAD	F	301	-	-	5/20/36/62	0/2/2/5
2	NAD	B	301	-	-	4/30/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	PA-O1A	3.88	1.62	1.50
2	F	301	NAD	C2N-N1N	3.76	1.39	1.35
2	C	301	NAD	C2N-N1N	3.38	1.38	1.35
2	A	301	NAD	C2N-N1N	3.26	1.38	1.35
2	F	301	NAD	O4D-C1D	2.75	1.44	1.40
2	B	301	NAD	C2N-N1N	2.21	1.37	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	C6N-N1N-C2N	-4.13	118.36	121.88
2	B	301	NAD	C6N-N1N-C2N	-3.28	119.08	121.88
2	A	301	NAD	C6N-N1N-C2N	-2.90	119.41	121.88
2	F	301	NAD	O5B-PA-O2A	2.74	118.08	107.80
2	C	301	NAD	C6N-N1N-C2N	-2.74	119.55	121.88
2	A	301	NAD	O2N-PN-O3	2.21	113.25	107.27
2	C	301	NAD	C3B-C2B-C1B	-2.18	97.34	101.46
2	F	301	NAD	O2A-PA-O3	2.05	111.51	104.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	C2D-C1D-N1N-C2N
2	B	301	NAD	C2D-C1D-N1N-C6N
2	C	301	NAD	C5B-O5B-PA-O1A
2	C	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	O4D-C1D-N1N-C6N
2	C	301	NAD	C2D-C1D-N1N-C6N
2	F	301	NAD	PN-O3-PA-O2A
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	C3B-C4B-C5B-O5B
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	C5B-O5B-PA-O2A
2	C	301	NAD	C5B-O5B-PA-O3
2	C	301	NAD	C2D-C1D-N1N-C2N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	F	301	NAD	O4D-C1D-N1N-C6N
2	F	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	PN-O3-PA-O1A
2	C	301	NAD	PN-O3-PA-O2A

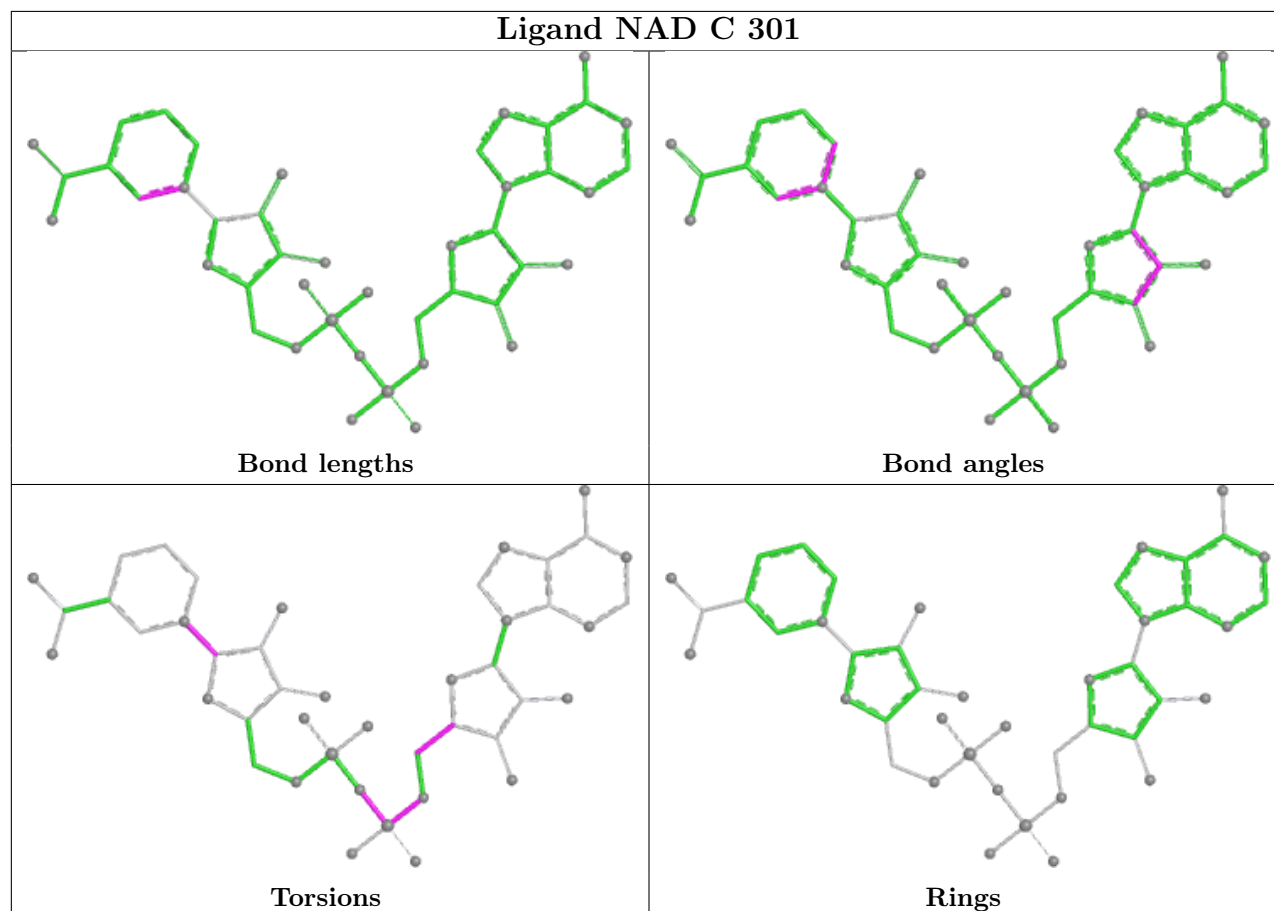
There are no ring outliers.

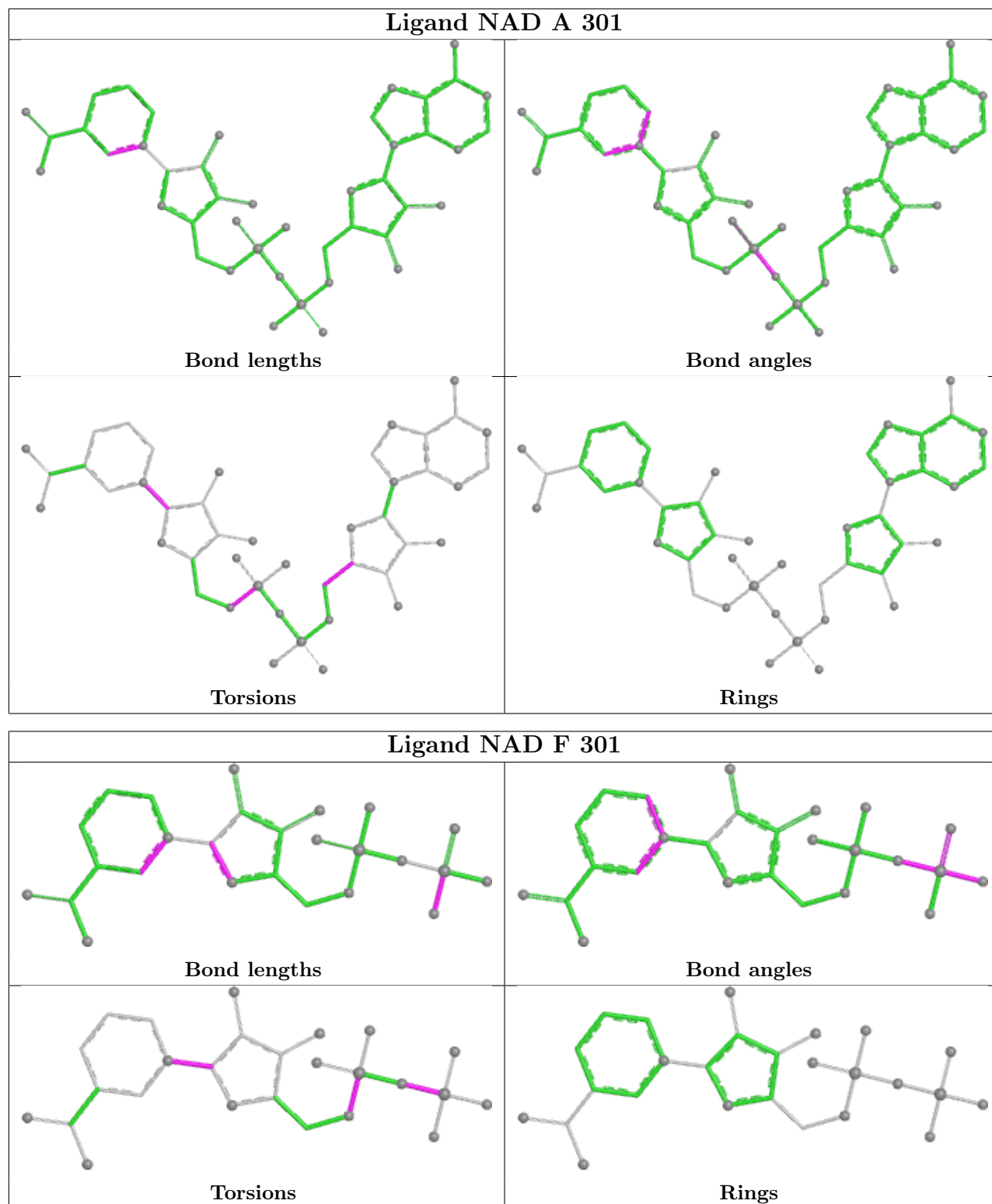
3 monomers are involved in 5 short contacts:

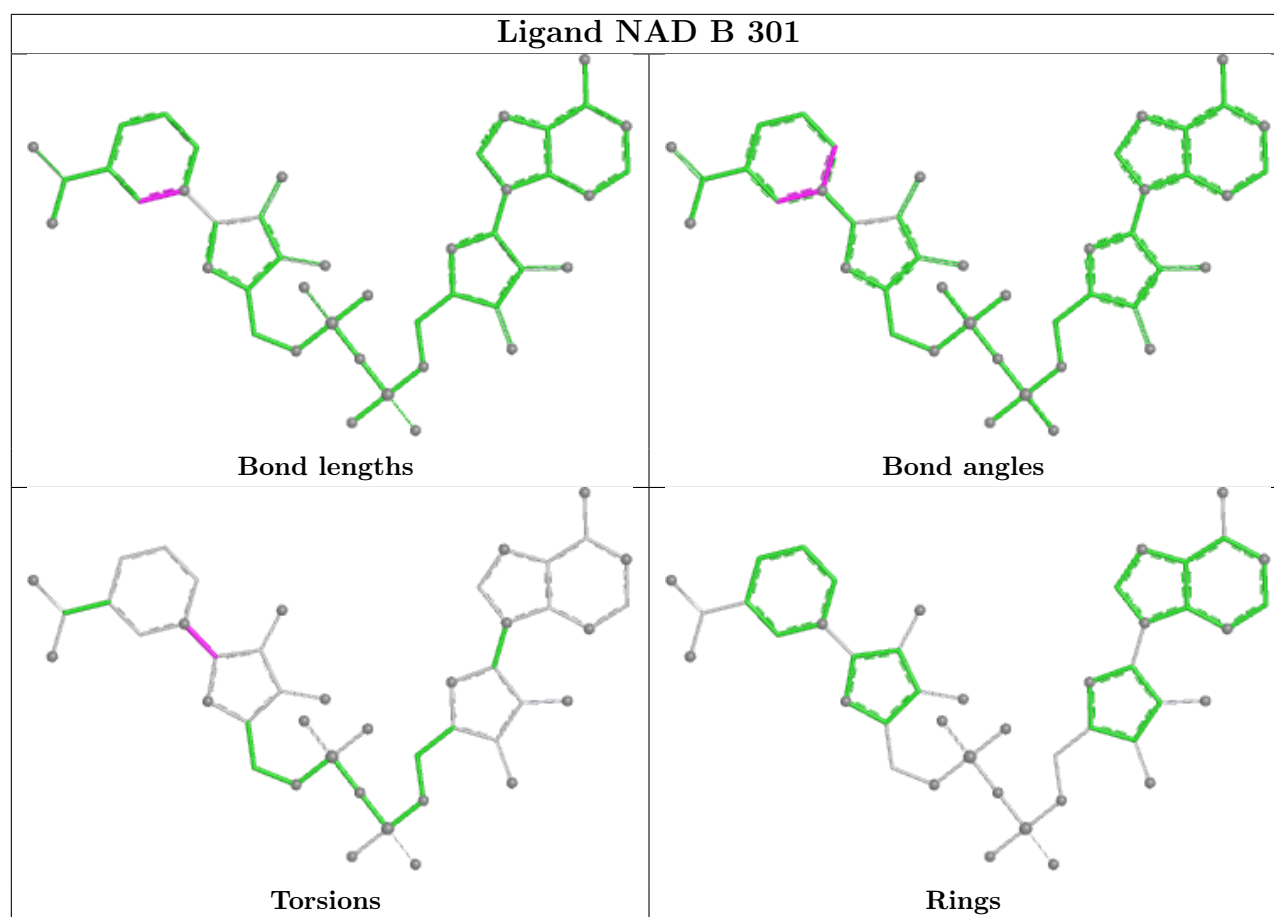
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
2	F	301	NAD	2	0
2	B	301	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	292/311 (93%)	-0.09	4 (1%) 73 67	27, 46, 71, 128	0
1	B	293/311 (94%)	-0.10	4 (1%) 73 67	22, 42, 72, 90	0
1	C	292/311 (93%)	0.13	8 (2%) 56 48	26, 49, 86, 104	0
1	D	286/311 (91%)	0.53	39 (13%) 7 5	25, 54, 113, 142	0
1	E	289/311 (92%)	-0.06	6 (2%) 63 56	28, 44, 71, 95	0
1	F	291/311 (93%)	-0.14	2 (0%) 84 79	25, 42, 61, 91	3 (1%)
All	All	1743/1866 (93%)	0.05	63 (3%) 46 39	22, 45, 86, 142	3 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	TRP	6.1
1	D	54	ASP	5.1
1	D	52	VAL	4.6
1	E	36	ALA	4.4
1	E	33	TYR	4.1
1	D	41	LEU	3.9
1	D	0	HIS	3.8
1	D	51	THR	3.7
1	D	86	ARG	3.5
1	D	15	SER	3.3
1	D	58	ARG	3.1
1	D	76	LEU	3.1
1	D	57	LYS	3.0
1	D	53	ARG	3.0
1	D	66	VAL	3.0
1	C	1	MET	2.9
1	D	30	VAL	2.8
1	E	10	ALA	2.8
1	D	44	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	62	ILE	2.7
1	D	67	ILE	2.7
1	E	37	ARG	2.7
1	A	236	LEU	2.7
1	D	56	VAL	2.6
1	D	113	ILE	2.6
1	C	85	LEU	2.6
1	D	29	THR	2.6
1	A	1	MET	2.6
1	B	233	ALA	2.6
1	C	234	GLN	2.6
1	C	67	ILE	2.5
1	F	255	GLU	2.5
1	D	47	HIS	2.5
1	E	1	MET	2.5
1	D	38	SER	2.5
1	B	79	ASP	2.5
1	B	4	THR	2.4
1	D	85	LEU	2.4
1	C	38	SER	2.4
1	D	50	ASP	2.4
1	D	49	ALA	2.4
1	D	27	THR	2.4
1	D	34	GLU	2.4
1	D	39	GLU	2.3
1	D	75	LEU	2.3
1	D	18	ILE	2.3
1	D	35	LYS	2.3
1	C	56	VAL	2.3
1	D	48	LEU	2.2
1	B	80	GLU	2.2
1	C	41	LEU	2.2
1	D	90	LEU	2.2
1	A	0	HIS	2.2
1	D	12	ARG	2.2
1	D	112	GLY	2.2
1	D	33	TYR	2.1
1	D	110	GLN	2.1
1	C	4	THR	2.1
1	F	1	MET	2.1
1	D	37	ARG	2.0
1	E	12	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	2.0
1	D	64	VAL	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](#)

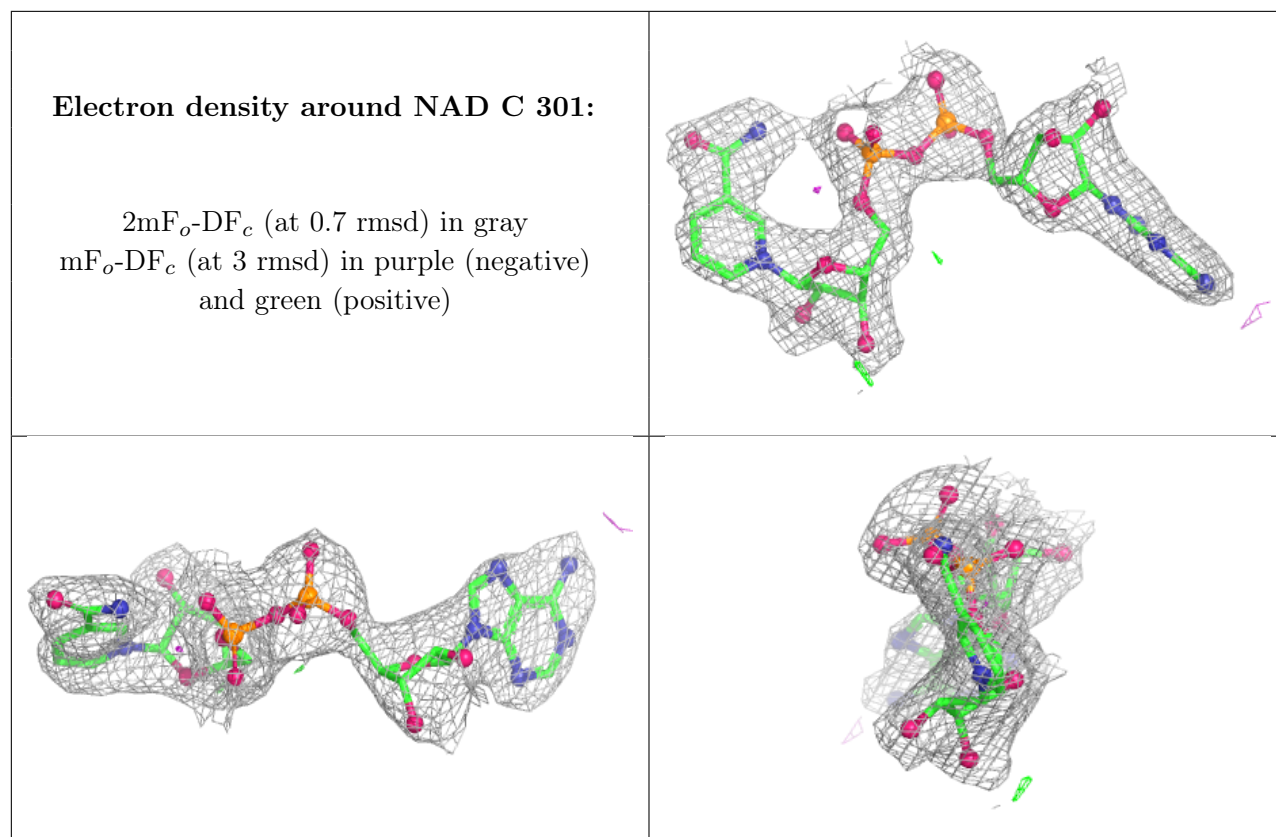
There are no oligosaccharides in this entry.

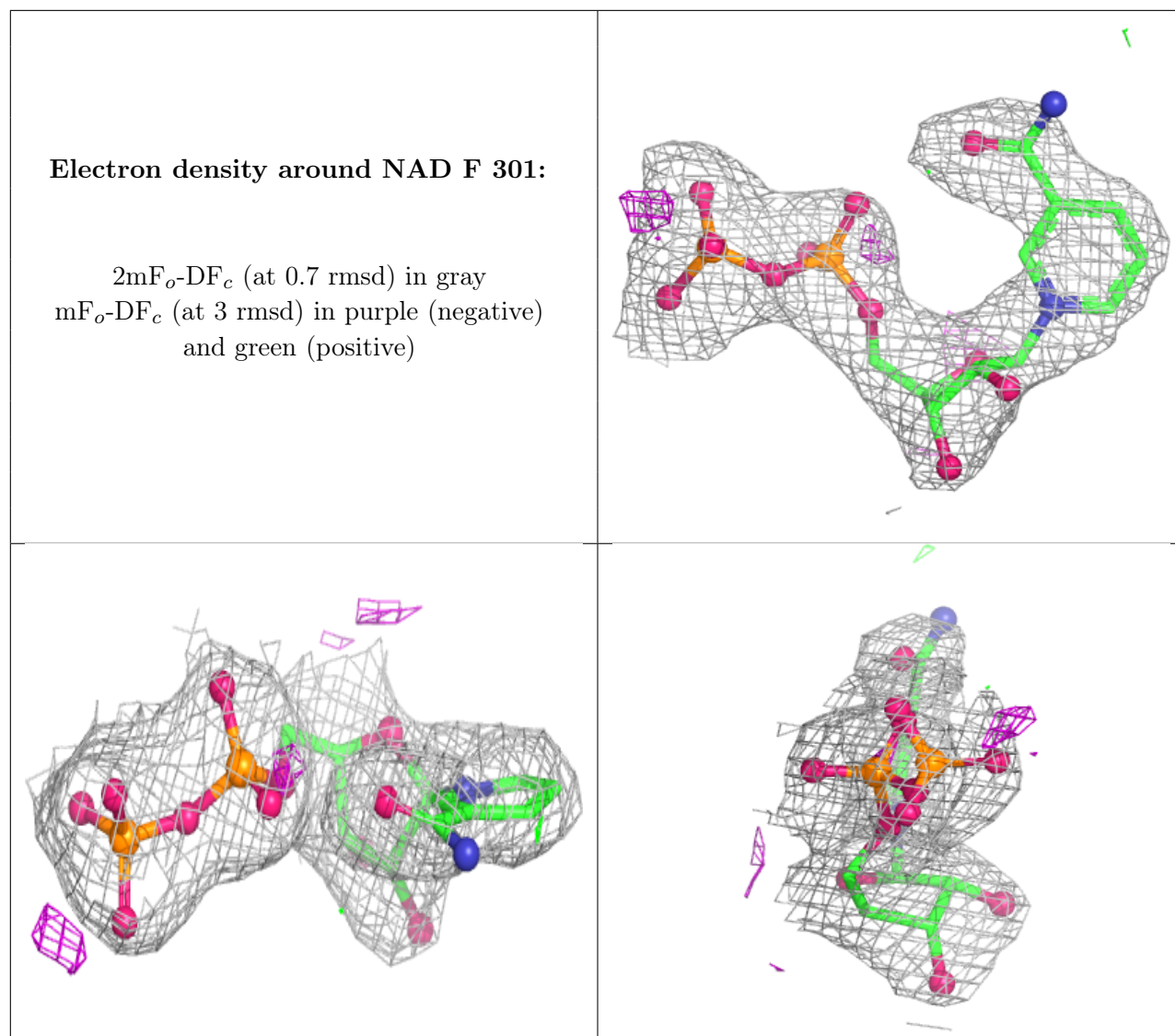
6.4 Ligands [i](#)

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	NAD	C	301	44/44	0.93	0.09	39,64,98,102	0
2	NAD	F	301	26/44	0.93	0.09	50,61,68,72	0
2	NAD	B	301	44/44	0.95	0.08	38,50,82,92	0
2	NAD	A	301	44/44	0.97	0.07	32,44,65,70	0

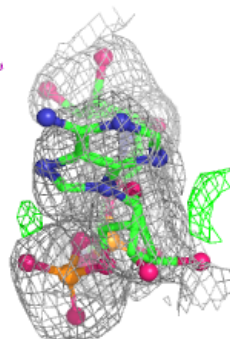
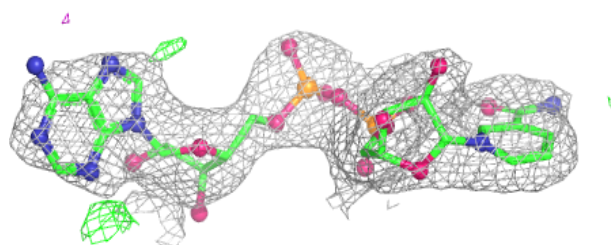
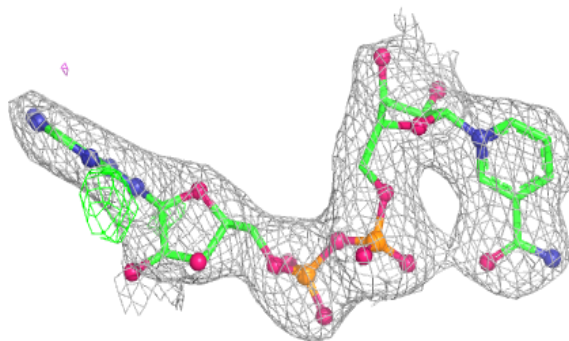
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



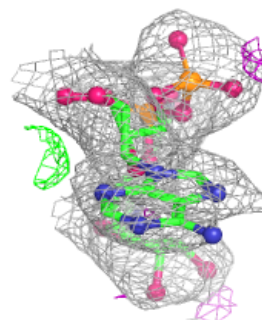
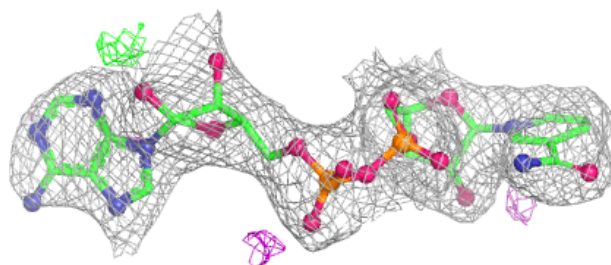
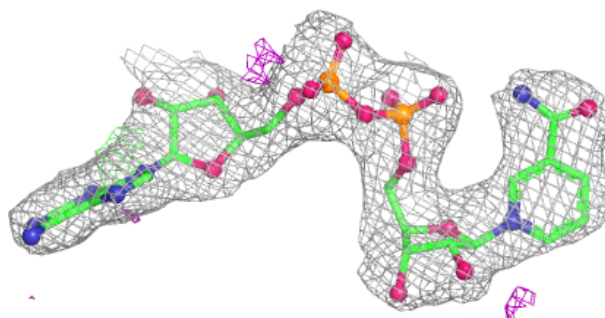


Electron density around NAD B 301:

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

**Electron density around NAD A 301:**

$2mF_o-DF_c$ (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.