



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 3WFJ / pdb_00003wfj
Title : The complex structure of D-mandelate dehydrogenase with NADH
Authors : Miyanaga, A.; Fujisawa, S.; Furukawa, N.; Arai, K.; Nakajima, M.; Taguchi, H.
Deposited on : 2013-07-19
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

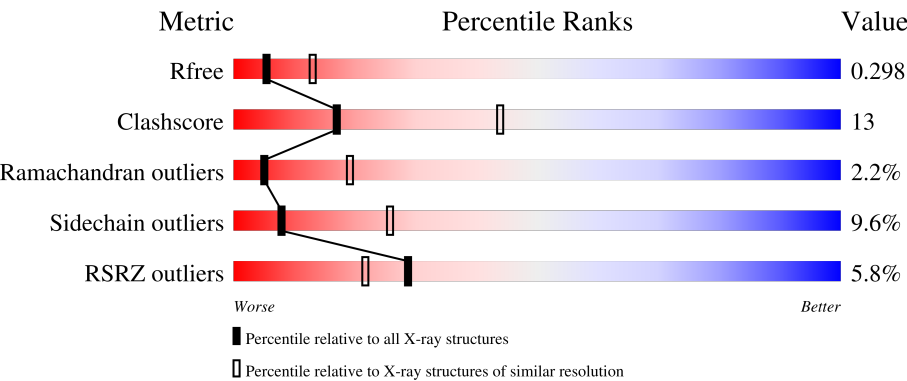
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	312	
1	B	312	
1	C	312	
1	D	312	
1	E	312	

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Mol	Chain	Length	Quality of chain
1	F	312	14% 56% 22% • • 16%
1	G	312	4% 64% 25% • • •
1	H	312	11% 56% 20% • 20%

2 Entry composition

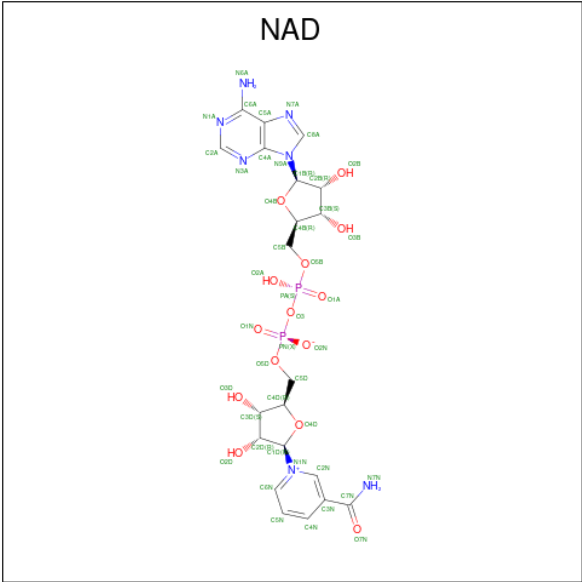
There are 3 unique types of molecules in this entry. The entry contains 18247 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2298	1458	382	441	17			
1	B	295	Total	C	N	O	S	0	0	0
			2267	1441	379	430	17			
1	C	295	Total	C	N	O	S	0	0	0
			2271	1444	379	431	17			
1	D	293	Total	C	N	O	S	0	0	0
			2254	1430	377	430	17			
1	E	299	Total	C	N	O	S	0	0	0
			2298	1460	384	437	17			
1	F	263	Total	C	N	O	S	0	0	0
			2024	1291	336	381	16			
1	G	298	Total	C	N	O	S	0	0	0
			2288	1453	384	434	17			
1	H	250	Total	C	N	O	S	0	0	0
			1916	1219	320	361	16			

- 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	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	33	Total	O	0	0
			33	33		
3	C	19	Total	O	0	0
			19	19		
3	D	38	Total	O	0	0
			38	38		

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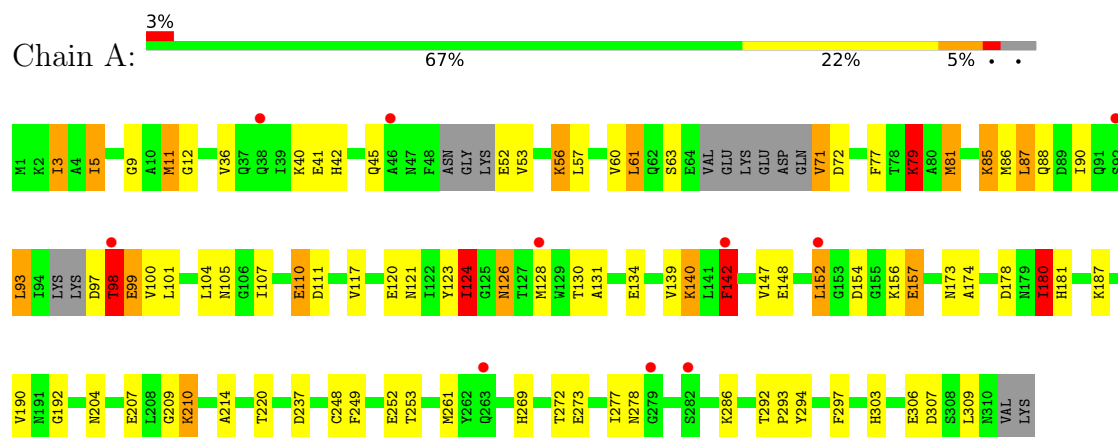
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	42	Total 42	O 42	0	0
3	F	38	Total 38	O 38	0	0
3	G	35	Total 35	O 35	0	0
3	H	29	Total 29	O 29	0	0

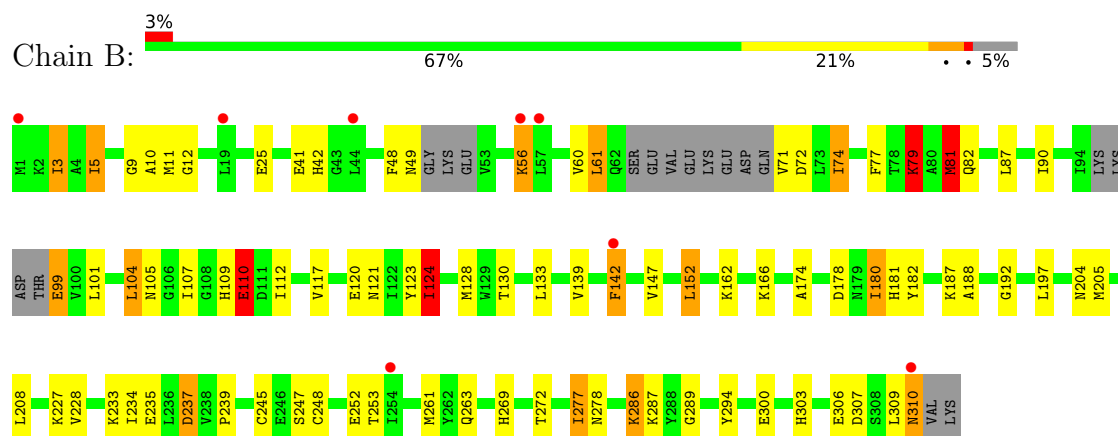
3 Residue-property plots [i](#)

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.

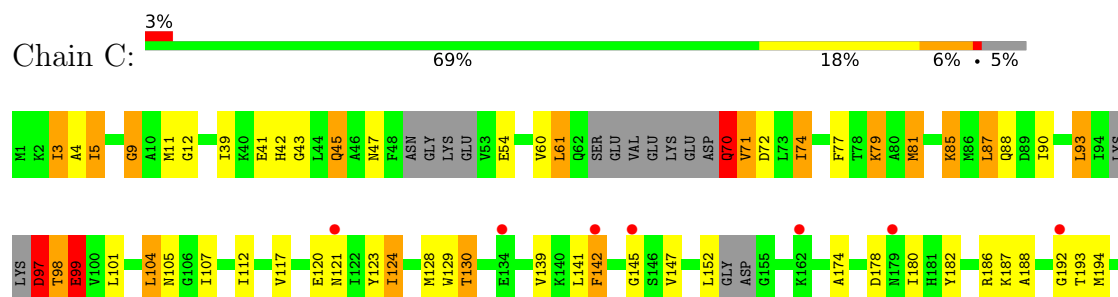
- Molecule 1: 2-dehydropantoate 2-reductase



- Molecule 1: 2-dehydropantoate 2-reductase

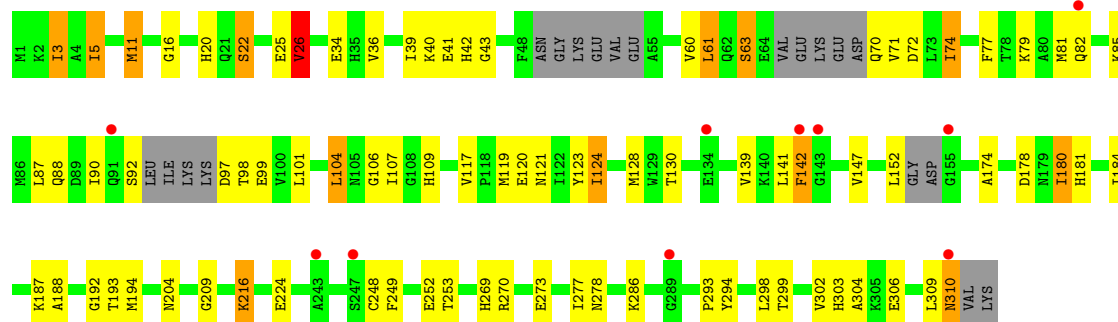


- Molecule 1: 2-dehydropantoate 2-reductase

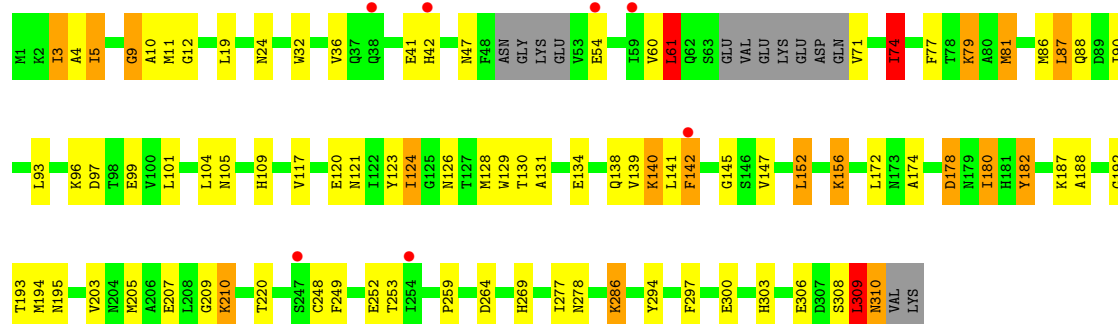




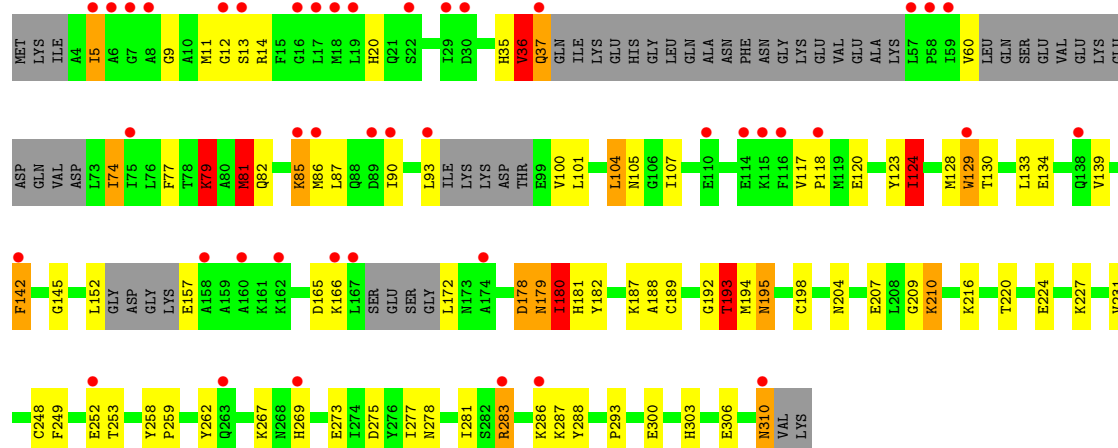
• Molecule 1: 2-dehydropantoate 2-reductase



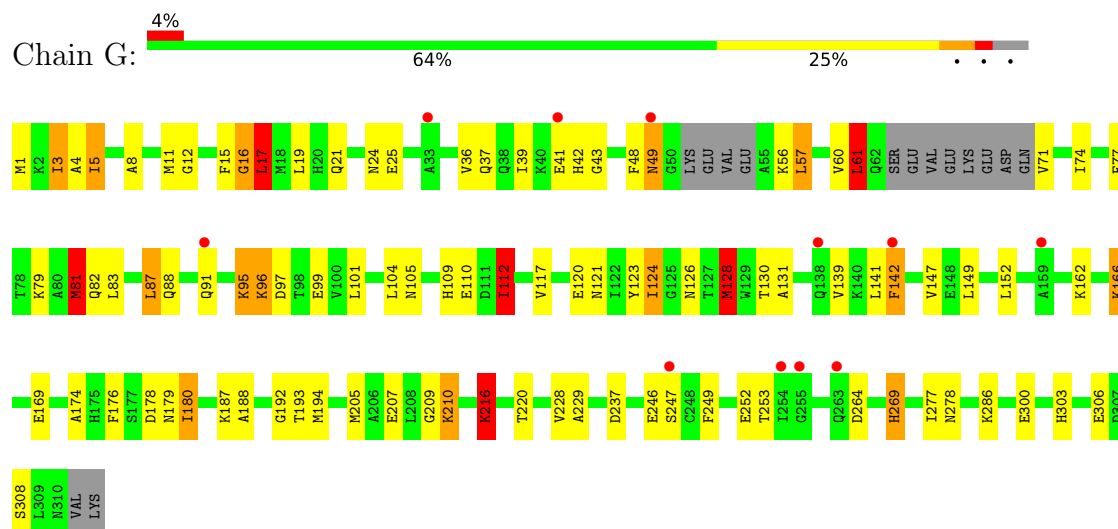
• Molecule 1: 2-dehydropantoate 2-reductase



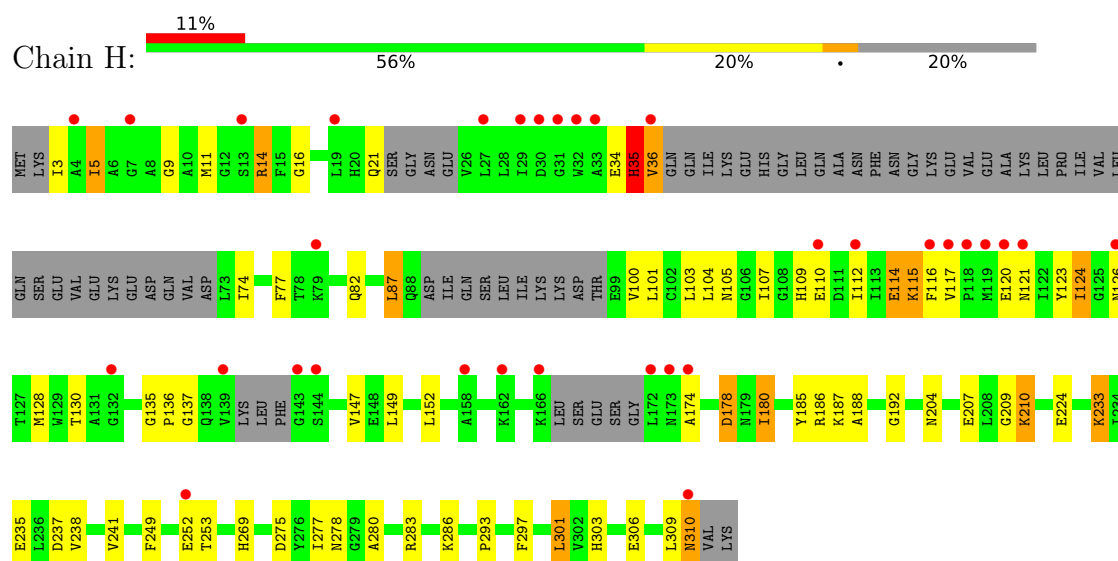
• Molecule 1: 2-dehydropantoate 2-reductase



• Molecule 1: 2-dehydropantoate 2-reductase



• Molecule 1: 2-dehydropantoate 2-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.65Å 103.44Å 119.74Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	19.97 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.97-2.80) 97.7 (19.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.306 (Not available) , 0.298	Depositor DCC
R_{free} test set	3513 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.087 for l,k,-h 0.337 for h,-k,-l 0.126 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	18247	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.47% 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

5.1 Standard geometry

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	1.35	15/2333 (0.6%)	1.33	21/3145 (0.7%)
1	B	1.38	10/2302 (0.4%)	1.30	14/3103 (0.5%)
1	C	1.32	9/2305 (0.4%)	1.30	9/3106 (0.3%)
1	D	1.34	9/2288 (0.4%)	1.31	11/3082 (0.4%)
1	E	1.39	9/2334 (0.4%)	1.29	9/3146 (0.3%)
1	F	1.32	3/2055 (0.1%)	1.32	18/2771 (0.6%)
1	G	1.45	16/2324 (0.7%)	1.32	16/3132 (0.5%)
1	H	1.30	3/1945 (0.2%)	1.30	10/2620 (0.4%)
All	All	1.36	74/17886 (0.4%)	1.31	108/24105 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
1	H	0	2
All	All	0	6

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	142	PHE	CA-CB	8.75	1.65	1.53
1	A	142	PHE	CA-CB	8.61	1.64	1.53
1	G	308	SER	C-O	-7.62	1.14	1.24
1	B	227	LYS	CA-C	7.35	1.62	1.52
1	E	54	GLU	CA-C	7.20	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	GLY	C-O	-6.81	1.16	1.24
1	G	49	ASN	CA-C	6.78	1.61	1.52
1	D	299	THR	N-CA	-6.67	1.38	1.46
1	B	235	GLU	C-O	-6.45	1.16	1.24
1	C	54	GLU	CA-C	6.40	1.60	1.52
1	C	301	LEU	N-CA	6.26	1.53	1.46
1	C	4	ALA	N-CA	6.20	1.54	1.46
1	A	214	ALA	N-CA	6.15	1.53	1.46
1	A	307	ASP	CA-C	6.08	1.60	1.52
1	E	126	ASN	CA-C	-6.04	1.45	1.52
1	D	72	ASP	N-CA	6.03	1.53	1.46
1	G	264	ASP	C-O	-5.95	1.17	1.24
1	A	110	GLU	N-CA	5.95	1.53	1.46
1	H	280	ALA	N-CA	-5.93	1.39	1.46
1	A	124	ILE	N-CA	5.90	1.53	1.46
1	A	72	ASP	N-CA	5.86	1.53	1.46
1	E	32	TRP	CA-CB	5.82	1.60	1.53
1	G	74	ILE	CA-CB	5.78	1.61	1.54
1	G	4	ALA	N-CA	5.76	1.53	1.46
1	B	245	CYS	N-CA	5.73	1.53	1.46
1	A	148	GLU	N-CA	-5.69	1.38	1.46
1	G	229	ALA	N-CA	5.67	1.53	1.46
1	D	63	SER	N-CA	-5.67	1.38	1.46
1	A	220	THR	N-CA	-5.66	1.39	1.46
1	D	302	VAL	CA-C	-5.63	1.45	1.52
1	A	190	VAL	CA-CB	-5.61	1.47	1.54
1	F	281	ILE	CA-CB	5.59	1.60	1.54
1	A	99	GLU	N-CA	5.58	1.53	1.46
1	G	162	LYS	N-CA	5.50	1.53	1.46
1	A	237	ASP	N-CA	-5.50	1.39	1.46
1	D	22	SER	CA-C	-5.50	1.45	1.52
1	G	61	LEU	CA-C	-5.49	1.45	1.53
1	A	126	ASN	CA-C	-5.49	1.45	1.52
1	G	216	LYS	CA-C	5.49	1.59	1.52
1	G	95	LYS	CA-C	5.47	1.60	1.53
1	B	277	ILE	N-CA	-5.46	1.39	1.46
1	D	270	ARG	CZ-NH2	-5.45	1.26	1.33
1	C	309	LEU	CA-C	5.43	1.59	1.52
1	C	186	ARG	CA-C	-5.42	1.46	1.52
1	D	92	SER	C-O	5.41	1.34	1.23
1	C	70	GLN	N-CA	5.39	1.56	1.46
1	B	237	ASP	N-CA	-5.39	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	241	VAL	CA-CB	-5.38	1.48	1.54
1	C	85	LYS	N-CA	-5.34	1.40	1.46
1	E	308	SER	C-O	-5.34	1.17	1.24
1	B	112	ILE	N-CA	-5.33	1.39	1.46
1	F	36	VAL	CA-C	5.32	1.59	1.52
1	B	197	LEU	N-CA	5.32	1.52	1.46
1	E	182	TYR	C-O	-5.29	1.18	1.24
1	D	11	MET	N-CA	-5.29	1.39	1.46
1	B	307	ASP	CA-C	5.28	1.59	1.52
1	A	57	LEU	CA-C	-5.24	1.45	1.52
1	E	152	LEU	C-O	-5.23	1.17	1.24
1	A	309	LEU	CA-C	5.21	1.59	1.52
1	C	99	GLU	N-CA	5.18	1.52	1.46
1	G	308	SER	CA-C	-5.17	1.45	1.52
1	F	198	CYS	CA-CB	-5.12	1.45	1.53
1	A	56	LYS	CA-C	5.12	1.59	1.52
1	B	152	LEU	C-O	-5.10	1.17	1.24
1	C	276	TYR	C-O	5.10	1.31	1.24
1	G	17	LEU	CB-CG	5.09	1.63	1.53
1	E	300	GLU	N-CA	5.07	1.52	1.46
1	D	97	ASP	CA-C	5.06	1.63	1.52
1	G	96	LYS	C-O	-5.05	1.18	1.24
1	E	61	LEU	CA-C	-5.05	1.46	1.53
1	H	238	VAL	N-CA	-5.05	1.40	1.46
1	G	8	ALA	N-CA	-5.03	1.40	1.46
1	G	176	PHE	N-CA	-5.03	1.39	1.45
1	E	4	ALA	N-CA	5.01	1.52	1.46

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	179	ASN	N-CA-C	11.68	125.00	108.54
1	H	114	GLU	N-CA-C	-10.45	96.66	110.24
1	A	152	LEU	N-CA-C	-9.09	96.33	110.42
1	D	98	THR	N-CA-C	7.80	122.18	110.64
1	G	269	HIS	CB-CA-C	-7.69	100.81	111.73
1	H	107	ILE	CB-CA-C	-7.26	98.81	110.28
1	B	79	LYS	N-CA-C	-7.13	100.93	110.55
1	A	79	LYS	N-CA-C	-7.03	101.06	110.55
1	A	140	LYS	CA-CB-CG	6.87	127.84	114.10
1	F	193	THR	CB-CA-C	6.81	123.97	110.42
1	G	179	ASN	CB-CA-C	-6.80	101.64	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	THR	N-CA-C	-6.77	103.83	111.14
1	G	112	ILE	N-CA-CB	6.77	121.86	110.56
1	H	5	ILE	CB-CA-C	-6.72	101.85	111.19
1	C	107	ILE	CB-CA-C	-6.70	99.69	110.28
1	A	139	VAL	N-CA-C	6.64	118.36	108.46
1	E	172	LEU	N-CA-C	-6.55	105.28	113.28
1	D	121	ASN	N-CA-C	6.45	121.30	113.17
1	E	220	THR	N-CA-C	-6.44	104.34	111.36
1	G	16	GLY	N-CA-C	-6.39	104.91	112.64
1	D	5	ILE	CB-CA-C	-6.39	102.31	111.19
1	G	228	VAL	N-CA-C	6.37	116.53	110.42
1	A	107	ILE	CB-CA-C	-6.35	99.47	110.65
1	B	107	ILE	CB-CA-C	-6.31	100.30	110.28
1	F	107	ILE	CB-CA-C	-6.31	100.31	110.28
1	A	157	GLU	CA-CB-CG	6.29	126.68	114.10
1	F	193	THR	N-CA-CB	-6.28	99.88	110.49
1	E	309	LEU	CA-CB-CG	6.22	138.06	116.30
1	G	180	ILE	N-CA-C	-6.19	104.25	111.00
1	A	53	VAL	N-CA-C	6.16	118.80	108.81
1	G	142	PHE	N-CA-C	6.16	118.78	108.73
1	E	121	ASN	N-CA-C	6.15	120.92	113.17
1	D	98	THR	CB-CA-C	-6.05	102.36	109.80
1	D	139	VAL	N-CA-C	6.03	117.37	108.45
1	E	74	ILE	N-CA-CB	5.99	118.17	110.99
1	A	85	LYS	CA-CB-CG	5.93	125.97	114.10
1	B	121	ASN	N-CA-C	5.93	120.64	113.17
1	H	297	PHE	N-CA-C	-5.85	104.49	111.69
1	F	79	LYS	N-CA-C	-5.83	102.67	110.55
1	G	128	MET	CG-SD-CE	5.83	113.72	100.90
1	B	228	VAL	N-CA-C	5.82	116.01	110.42
1	A	121	ASN	N-CA-C	5.81	120.49	113.17
1	B	124	ILE	CB-CA-C	-5.77	103.30	111.38
1	G	121	ASN	N-CA-C	5.76	120.30	113.16
1	F	220	THR	N-CA-C	-5.75	105.09	111.36
1	F	287	LYS	N-CA-C	5.74	117.21	111.07
1	G	139	VAL	N-CA-C	5.72	118.08	108.81
1	H	233	LYS	CA-CB-CG	5.72	125.54	114.10
1	F	81	MET	CA-CB-CG	-5.71	102.67	114.10
1	A	100	VAL	N-CA-C	5.70	116.09	108.11
1	B	81	MET	CA-CB-CG	-5.67	102.77	114.10
1	D	25	GLU	N-CA-C	-5.64	99.32	108.41
1	A	110	GLU	N-CA-CB	5.63	118.51	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	GLU	N-CA-CB	5.61	118.47	110.06
1	D	224	GLU	N-CA-C	-5.61	105.09	111.14
1	D	107	ILE	CB-CA-C	-5.60	101.03	110.71
1	F	283	ARG	CB-CG-CD	5.59	124.16	111.30
1	F	93	LEU	CB-CG-CD2	-5.54	94.07	110.70
1	D	26	VAL	CB-CA-C	5.53	119.07	110.83
1	C	3	ILE	N-CA-C	5.53	115.96	107.77
1	A	3	ILE	N-CA-C	5.53	115.95	107.77
1	A	140	LYS	CB-CA-C	5.50	118.83	109.75
1	B	182	TYR	N-CA-C	-5.49	105.38	111.36
1	A	124	ILE	CB-CA-C	-5.48	103.35	111.19
1	C	224	GLU	N-CA-C	-5.48	105.22	111.14
1	H	126	ASN	CB-CA-C	-5.48	98.02	110.07
1	B	208	LEU	CB-CA-C	-5.43	102.12	110.81
1	C	210	LYS	N-CA-CB	5.41	118.67	110.28
1	E	139	VAL	N-CA-C	5.40	117.56	108.81
1	G	81	MET	CA-CB-CG	-5.38	103.33	114.10
1	F	124	ILE	CB-CA-C	-5.35	103.90	111.38
1	F	100	VAL	N-CA-C	5.34	115.59	108.11
1	G	3	ILE	N-CA-C	5.33	116.19	107.24
1	F	216	LYS	N-CA-C	-5.26	105.63	111.36
1	C	182	TYR	N-CA-C	-5.26	105.63	111.36
1	A	99	GLU	N-CA-C	5.25	121.99	110.80
1	F	227	LYS	CB-CG-CD	5.25	123.39	111.30
1	H	100	VAL	N-CA-C	5.25	115.45	108.11
1	A	11	MET	N-CA-C	-5.23	105.26	111.69
1	E	54	GLU	CB-CA-C	5.21	120.28	109.38
1	F	85	LYS	N-CA-CB	5.21	117.77	110.12
1	E	96	LYS	N-CA-C	-5.20	105.06	111.40
1	H	14	ARG	CG-CD-NE	5.19	123.43	112.00
1	B	286	LYS	CB-CA-C	5.17	119.00	110.88
1	B	3	ILE	N-CA-C	5.17	115.42	107.77
1	A	142	PHE	CA-CB-CG	5.16	118.96	113.80
1	F	139	VAL	N-CA-C	5.16	116.08	108.45
1	A	63	SER	CA-C-N	5.13	130.94	121.70
1	A	63	SER	C-N-CA	5.13	130.94	121.70
1	C	121	ASN	N-CA-C	5.13	119.52	113.16
1	A	81	MET	CA-CB-CG	-5.13	103.84	114.10
1	F	13	SER	N-CA-C	5.12	116.87	111.28
1	D	298	LEU	N-CA-C	-5.12	105.59	111.07
1	H	224	GLU	N-CA-C	-5.12	105.61	111.14
1	C	112	ILE	N-CA-C	-5.12	105.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	VAL	N-CA-C	5.12	115.73	110.36
1	F	193	THR	CA-CB-CG2	5.12	119.20	110.50
1	G	142	PHE	CA-CB-CG	5.09	118.89	113.80
1	F	224	GLU	N-CA-C	-5.07	105.67	111.14
1	D	3	ILE	N-CA-C	5.06	115.26	107.77
1	B	162	LYS	CB-CA-C	-5.05	102.93	110.90
1	C	139	VAL	N-CA-C	5.04	116.97	108.81
1	B	56	LYS	N-CA-CB	5.04	117.86	110.35
1	E	3	ILE	N-CA-C	5.03	115.21	107.77
1	G	220	THR	N-CA-C	-5.02	105.72	111.14
1	H	35	HIS	N-CA-CB	-5.02	101.69	109.87
1	G	36	VAL	CB-CA-C	-5.02	105.54	111.81
1	B	287	LYS	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ASN	Mainchain
1	C	97	ASP	Peptide
1	E	97	ASP	Peptide
1	G	97	ASP	Peptide
1	H	103	LEU	Peptide
1	H	35	HIS	Peptide

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	2298	0	2304	48	0
1	B	2267	0	2282	50	0
1	C	2271	0	2287	62	0
1	D	2254	0	2261	64	0
1	E	2298	0	2319	67	0
1	F	2024	0	2033	75	0
1	G	2288	0	2308	58	0
1	H	1916	0	1918	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	7	0
2	B	44	0	26	8	0
2	C	44	0	26	12	0
2	D	44	0	26	6	0
2	E	44	0	26	10	0
2	F	44	0	26	15	0
2	G	44	0	26	7	0
2	H	44	0	26	8	0
3	A	45	0	0	4	0
3	B	33	0	0	6	0
3	C	19	0	0	2	0
3	D	38	0	0	2	0
3	E	42	0	0	2	0
3	F	38	0	0	2	0
3	G	35	0	0	7	0
3	H	29	0	0	1	0
All	All	18247	0	17920	454	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 13.

All (454) 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:F:179:ASN:OD1	1:F:180:ILE:N	2.00	0.94
1:B:99:GLU:HG2	3:B:522:HOH:O	1.69	0.91
1:H:34:GLU:O	1:H:36:VAL:HG12	1.72	0.90
1:H:310:ASN:N	1:H:310:ASN:HD22	1.71	0.89
1:B:239:PRO:HG3	1:D:22:SER:HB2	1.55	0.89
1:H:235:GLU:O	1:H:235:GLU:HG2	1.72	0.89
1:C:130:THR:HG21	1:C:142:PHE:CD1	2.08	0.88
1:E:269:HIS:CD2	1:F:269:HIS:CD2	2.62	0.87
1:F:275:ASP:O	1:F:283:ARG:NH1	2.10	0.84
1:H:112:ILE:O	1:H:114:GLU:O	1.95	0.84
1:H:114:GLU:O	1:H:115:LYS:HB2	1.79	0.83
1:B:11:MET:HE3	2:B:401:NAD:C3N	2.09	0.82
1:E:269:HIS:CD2	1:F:269:HIS:NE2	2.48	0.82
1:E:269:HIS:NE2	1:F:269:HIS:CD2	2.48	0.82
1:F:129:TRP:HZ3	1:F:172:LEU:O	1.65	0.80
1:C:71:VAL:HG22	1:C:93:LEU:HD23	1.63	0.79
1:H:36:VAL:HG22	1:H:36:VAL:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:MET:SD	1:G:187:LYS:HE3	2.22	0.79
1:C:97:ASP:HB2	1:C:98:THR:OG1	1.84	0.78
1:A:111:ASP:OD2	1:A:111:ASP:C	2.27	0.78
1:G:1:MET:SD	1:G:166:LYS:HD2	2.25	0.77
1:C:93:LEU:HD22	1:C:93:LEU:O	1.84	0.77
1:E:269:HIS:CE1	1:F:269:HIS:CD2	2.73	0.77
1:E:105:ASN:ND2	2:E:401:NAD:C6N	2.49	0.76
1:C:130:THR:CG2	1:C:142:PHE:CD1	2.68	0.76
1:C:93:LEU:HD13	1:C:93:LEU:C	2.09	0.76
1:G:1:MET:SD	1:G:166:LYS:CD	2.74	0.76
1:C:11:MET:CE	2:C:401:NAD:C3N	2.64	0.74
1:D:119:MET:CE	1:D:152:LEU:HB2	2.18	0.74
1:G:1:MET:HE3	1:G:166:LYS:HD2	1.70	0.73
1:A:111:ASP:OD2	1:A:111:ASP:O	2.06	0.73
1:C:71:VAL:HG22	1:C:93:LEU:CD2	2.18	0.72
1:H:5:ILE:HD11	1:H:16:GLY:HA2	1.72	0.72
1:C:11:MET:HE3	2:C:401:NAD:C4N	2.20	0.72
1:H:82:GLN:OE1	2:H:401:NAD:H4B	1.89	0.72
1:H:309:LEU:C	1:H:310:ASN:HD22	1.98	0.71
1:C:74:ILE:HG21	1:C:93:LEU:HD11	1.72	0.71
1:F:36:VAL:HG22	1:F:37:GLN:OE1	1.90	0.71
1:C:310:ASN:C	3:C:503:HOH:O	2.33	0.70
1:C:70:GLN:HG2	3:C:501:HOH:O	1.91	0.70
1:H:235:GLU:O	1:H:235:GLU:CG	2.39	0.70
1:G:1:MET:CE	1:G:166:LYS:HD2	2.21	0.69
1:H:35:HIS:CD2	1:H:137:GLY:H	2.10	0.69
1:H:5:ILE:HD11	1:H:16:GLY:CA	2.23	0.69
1:D:119:MET:CE	1:D:152:LEU:CB	2.70	0.69
1:D:5:ILE:HD11	1:D:16:GLY:HA2	1.75	0.68
1:A:11:MET:HE3	2:A:401:NAD:C3N	2.23	0.68
1:F:189:CYS:O	1:F:193:THR:HB	1.93	0.68
1:D:11:MET:HE3	2:D:401:NAD:C3N	2.24	0.68
1:C:11:MET:HE3	2:C:401:NAD:C3N	2.22	0.68
1:D:40:LYS:HE3	3:D:505:HOH:O	1.93	0.68
1:A:105:ASN:HB2	2:A:401:NAD:O2D	1.94	0.67
1:D:119:MET:HE2	1:D:152:LEU:CB	2.25	0.67
1:H:235:GLU:N	1:H:235:GLU:OE1	2.27	0.67
1:G:91:GLN:HB3	3:G:528:HOH:O	1.95	0.66
1:G:25:GLU:HG3	3:G:532:HOH:O	1.94	0.66
1:H:11:MET:HE3	2:H:401:NAD:C3N	2.25	0.66
1:A:5:ILE:CD1	1:A:12:GLY:O	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HD11	1:D:16:GLY:CA	2.26	0.65
1:F:105:ASN:HB2	2:F:401:NAD:O2D	1.96	0.65
1:B:300:GLU:OE2	1:G:216:LYS:HE2	1.96	0.65
1:D:11:MET:HE3	2:D:401:NAD:C7N	2.26	0.65
1:E:5:ILE:CD1	1:E:12:GLY:O	2.45	0.65
1:D:310:ASN:OD1	1:D:310:ASN:N	2.30	0.64
1:E:128:MET:HE1	1:E:187:LYS:HG3	1.79	0.64
1:G:1:MET:SD	1:G:166:LYS:HD3	2.36	0.64
1:A:273:GLU:OE2	2:A:401:NAD:O3D	2.15	0.64
1:D:34:GLU:HG3	3:D:525:HOH:O	1.97	0.64
1:G:11:MET:HE3	2:G:401:NAD:C7N	2.28	0.64
1:D:309:LEU:C	1:D:310:ASN:OD1	2.41	0.64
1:C:310:ASN:N	1:C:310:ASN:OD1	2.31	0.64
1:B:5:ILE:CD1	1:B:12:GLY:O	2.46	0.63
1:E:269:HIS:CG	1:F:269:HIS:CG	2.87	0.63
1:G:5:ILE:CD1	1:G:12:GLY:O	2.46	0.63
1:H:114:GLU:O	1:H:115:LYS:CB	2.46	0.63
1:F:14:ARG:NH2	1:F:130:THR:O	2.32	0.63
1:G:11:MET:HE3	2:G:401:NAD:C3N	2.29	0.63
1:A:269:HIS:CD2	1:D:269:HIS:CD2	2.87	0.63
1:H:105:ASN:ND2	2:H:401:NAD:C6N	2.62	0.62
1:F:5:ILE:CD1	1:F:12:GLY:O	2.46	0.62
1:D:124:ILE:HG23	1:D:184:ILE:HD11	1.82	0.62
1:F:118:PRO:HD2	3:F:531:HOH:O	2.00	0.62
1:H:14:ARG:NH2	1:H:130:THR:O	2.31	0.62
1:F:11:MET:HE3	2:F:401:NAD:C3N	2.29	0.62
1:C:130:THR:HG22	1:C:142:PHE:CG	2.35	0.62
1:H:35:HIS:HD2	1:H:137:GLY:H	1.48	0.61
1:C:11:MET:HE2	2:C:401:NAD:C7N	2.30	0.61
1:C:104:LEU:HD13	2:C:401:NAD:O3D	2.00	0.61
1:C:11:MET:CE	2:C:401:NAD:C7N	2.79	0.61
1:F:11:MET:HE3	2:F:401:NAD:C7N	2.30	0.61
1:A:134:GLU:OE1	1:A:140:LYS:HD3	2.01	0.61
1:G:91:GLN:CB	3:G:528:HOH:O	2.48	0.61
1:C:5:ILE:CD1	1:C:12:GLY:O	2.48	0.61
1:B:269:HIS:CD2	1:C:269:HIS:CD2	2.89	0.60
1:B:263:GLN:HG3	3:B:524:HOH:O	2.02	0.60
1:H:310:ASN:N	1:H:310:ASN:ND2	2.48	0.60
1:A:40:LYS:O	1:A:56:LYS:HE3	2.02	0.60
1:H:235:GLU:H	1:H:235:GLU:CD	2.10	0.59
1:F:179:ASN:OD1	1:F:179:ASN:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:HIS:O	1:F:20:HIS:CD2	2.56	0.58
1:F:129:TRP:HZ3	1:F:172:LEU:C	2.12	0.58
1:C:74:ILE:HG22	1:C:93:LEU:HD21	1.84	0.58
1:A:11:MET:HE3	2:A:401:NAD:C7N	2.34	0.58
1:D:119:MET:HE1	1:D:152:LEU:HB2	1.86	0.58
1:B:82:GLN:HE22	2:B:401:NAD:H4B	1.69	0.58
1:E:134:GLU:OE1	1:E:140:LYS:HD3	2.04	0.58
1:F:82:GLN:HE22	2:F:401:NAD:C4B	2.16	0.58
1:F:165:ASP:O	1:F:166:LYS:C	2.45	0.58
1:H:36:VAL:O	1:H:36:VAL:CG2	2.46	0.58
1:H:105:ASN:HB2	2:H:401:NAD:O2D	2.03	0.57
1:B:247:SER:OG	3:B:505:HOH:O	2.13	0.57
1:D:119:MET:HE1	1:D:152:LEU:CB	2.34	0.57
1:C:217:MET:SD	1:H:301:LEU:HD13	2.44	0.57
1:D:79:LYS:HB3	1:D:81:MET:HE3	1.85	0.57
1:E:124:ILE:HD11	1:E:152:LEU:HD21	1.86	0.57
1:F:129:TRP:CZ3	1:F:172:LEU:HA	2.40	0.57
1:E:269:HIS:ND1	1:F:269:HIS:CG	2.73	0.56
1:F:273:GLU:OE1	2:F:401:NAD:O2D	2.19	0.56
2:F:401:NAD:H2B	2:F:401:NAD:O5B	2.05	0.56
1:D:119:MET:CE	1:D:152:LEU:HB3	2.36	0.56
1:B:74:ILE:HD13	1:B:90:ILE:CD1	2.36	0.56
1:G:124:ILE:HD11	1:G:152:LEU:HD21	1.88	0.56
1:E:11:MET:HE3	2:E:401:NAD:C7N	2.37	0.55
1:G:109:HIS:O	1:G:112:ILE:HD12	2.06	0.55
1:F:74:ILE:HD13	1:F:90:ILE:CD1	2.36	0.55
1:F:9:GLY:HA3	2:F:401:NAD:H2B	1.87	0.55
2:F:401:NAD:C2A	3:F:527:HOH:O	2.55	0.55
2:H:401:NAD:O5B	2:H:401:NAD:H2B	2.07	0.55
1:D:81:MET:CE	1:D:273:GLU:HG2	2.36	0.55
1:A:5:ILE:HD11	1:A:12:GLY:C	2.31	0.55
1:A:124:ILE:HD11	1:A:152:LEU:HD21	1.89	0.55
1:E:269:HIS:CG	1:F:269:HIS:CD2	2.95	0.55
1:F:5:ILE:HD11	1:F:12:GLY:C	2.31	0.55
1:B:178:ASP:OD2	1:B:178:ASP:N	2.39	0.55
1:F:193:THR:HG23	1:F:194:MET:HE2	1.89	0.55
1:C:309:LEU:C	1:C:310:ASN:OD1	2.51	0.54
1:B:124:ILE:HD11	1:B:152:LEU:HD21	1.89	0.54
1:D:74:ILE:HD13	1:D:90:ILE:CD1	2.38	0.54
1:F:124:ILE:HD11	1:F:152:LEU:HD21	1.89	0.54
1:G:79:LYS:NZ	2:G:401:NAD:O1A	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:OD1	1:B:310:ASN:N	2.40	0.53
1:C:124:ILE:HD11	1:C:152:LEU:HD21	1.88	0.53
1:E:74:ILE:HD13	1:E:90:ILE:CD1	2.38	0.53
1:C:11:MET:CE	2:C:401:NAD:C4N	2.87	0.53
1:H:178:ASP:OD1	1:H:178:ASP:N	2.41	0.53
1:D:178:ASP:OD1	1:D:178:ASP:N	2.40	0.53
1:E:269:HIS:CE1	1:F:269:HIS:CG	2.96	0.53
1:F:179:ASN:CG	1:F:182:TYR:HB3	2.33	0.53
1:E:207:GLU:HA	1:E:210:LYS:HE2	1.91	0.53
1:E:303:HIS:HD2	1:E:306:GLU:OE1	1.92	0.53
1:C:105:ASN:ND2	2:C:401:NAD:C6N	2.72	0.53
1:E:310:ASN:N	1:E:310:ASN:OD1	2.42	0.53
1:F:178:ASP:OD1	1:F:178:ASP:N	2.38	0.53
1:C:130:THR:CG2	1:C:142:PHE:CG	2.92	0.53
1:H:124:ILE:HD11	1:H:152:LEU:HD21	1.89	0.53
2:H:401:NAD:O5B	2:H:401:NAD:C2B	2.57	0.53
1:F:193:THR:CG2	1:F:194:MET:HE2	2.39	0.52
1:A:5:ILE:CD1	1:A:12:GLY:C	2.82	0.52
2:F:401:NAD:O5B	2:F:401:NAD:C2B	2.57	0.52
1:G:101:LEU:HD12	1:G:123:TYR:O	2.09	0.52
1:A:9:GLY:HA3	2:A:401:NAD:O5B	2.09	0.52
1:A:154:ASP:N	3:A:525:HOH:O	2.42	0.52
1:E:9:GLY:N	2:E:401:NAD:H3B	2.25	0.52
1:F:14:ARG:CZ	1:F:129:TRP:CD1	2.92	0.52
1:H:35:HIS:HD2	1:H:137:GLY:N	2.07	0.52
1:H:188:ALA:O	1:H:192:GLY:N	2.43	0.52
1:B:303:HIS:HD2	1:B:306:GLU:OE1	1.93	0.51
1:A:134:GLU:OE1	1:A:140:LYS:CD	2.58	0.51
1:A:178:ASP:OD1	1:A:178:ASP:N	2.39	0.51
1:E:269:HIS:CD2	1:F:269:HIS:CE1	2.98	0.51
1:F:130:THR:OG1	1:F:142:PHE:HB2	2.11	0.51
1:G:25:GLU:CG	3:G:532:HOH:O	2.54	0.51
1:C:9:GLY:CA	2:C:401:NAD:H3B	2.40	0.51
1:A:93:LEU:O	1:A:98:THR:HG21	2.10	0.51
1:C:9:GLY:HA3	2:C:401:NAD:H3B	1.93	0.51
1:C:101:LEU:HD12	1:C:123:TYR:O	2.11	0.51
1:D:130:THR:OG1	1:D:142:PHE:HB2	2.10	0.51
1:E:269:HIS:CG	1:F:269:HIS:CE1	2.99	0.51
1:H:87:LEU:HB3	1:H:116:PHE:CD2	2.46	0.51
1:B:105:ASN:HB2	2:B:401:NAD:O2D	2.11	0.51
1:D:101:LEU:HD12	1:D:123:TYR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:MET:HE2	1:D:152:LEU:HB3	1.89	0.51
1:D:128:MET:HE1	1:D:187:LYS:HG3	1.93	0.51
1:F:5:ILE:CD1	1:F:12:GLY:C	2.84	0.51
1:D:11:MET:CE	2:D:401:NAD:C7N	2.89	0.51
1:B:5:ILE:HD11	1:B:12:GLY:C	2.36	0.51
1:B:9:GLY:HA3	2:B:401:NAD:H3B	1.92	0.51
1:D:81:MET:HE2	1:D:273:GLU:HG2	1.93	0.51
1:G:303:HIS:HD2	1:G:306:GLU:OE1	1.94	0.51
1:B:11:MET:HE3	2:B:401:NAD:C7N	2.40	0.51
1:E:41:GLU:HB3	1:E:42:HIS:CD2	2.46	0.51
1:E:134:GLU:OE1	1:E:140:LYS:CD	2.59	0.50
1:F:101:LEU:HD12	1:F:123:TYR:O	2.11	0.50
1:F:303:HIS:HD2	1:F:306:GLU:OE1	1.94	0.50
1:B:130:THR:OG1	1:B:142:PHE:HB2	2.11	0.50
1:B:239:PRO:HG3	1:D:22:SER:CB	2.35	0.50
1:G:1:MET:CE	3:G:515:HOH:O	2.59	0.50
1:H:101:LEU:HD12	1:H:123:TYR:O	2.11	0.50
1:C:74:ILE:HD13	1:C:90:ILE:CD1	2.41	0.50
1:A:71:VAL:N	3:A:530:HOH:O	2.45	0.50
1:C:303:HIS:HD2	1:C:306:GLU:OE1	1.94	0.50
1:D:293:PRO:HG3	1:F:293:PRO:HG3	1.93	0.50
1:A:60:VAL:HG22	1:A:61:LEU:O	2.12	0.50
1:A:128:MET:HE1	1:A:187:LYS:HG3	1.94	0.50
1:B:99:GLU:HB3	3:B:522:HOH:O	2.11	0.50
1:D:303:HIS:HD2	1:D:306:GLU:OE1	1.95	0.50
1:A:207:GLU:HA	1:A:210:LYS:HE2	1.94	0.50
1:E:101:LEU:HD12	1:E:123:TYR:O	2.12	0.50
1:H:207:GLU:HA	1:H:210:LYS:HE2	1.94	0.50
1:E:79:LYS:HD3	2:E:401:NAD:H3D	1.93	0.49
1:A:204:ASN:OD1	1:A:204:ASN:C	2.54	0.49
1:G:79:LYS:C	1:G:81:MET:H	2.20	0.49
1:A:142:PHE:H	1:A:142:PHE:HD2	1.59	0.49
1:E:11:MET:HE3	2:E:401:NAD:C3N	2.42	0.49
1:E:11:MET:HE1	1:E:130:THR:C	2.37	0.49
1:H:209:GLY:HA3	1:H:249:PHE:CG	2.47	0.49
1:F:310:ASN:N	1:F:310:ASN:OD1	2.44	0.49
1:C:47:ASN:HD22	1:C:47:ASN:C	2.19	0.49
1:D:41:GLU:HB3	1:D:42:HIS:CD2	2.48	0.49
1:G:207:GLU:HA	1:G:210:LYS:HE2	1.95	0.49
1:A:303:HIS:HD2	1:A:306:GLU:OE1	1.96	0.49
1:C:60:VAL:HG22	1:C:61:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLU:HG3	1:D:123:TYR:CE1	2.47	0.49
1:E:5:ILE:HD11	1:E:12:GLY:C	2.38	0.49
1:H:303:HIS:HD2	1:H:306:GLU:OE1	1.93	0.49
1:H:309:LEU:C	1:H:310:ASN:ND2	2.68	0.49
1:A:173:ASN:HB2	3:A:520:HOH:O	2.13	0.49
1:D:119:MET:O	1:D:119:MET:HE3	2.13	0.49
1:E:10:ALA:HB3	2:E:401:NAD:O1N	2.12	0.49
1:E:109:HIS:HA	3:E:502:HOH:O	2.13	0.49
1:F:204:ASN:OD1	1:F:204:ASN:C	2.56	0.49
1:C:93:LEU:O	1:C:98:THR:HG21	2.13	0.48
1:B:11:MET:CE	2:B:401:NAD:C7N	2.91	0.48
1:C:11:MET:HE2	2:C:401:NAD:C3N	2.43	0.48
1:E:9:GLY:H	2:E:401:NAD:H3B	1.78	0.48
1:F:82:GLN:HE22	2:F:401:NAD:H4B	1.77	0.48
1:G:41:GLU:HB3	1:G:42:HIS:CD2	2.48	0.48
1:B:48:PHE:HD1	1:B:49:ASN:ND2	2.11	0.48
1:F:128:MET:HE1	1:F:187:LYS:HG3	1.94	0.48
1:F:188:ALA:O	1:F:192:GLY:N	2.46	0.48
1:D:20:HIS:HB2	1:D:26:VAL:HG13	1.96	0.48
1:G:216:LYS:HD2	1:G:216:LYS:C	2.38	0.48
1:B:101:LEU:HD12	1:B:123:TYR:O	2.14	0.48
1:C:41:GLU:HB3	1:C:42:HIS:CD2	2.49	0.48
1:D:119:MET:HE2	1:D:152:LEU:HB2	1.88	0.48
1:G:105:ASN:ND2	2:G:401:NAD:C6N	2.75	0.48
1:A:5:ILE:HD12	1:A:12:GLY:O	2.13	0.48
1:A:11:MET:CE	2:A:401:NAD:C7N	2.92	0.48
1:C:128:MET:HE1	1:C:187:LYS:HG3	1.95	0.48
1:E:269:HIS:HB3	1:F:269:HIS:CE1	2.47	0.48
1:F:207:GLU:HA	1:F:210:LYS:HE2	1.95	0.48
1:G:192:GLY:HA2	1:G:278:ASN:HD21	1.79	0.48
1:H:11:MET:HE3	2:H:401:NAD:C7N	2.44	0.48
1:B:166:LYS:NZ	3:B:525:HOH:O	2.45	0.48
1:G:178:ASP:OD1	1:G:178:ASP:N	2.37	0.48
1:H:5:ILE:CD1	1:H:16:GLY:CA	2.91	0.48
1:D:5:ILE:CD1	1:D:16:GLY:CA	2.92	0.48
1:G:188:ALA:O	1:G:192:GLY:N	2.46	0.48
1:B:5:ILE:CD1	1:B:12:GLY:C	2.87	0.47
1:D:204:ASN:OD1	1:D:204:ASN:C	2.58	0.47
1:F:165:ASP:O	1:F:166:LYS:O	2.31	0.47
1:A:79:LYS:HD3	2:A:401:NAD:H3D	1.96	0.47
1:E:178:ASP:OD1	1:E:178:ASP:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLN:H	1:C:45:GLN:HG2	1.47	0.47
1:G:60:VAL:HG22	1:G:61:LEU:O	2.13	0.47
1:B:5:ILE:HD12	1:B:12:GLY:O	2.13	0.47
1:H:192:GLY:HA2	1:H:278:ASN:HD21	1.79	0.47
1:B:41:GLU:HB3	1:B:42:HIS:CD2	2.50	0.47
1:A:101:LEU:HD12	1:A:123:TYR:O	2.14	0.47
1:C:188:ALA:O	1:C:192:GLY:N	2.48	0.47
1:D:60:VAL:HG22	1:D:61:LEU:O	2.14	0.47
1:D:188:ALA:O	1:D:192:GLY:N	2.48	0.47
1:G:216:LYS:C	1:G:216:LYS:CD	2.88	0.47
1:G:19:LEU:O	1:G:24:ASN:HB2	2.15	0.47
1:C:129:TRP:CD2	1:C:145:GLY:HA3	2.49	0.47
1:E:105:ASN:HD21	2:E:401:NAD:C5N	2.27	0.47
1:H:128:MET:HE1	1:H:187:LYS:HG3	1.96	0.47
1:G:109:HIS:O	1:G:110:GLU:C	2.56	0.46
1:B:72:ASP:O	1:B:99:GLU:HB2	2.14	0.46
1:C:72:ASP:O	1:C:99:GLU:HB2	2.15	0.46
1:G:5:ILE:HD11	1:G:12:GLY:C	2.40	0.46
1:H:204:ASN:OD1	1:H:204:ASN:C	2.58	0.46
1:B:128:MET:HE1	1:B:187:LYS:HG3	1.98	0.46
1:E:130:THR:OG1	1:E:142:PHE:HB2	2.14	0.46
1:E:195:ASN:HD22	1:E:259:PRO:HB2	1.79	0.46
1:F:35:HIS:O	1:F:36:VAL:C	2.58	0.46
1:A:180:ILE:CG2	1:A:181:HIS:N	2.78	0.46
1:B:79:LYS:H	1:B:82:GLN:HE21	1.63	0.46
1:B:192:GLY:HA2	1:B:278:ASN:HD21	1.80	0.46
1:E:5:ILE:HD12	1:E:12:GLY:O	2.14	0.46
1:G:180:ILE:HD12	1:G:180:ILE:HA	1.80	0.46
1:B:147:VAL:HB	1:B:174:ALA:CB	2.46	0.46
1:F:5:ILE:HD12	1:F:12:GLY:O	2.15	0.46
1:C:206:ALA:O	1:C:210:LYS:HG2	2.16	0.45
1:D:87:LEU:O	1:D:88:GLN:C	2.59	0.45
1:E:60:VAL:HG22	1:E:61:LEU:O	2.16	0.45
1:A:292:THR:N	1:A:293:PRO:CD	2.78	0.45
1:G:11:MET:HE2	1:G:131:ALA:HB3	1.99	0.45
1:H:149:LEU:HD12	1:H:149:LEU:C	2.41	0.45
1:D:216:LYS:O	1:D:216:LYS:HD3	2.16	0.45
1:C:192:GLY:HA2	1:C:278:ASN:HD21	1.82	0.45
1:C:97:ASP:OD1	1:C:97:ASP:N	2.49	0.45
1:G:147:VAL:HB	1:G:174:ALA:CB	2.46	0.45
1:B:60:VAL:HG22	1:B:61:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:C	1:B:204:ASN:OD1	2.60	0.45
1:C:74:ILE:CG2	1:C:93:LEU:HD21	2.46	0.45
1:E:156:LYS:HB3	1:E:156:LYS:HE2	1.70	0.45
1:G:82:GLN:HE22	2:G:401:NAD:C4B	2.30	0.45
1:B:109:HIS:O	1:B:110:GLU:C	2.60	0.45
1:F:11:MET:HE1	1:F:130:THR:C	2.42	0.45
1:H:21:GLN:HG2	3:H:520:HOH:O	2.17	0.45
1:C:293:PRO:HG3	1:H:293:PRO:HG3	1.99	0.45
1:B:11:MET:HE1	1:B:130:THR:C	2.42	0.44
1:D:20:HIS:HB2	1:D:26:VAL:CG1	2.47	0.44
1:E:47:ASN:HB3	1:E:140:LYS:HD2	1.99	0.44
1:F:267:LYS:HE3	1:F:267:LYS:HB3	1.83	0.44
1:E:138:GLN:OE1	1:E:138:GLN:HA	2.17	0.44
1:C:47:ASN:C	1:C:47:ASN:ND2	2.74	0.44
1:G:209:GLY:HA3	1:G:249:PHE:CG	2.53	0.44
1:B:5:ILE:HG21	1:B:5:ILE:HD13	1.73	0.44
1:F:129:TRP:CZ3	1:F:172:LEU:C	2.93	0.44
1:G:5:ILE:HD12	1:G:12:GLY:O	2.15	0.44
1:G:149:LEU:C	1:G:149:LEU:HD12	2.43	0.44
1:B:237:ASP:OD1	1:B:237:ASP:C	2.59	0.44
1:F:133:LEU:CD2	2:F:401:NAD:H8A	2.48	0.44
1:G:237:ASP:OD1	1:G:237:ASP:C	2.59	0.44
1:D:209:GLY:HA3	1:D:249:PHE:CG	2.52	0.44
1:G:87:LEU:O	1:G:88:GLN:C	2.60	0.44
1:A:209:GLY:HA3	1:A:249:PHE:CG	2.53	0.44
1:B:294:TYR:OH	1:G:300:GLU:OE1	2.33	0.44
1:C:178:ASP:OD1	1:C:178:ASP:N	2.38	0.44
1:G:11:MET:CE	2:G:401:NAD:C7N	2.96	0.44
1:G:17:LEU:HD22	1:G:17:LEU:O	2.18	0.44
1:D:180:ILE:HD12	1:D:180:ILE:HA	1.87	0.44
1:B:180:ILE:CG2	1:B:181:HIS:N	2.80	0.43
1:F:192:GLY:HA2	1:F:278:ASN:HD21	1.82	0.43
1:B:10:ALA:HB3	2:B:401:NAD:O1N	2.18	0.43
1:C:5:ILE:HD11	1:C:12:GLY:C	2.43	0.43
1:D:99:GLU:HG3	1:D:123:TYR:HE1	1.83	0.43
1:A:87:LEU:O	1:A:88:GLN:C	2.62	0.43
1:E:195:ASN:ND2	1:E:259:PRO:HB2	2.32	0.43
1:A:41:GLU:HB3	1:A:42:HIS:CD2	2.53	0.43
1:E:182:TYR:HE2	3:E:510:HOH:O	2.01	0.43
1:H:185:TYR:O	1:H:186:ARG:C	2.60	0.43
1:D:104:LEU:HA	2:D:401:NAD:O3D	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLY:HA2	1:D:278:ASN:HD21	1.83	0.43
1:D:79:LYS:H	1:D:82:GLN:HE21	1.67	0.43
1:F:179:ASN:CG	1:F:180:ILE:N	2.73	0.43
1:D:104:LEU:HG	2:D:401:NAD:O3D	2.18	0.43
1:E:105:ASN:HB2	2:E:401:NAD:O2D	2.18	0.43
1:G:169:GLU:HG2	3:G:506:HOH:O	2.18	0.43
1:A:11:MET:HE2	1:A:131:ALA:HB3	2.00	0.43
1:F:129:TRP:CD2	1:F:145:GLY:HA3	2.54	0.43
1:G:5:ILE:CD1	1:G:12:GLY:C	2.92	0.43
1:G:5:ILE:HD13	1:G:5:ILE:HG21	1.73	0.43
1:H:306:GLU:O	1:H:310:ASN:N	2.38	0.42
1:C:5:ILE:HD12	1:C:12:GLY:O	2.19	0.42
1:F:104:LEU:HD13	2:F:401:NAD:O3D	2.19	0.42
1:F:209:GLY:HA3	1:F:249:PHE:CG	2.54	0.42
1:A:187:LYS:HB3	3:A:504:HOH:O	2.18	0.42
1:A:294:TYR:CZ	1:E:297:PHE:HB2	2.54	0.42
1:D:85:LYS:HD2	1:D:85:LYS:HA	1.88	0.42
1:G:193:THR:O	1:G:194:MET:C	2.61	0.42
1:D:294:TYR:OH	1:F:300:GLU:OE1	2.35	0.42
2:H:401:NAD:O2N	2:H:401:NAD:O2A	2.37	0.42
1:E:5:ILE:CD1	1:E:12:GLY:C	2.92	0.42
1:E:134:GLU:HB2	1:E:138:GLN:HG3	2.02	0.42
1:E:36:VAL:HG11	1:E:61:LEU:HD12	2.01	0.42
1:F:9:GLY:CA	2:F:401:NAD:H2B	2.50	0.42
1:G:83:LEU:HD21	1:G:112:ILE:HD13	2.02	0.42
1:B:104:LEU:HD13	2:B:401:NAD:O3D	2.19	0.42
1:B:133:LEU:HD12	1:B:139:VAL:HG12	2.01	0.42
1:C:147:VAL:HB	1:C:174:ALA:CB	2.50	0.42
1:D:39:ILE:HA	1:D:43:GLY:O	2.20	0.42
1:E:79:LYS:HE2	1:E:264:ASP:OD2	2.20	0.42
1:E:86:MET:O	1:E:90:ILE:HG12	2.20	0.42
1:G:17:LEU:CD1	1:G:48:PHE:CE2	3.02	0.42
1:H:120:GLU:HG3	1:H:121:ASN:OD1	2.19	0.42
1:H:237:ASP:C	1:H:237:ASP:OD1	2.62	0.42
1:B:79:LYS:C	1:B:81:MET:H	2.28	0.42
1:B:188:ALA:O	1:B:192:GLY:N	2.53	0.42
1:D:147:VAL:HB	1:D:174:ALA:CB	2.49	0.42
1:A:192:GLY:HA2	1:A:278:ASN:HD21	1.85	0.41
1:C:39:ILE:HA	1:C:43:GLY:O	2.20	0.41
1:C:79:LYS:C	1:C:81:MET:H	2.27	0.41
1:D:11:MET:HE1	1:D:130:THR:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD23	1:D:87:LEU:HA	1.78	0.41
1:E:269:HIS:CG	1:F:269:HIS:ND1	2.88	0.41
1:G:11:MET:HE1	1:G:130:THR:C	2.45	0.41
1:C:5:ILE:HD13	1:C:5:ILE:HG21	1.72	0.41
1:E:11:MET:HE2	1:E:131:ALA:HB3	2.01	0.41
1:E:129:TRP:CD2	1:E:145:GLY:HA3	2.54	0.41
1:E:147:VAL:HB	1:E:174:ALA:CB	2.50	0.41
1:E:192:GLY:HA2	1:E:278:ASN:HD21	1.84	0.41
1:A:36:VAL:HG11	1:A:61:LEU:HD12	2.02	0.41
1:A:180:ILE:HG23	1:A:181:HIS:N	2.35	0.41
1:C:85:LYS:HA	1:C:85:LYS:HD2	1.88	0.41
1:D:36:VAL:HG11	1:D:61:LEU:HD12	2.01	0.41
1:F:5:ILE:HD13	1:F:5:ILE:HG21	1.74	0.41
1:C:93:LEU:C	1:C:93:LEU:CD1	2.80	0.41
1:E:193:THR:O	1:E:194:MET:C	2.61	0.41
1:F:11:MET:CE	2:F:401:NAD:C7N	2.99	0.41
1:F:258:TYR:CD1	1:F:262:TYR:CE2	3.09	0.41
1:C:193:THR:O	1:C:194:MET:C	2.60	0.41
1:H:109:HIS:O	1:H:110:GLU:C	2.63	0.41
1:A:5:ILE:HD13	1:A:5:ILE:HG21	1.76	0.41
1:A:11:MET:HE1	1:A:130:THR:C	2.45	0.41
1:F:86:MET:O	1:F:90:ILE:HG12	2.21	0.41
1:A:147:VAL:HB	1:A:174:ALA:CB	2.51	0.41
1:B:99:GLU:CG	3:B:522:HOH:O	2.46	0.41
1:G:246:GLU:O	1:G:247:SER:C	2.63	0.41
1:H:147:VAL:HB	1:H:174:ALA:CB	2.51	0.41
1:A:261:MET:HG3	1:A:272:THR:CG2	2.50	0.41
1:D:11:MET:CE	2:D:401:NAD:O7N	2.69	0.41
1:D:193:THR:O	1:D:194:MET:C	2.63	0.41
1:D:303:HIS:O	1:D:304:ALA:C	2.61	0.41
1:A:86:MET:O	1:A:90:ILE:HG12	2.20	0.41
1:B:233:LYS:C	1:B:234:ILE:HG13	2.46	0.41
1:E:309:LEU:C	1:E:310:ASN:OD1	2.64	0.41
1:F:20:HIS:O	1:F:20:HIS:HD2	2.02	0.41
1:F:231:VAL:HG11	1:F:288:TYR:CG	2.55	0.41
1:G:15:PHE:O	1:G:16:GLY:C	2.63	0.41
1:G:39:ILE:HA	1:G:43:GLY:O	2.21	0.41
1:C:87:LEU:O	1:C:88:GLN:C	2.64	0.41
1:C:204:ASN:OD1	1:C:204:ASN:C	2.63	0.41
1:D:216:LYS:C	1:D:216:LYS:CD	2.94	0.41
1:E:19:LEU:O	1:E:24:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ASN:ND2	1:F:259:PRO:HB2	2.36	0.41
1:C:5:ILE:CD1	1:C:12:GLY:C	2.94	0.40
1:C:9:GLY:N	2:C:401:NAD:H3B	2.35	0.40
1:E:105:ASN:ND2	2:E:401:NAD:C5N	2.84	0.40
1:E:188:ALA:O	1:E:192:GLY:N	2.55	0.40
1:H:135:GLY:O	1:H:136:PRO:C	2.64	0.40
1:B:261:MET:HG3	1:B:272:THR:CG2	2.51	0.40
1:D:106:GLY:H	1:D:109:HIS:HE1	1.70	0.40
1:F:79:LYS:C	1:F:81:MET:H	2.29	0.40
1:G:11:MET:CE	2:G:401:NAD:N7N	2.84	0.40
1:G:83:LEU:O	1:G:87:LEU:HD22	2.21	0.40
1:F:79:LYS:H	1:F:82:GLN:HE21	1.68	0.40
1:F:180:ILE:CG2	1:F:181:HIS:N	2.85	0.40
1:A:269:HIS:CG	1:D:269:HIS:CG	3.09	0.40
1:B:309:LEU:C	1:B:310:ASN:OD1	2.64	0.40
1:D:119:MET:HE3	1:D:119:MET:HA	2.02	0.40
1:D:180:ILE:CG2	1:D:181:HIS:N	2.84	0.40
1:E:11:MET:HE1	1:E:131:ALA:N	2.36	0.40
1:E:79:LYS:C	1:E:81:MET:H	2.29	0.40
1:E:203:VAL:HB	1:E:207:GLU:HB2	2.02	0.40
1:G:91:GLN:HB2	3:G:528:HOH:O	2.18	0.40
1:A:297:PHE:HB2	1:E:294:TYR:CZ	2.57	0.40
1:E:87:LEU:O	1:E:88:GLN:C	2.64	0.40
1:E:209:GLY:HA3	1:E:249:PHE:CG	2.57	0.40
1:E:286:LYS:HE2	1:E:286:LYS:HB3	1.89	0.40
1:F:105:ASN:ND2	2:F:401:NAD:C6N	2.85	0.40
1:H:275:ASP:O	1:H:283:ARG:NH2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/312 (93%)	265 (91%)	19 (6%)	7 (2%)	4	17
1	B	287/312 (92%)	262 (91%)	20 (7%)	5 (2%)	7	25
1	C	285/312 (91%)	257 (90%)	21 (7%)	7 (2%)	4	16
1	D	283/312 (91%)	256 (90%)	22 (8%)	5 (2%)	6	23
1	E	293/312 (94%)	269 (92%)	17 (6%)	7 (2%)	4	17
1	F	251/312 (80%)	226 (90%)	18 (7%)	7 (3%)	4	14
1	G	292/312 (94%)	266 (91%)	21 (7%)	5 (2%)	7	25
1	H	238/312 (76%)	218 (92%)	14 (6%)	6 (2%)	4	16
All	All	2220/2496 (89%)	2019 (91%)	152 (7%)	49 (2%)	5	19

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	LEU
1	B	142	PHE
1	C	104	LEU
1	C	142	PHE
1	D	104	LEU
1	D	142	PHE
1	E	142	PHE
1	F	104	LEU
1	F	142	PHE
1	G	104	LEU
1	H	104	LEU
1	A	98	THR
1	A	104	LEU
1	A	253	THR
1	B	253	THR
1	C	253	THR
1	D	253	THR
1	E	104	LEU
1	E	253	THR
1	F	253	THR
1	G	253	THR
1	H	115	LYS
1	H	253	THR
1	F	248	CYS
1	G	57	LEU
1	A	99	GLU
1	B	248	CYS

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Mol	Chain	Res	Type
1	C	99	GLU
1	F	195	ASN
1	G	49	ASN
1	C	277	ILE
1	D	248	CYS
1	D	277	ILE
1	E	248	CYS
1	A	248	CYS
1	C	248	CYS
1	E	277	ILE
1	H	277	ILE
1	A	277	ILE
1	B	277	ILE
1	F	180	ILE
1	G	277	ILE
1	F	277	ILE
1	E	180	ILE
1	A	180	ILE
1	E	9	GLY
1	H	9	GLY
1	C	9	GLY
1	H	180	ILE

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	249/261 (95%)	224 (90%)	25 (10%)	7	24
1	B	245/261 (94%)	224 (91%)	21 (9%)	10	31
1	C	246/261 (94%)	221 (90%)	25 (10%)	7	23
1	D	244/261 (94%)	227 (93%)	17 (7%)	14	40
1	E	249/261 (95%)	224 (90%)	25 (10%)	7	24
1	F	219/261 (84%)	195 (89%)	24 (11%)	6	20
1	G	247/261 (95%)	217 (88%)	30 (12%)	5	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	205/261 (78%)	189 (92%)	16 (8%)	11	35
All	All	1904/2088 (91%)	1721 (90%)	183 (10%)	8	26

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	ILE
1	A	45	GLN
1	A	52	GLU
1	A	61	LEU
1	A	71	VAL
1	A	77	PHE
1	A	79	LYS
1	A	81	MET
1	A	85	LYS
1	A	87	LEU
1	A	93	LEU
1	A	97	ASP
1	A	98	THR
1	A	110	GLU
1	A	117	VAL
1	A	120	GLU
1	A	124	ILE
1	A	142	PHE
1	A	156	LYS
1	A	157	GLU
1	A	180	ILE
1	A	210	LYS
1	A	252	GLU
1	A	286	LYS
1	B	3	ILE
1	B	5	ILE
1	B	25	GLU
1	B	56	LYS
1	B	61	LEU
1	B	71	VAL
1	B	74	ILE
1	B	77	PHE
1	B	79	LYS
1	B	81	MET
1	B	87	LEU

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Mol	Chain	Res	Type
1	B	99	GLU
1	B	110	GLU
1	B	117	VAL
1	B	120	GLU
1	B	124	ILE
1	B	180	ILE
1	B	205	MET
1	B	252	GLU
1	B	286	LYS
1	B	310	ASN
1	C	3	ILE
1	C	5	ILE
1	C	45	GLN
1	C	61	LEU
1	C	70	GLN
1	C	71	VAL
1	C	74	ILE
1	C	77	PHE
1	C	79	LYS
1	C	81	MET
1	C	87	LEU
1	C	93	LEU
1	C	97	ASP
1	C	98	THR
1	C	117	VAL
1	C	120	GLU
1	C	124	ILE
1	C	130	THR
1	C	141	LEU
1	C	180	ILE
1	C	205	MET
1	C	210	LYS
1	C	252	GLU
1	C	286	LYS
1	C	310	ASN
1	D	3	ILE
1	D	26	VAL
1	D	61	LEU
1	D	63	SER
1	D	70	GLN
1	D	71	VAL
1	D	74	ILE

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Mol	Chain	Res	Type
1	D	77	PHE
1	D	117	VAL
1	D	120	GLU
1	D	124	ILE
1	D	141	LEU
1	D	180	ILE
1	D	216	LYS
1	D	252	GLU
1	D	286	LYS
1	D	310	ASN
1	E	3	ILE
1	E	5	ILE
1	E	61	LEU
1	E	71	VAL
1	E	74	ILE
1	E	77	PHE
1	E	79	LYS
1	E	81	MET
1	E	87	LEU
1	E	93	LEU
1	E	99	GLU
1	E	117	VAL
1	E	120	GLU
1	E	124	ILE
1	E	140	LYS
1	E	141	LEU
1	E	156	LYS
1	E	178	ASP
1	E	180	ILE
1	E	205	MET
1	E	210	LYS
1	E	252	GLU
1	E	286	LYS
1	E	309	LEU
1	E	310	ASN
1	F	5	ILE
1	F	36	VAL
1	F	37	GLN
1	F	60	VAL
1	F	74	ILE
1	F	77	PHE
1	F	79	LYS

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Mol	Chain	Res	Type
1	F	81	MET
1	F	85	LYS
1	F	87	LEU
1	F	117	VAL
1	F	120	GLU
1	F	124	ILE
1	F	129	TRP
1	F	134	GLU
1	F	157	GLU
1	F	178	ASP
1	F	179	ASN
1	F	180	ILE
1	F	193	THR
1	F	210	LYS
1	F	252	GLU
1	F	286	LYS
1	F	310	ASN
1	G	3	ILE
1	G	5	ILE
1	G	17	LEU
1	G	21	GLN
1	G	37	GLN
1	G	56	LYS
1	G	57	LEU
1	G	61	LEU
1	G	71	VAL
1	G	77	PHE
1	G	81	MET
1	G	87	LEU
1	G	95	LYS
1	G	96	LYS
1	G	99	GLU
1	G	112	ILE
1	G	117	VAL
1	G	120	GLU
1	G	124	ILE
1	G	126	ASN
1	G	128	MET
1	G	141	LEU
1	G	142	PHE
1	G	166	LYS
1	G	205	MET

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Mol	Chain	Res	Type
1	G	210	LYS
1	G	216	LYS
1	G	252	GLU
1	G	269	HIS
1	G	286	LYS
1	H	3	ILE
1	H	36	VAL
1	H	74	ILE
1	H	77	PHE
1	H	87	LEU
1	H	117	VAL
1	H	124	ILE
1	H	178	ASP
1	H	180	ILE
1	H	210	LYS
1	H	233	LYS
1	H	252	GLU
1	H	269	HIS
1	H	286	LYS
1	H	301	LEU
1	H	310	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	42	HIS
1	A	88	GLN
1	A	109	HIS
1	A	175	HIS
1	A	195	ASN
1	A	223	ASN
1	A	269	HIS
1	A	278	ASN
1	A	303	HIS
1	B	24	ASN
1	B	42	HIS
1	B	82	GLN
1	B	88	GLN
1	B	91	GLN
1	B	109	HIS
1	B	175	HIS

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Mol	Chain	Res	Type
1	B	195	ASN
1	B	268	ASN
1	B	269	HIS
1	B	278	ASN
1	B	303	HIS
1	C	24	ASN
1	C	42	HIS
1	C	47	ASN
1	C	91	GLN
1	C	109	HIS
1	C	173	ASN
1	C	175	HIS
1	C	181	HIS
1	C	195	ASN
1	C	223	ASN
1	C	269	HIS
1	C	278	ASN
1	C	303	HIS
1	D	24	ASN
1	D	42	HIS
1	D	45	GLN
1	D	82	GLN
1	D	91	GLN
1	D	109	HIS
1	D	175	HIS
1	D	195	ASN
1	D	223	ASN
1	D	269	HIS
1	D	278	ASN
1	D	303	HIS
1	E	42	HIS
1	E	91	GLN
1	E	109	HIS
1	E	195	ASN
1	E	223	ASN
1	E	269	HIS
1	E	278	ASN
1	E	303	HIS
1	F	20	HIS
1	F	82	GLN
1	F	109	HIS
1	F	195	ASN

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Mol	Chain	Res	Type
1	F	269	HIS
1	F	278	ASN
1	F	303	HIS
1	G	21	GLN
1	G	42	HIS
1	G	82	GLN
1	G	109	HIS
1	G	175	HIS
1	G	195	ASN
1	G	223	ASN
1	G	269	HIS
1	G	278	ASN
1	G	303	HIS
1	H	35	HIS
1	H	88	GLN
1	H	109	HIS
1	H	173	ASN
1	H	175	HIS
1	H	195	ASN
1	H	278	ASN
1	H	310	ASN

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](#)

8 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	401	-	46,48,48	1.91	11 (23%)	64,73,73	2.22	21 (32%)
2	NAD	E	401	-	46,48,48	2.02	11 (23%)	64,73,73	3.08	30 (46%)
2	NAD	G	401	-	46,48,48	1.69	8 (17%)	64,73,73	2.76	29 (45%)
2	NAD	F	401	-	46,48,48	1.79	11 (23%)	64,73,73	3.26	28 (43%)
2	NAD	B	401	-	46,48,48	1.88	13 (28%)	64,73,73	2.43	30 (46%)
2	NAD	H	401	-	46,48,48	1.97	8 (17%)	64,73,73	2.19	24 (37%)
2	NAD	D	401	-	46,48,48	1.78	9 (19%)	64,73,73	2.43	23 (35%)
2	NAD	A	401	-	46,48,48	2.11	12 (26%)	64,73,73	2.62	25 (39%)

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	401	-	-	4/30/62/62	0/5/5/5
2	NAD	E	401	-	-	4/30/62/62	0/5/5/5
2	NAD	G	401	-	-	8/30/62/62	0/5/5/5
2	NAD	F	401	-	-	8/30/62/62	0/5/5/5
2	NAD	B	401	-	-	7/30/62/62	0/5/5/5
2	NAD	H	401	-	-	13/30/62/62	0/5/5/5
2	NAD	D	401	-	-	9/30/62/62	0/5/5/5
2	NAD	A	401	-	-	5/30/62/62	0/5/5/5

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	PA-O3	10.52	1.70	1.59
2	H	401	NAD	PA-O3	7.59	1.67	1.59
2	E	401	NAD	C5A-C4A	6.65	1.50	1.39
2	G	401	NAD	C5A-C4A	5.99	1.49	1.39
2	F	401	NAD	PA-O3	5.50	1.65	1.59
2	B	401	NAD	PA-O3	5.37	1.65	1.59
2	D	401	NAD	C5A-N7A	-5.23	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAD	PN-O3	5.22	1.65	1.59
2	D	401	NAD	PN-O3	4.89	1.64	1.59
2	C	401	NAD	C8A-N7A	4.88	1.41	1.31
2	H	401	NAD	C5A-C4A	4.78	1.47	1.39
2	E	401	NAD	C2A-N1A	4.62	1.42	1.33
2	C	401	NAD	PN-O3	4.59	1.64	1.59
2	C	401	NAD	C5A-C4A	4.31	1.46	1.39
2	F	401	NAD	O3B-C3B	4.31	1.53	1.43
2	B	401	NAD	C4A-N9A	-4.19	1.29	1.37
2	E	401	NAD	C4A-N3A	4.15	1.42	1.34
2	E	401	NAD	C7N-N7N	4.15	1.40	1.33
2	F	401	NAD	C5A-C4A	3.88	1.46	1.39
2	F	401	NAD	C4A-N3A	3.82	1.41	1.34
2	C	401	NAD	C1B-N9A	3.66	1.56	1.46
2	B	401	NAD	PN-O3	3.65	1.63	1.59
2	E	401	NAD	O7N-C7N	3.63	1.30	1.24
2	G	401	NAD	C4A-N9A	-3.58	1.30	1.37
2	F	401	NAD	C3B-C4B	3.49	1.61	1.53
2	B	401	NAD	C2B-C3B	-3.48	1.43	1.53
2	C	401	NAD	PA-O3	3.47	1.63	1.59
2	C	401	NAD	C2N-C3N	3.45	1.44	1.39
2	H	401	NAD	C8A-N7A	3.44	1.38	1.31
2	E	401	NAD	C4A-N9A	-3.41	1.30	1.37
2	F	401	NAD	C8A-N7A	3.31	1.38	1.31
2	A	401	NAD	C5A-C4A	3.25	1.44	1.39
2	A	401	NAD	O4D-C1D	3.23	1.45	1.40
2	H	401	NAD	C4A-N9A	-3.23	1.31	1.37
2	G	401	NAD	C8A-N7A	3.17	1.37	1.31
2	D	401	NAD	C5A-C4A	3.14	1.44	1.39
2	C	401	NAD	C4A-N9A	-3.11	1.31	1.37
2	B	401	NAD	C5A-C4A	3.09	1.44	1.39
2	D	401	NAD	C8A-N9A	-2.96	1.32	1.37
2	G	401	NAD	C7N-N7N	2.90	1.38	1.33
2	D	401	NAD	O4D-C1D	2.86	1.44	1.40
2	E	401	NAD	C6A-N1A	2.79	1.43	1.35
2	F	401	NAD	O4D-C1D	2.75	1.44	1.40
2	B	401	NAD	C8A-N7A	2.73	1.36	1.31
2	B	401	NAD	C7N-N7N	2.73	1.38	1.33
2	A	401	NAD	C8A-N9A	-2.66	1.33	1.37
2	G	401	NAD	C4A-N3A	2.64	1.39	1.34
2	E	401	NAD	C2A-N3A	2.61	1.38	1.33
2	G	401	NAD	C2A-N1A	2.57	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAD	O4D-C4D	2.54	1.50	1.45
2	A	401	NAD	C5A-C6A	2.53	1.48	1.41
2	C	401	NAD	C4A-N3A	2.50	1.39	1.34
2	F	401	NAD	C4A-N9A	-2.45	1.32	1.37
2	B	401	NAD	PN-O1N	2.43	1.59	1.50
2	A	401	NAD	O2D-C2D	-2.42	1.37	1.43
2	A	401	NAD	C4A-N9A	-2.41	1.32	1.37
2	H	401	NAD	O4D-C1D	2.39	1.44	1.40
2	B	401	NAD	C4A-N3A	-2.39	1.29	1.34
2	F	401	NAD	C5A-C6A	2.39	1.47	1.41
2	D	401	NAD	C4A-N3A	2.36	1.38	1.34
2	C	401	NAD	C5A-C6A	2.35	1.47	1.41
2	G	401	NAD	O4D-C1D	2.34	1.44	1.40
2	E	401	NAD	O4D-C1D	2.33	1.43	1.40
2	E	401	NAD	C3N-C7N	2.30	1.54	1.50
2	A	401	NAD	C2B-C3B	-2.28	1.47	1.53
2	B	401	NAD	C8A-N9A	-2.24	1.33	1.37
2	C	401	NAD	C5N-C4N	2.23	1.42	1.38
2	C	401	NAD	C2B-C3B	-2.20	1.47	1.53
2	E	401	NAD	C4N-C3N	2.18	1.42	1.39
2	F	401	NAD	C7N-N7N	2.18	1.37	1.33
2	A	401	NAD	C8A-N7A	2.17	1.35	1.31
2	D	401	NAD	C6A-N6A	2.17	1.39	1.34
2	A	401	NAD	C2N-C3N	-2.16	1.35	1.39
2	B	401	NAD	C6N-N1N	-2.15	1.30	1.35
2	H	401	NAD	C7N-N7N	2.12	1.36	1.33
2	D	401	NAD	C8A-N7A	2.12	1.35	1.31
2	B	401	NAD	C5A-C6A	2.12	1.46	1.41
2	F	401	NAD	O4B-C1B	2.10	1.46	1.42
2	B	401	NAD	O4D-C1D	-2.09	1.38	1.40
2	G	401	NAD	C5A-N7A	-2.06	1.35	1.39
2	H	401	NAD	C5A-N7A	-2.03	1.35	1.39
2	A	401	NAD	C4N-C3N	2.02	1.42	1.39
2	A	401	NAD	C5D-C4D	-2.02	1.45	1.51

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	O4B-C1B-N9A	10.77	128.78	108.09
2	E	401	NAD	C4A-N9A-C8A	9.16	115.36	105.74
2	F	401	NAD	C4A-N9A-C8A	7.83	113.96	105.74
2	A	401	NAD	C5A-C4A-N3A	-7.55	116.32	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	N3A-C2A-N1A	-7.53	117.19	128.58
2	E	401	NAD	O5B-PA-O1A	-7.13	80.67	108.94
2	E	401	NAD	C5A-C4A-N9A	-6.75	98.45	105.81
2	G	401	NAD	N6A-C6A-N1A	6.46	132.76	118.38
2	F	401	NAD	C4A-N9A-C1B	-6.45	111.55	126.63
2	C	401	NAD	O2A-PA-O3	6.35	124.44	107.27
2	A	401	NAD	O2N-PN-O3	-6.17	90.58	107.27
2	D	401	NAD	C5A-C4A-N3A	-6.13	118.28	126.72
2	D	401	NAD	C3N-C7N-N7N	6.09	125.25	117.74
2	G	401	NAD	O4B-C1B-N9A	6.03	119.68	108.09
2	D	401	NAD	N3A-C4A-N9A	5.99	137.35	127.17
2	F	401	NAD	C4B-O4B-C1B	-5.96	96.31	109.47
2	E	401	NAD	N6A-C6A-N1A	5.94	131.60	118.38
2	H	401	NAD	O4B-C1B-N9A	5.93	119.47	108.09
2	C	401	NAD	C1B-N9A-C8A	5.91	140.21	127.09
2	A	401	NAD	N3A-C4A-N9A	5.78	137.00	127.17
2	E	401	NAD	N3A-C2A-N1A	-5.76	119.87	128.58
2	C	401	NAD	C4A-N9A-C1B	-5.72	113.25	126.63
2	G	401	NAD	O3-PA-O1A	-5.58	93.92	110.70
2	B	401	NAD	C4A-N9A-C8A	5.49	111.50	105.74
2	F	401	NAD	C2B-C1B-N9A	-5.46	99.73	113.30
2	F	401	NAD	O4B-C1B-C2B	5.46	118.30	106.62
2	E	401	NAD	O7N-C7N-C3N	-5.37	113.03	119.60
2	A	401	NAD	O7N-C7N-N7N	-5.29	114.97	122.62
2	D	401	NAD	N3A-C2A-N1A	-5.20	120.71	128.58
2	F	401	NAD	O7N-C7N-C3N	-5.05	113.42	119.60
2	F	401	NAD	C6A-C5A-C4A	-5.04	110.29	117.18
2	G	401	NAD	C5A-C4A-N9A	-4.97	100.39	105.81
2	G	401	NAD	O4B-C4B-C5B	-4.96	93.46	109.33
2	F	401	NAD	C2A-N1A-C6A	4.94	126.85	118.73
2	D	401	NAD	O3-PN-O1N	4.93	125.53	110.70
2	G	401	NAD	C4A-N9A-C1B	-4.91	115.14	126.63
2	G	401	NAD	C4A-N9A-C8A	4.89	110.87	105.74
2	A	401	NAD	O3-PA-O1A	-4.88	96.02	110.70
2	E	401	NAD	C5A-C6A-N6A	-4.84	111.30	123.29
2	G	401	NAD	C2A-N1A-C6A	4.80	126.62	118.73
2	H	401	NAD	C4A-N9A-C8A	4.67	110.64	105.74
2	A	401	NAD	O3-PN-O1N	4.66	124.73	110.70
2	F	401	NAD	O3-PN-O1N	4.65	124.68	110.70
2	B	401	NAD	N6A-C6A-N1A	4.63	128.69	118.38
2	E	401	NAD	C5B-C4B-C3B	4.62	131.86	115.21
2	E	401	NAD	N3A-C4A-N9A	4.59	134.98	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	O2D-C2D-C3D	-4.55	97.24	111.82
2	E	401	NAD	O2B-C2B-C3B	4.52	126.30	111.82
2	B	401	NAD	C5A-C4A-N3A	-4.51	120.51	126.72
2	A	401	NAD	C6N-N1N-C2N	4.50	125.70	121.88
2	D	401	NAD	C2A-N3A-C4A	4.48	122.76	111.83
2	H	401	NAD	C2B-C1B-N9A	-4.46	102.23	113.30
2	E	401	NAD	C2A-N1A-C6A	4.40	125.96	118.73
2	G	401	NAD	O7N-C7N-C3N	-4.37	114.26	119.60
2	G	401	NAD	C5A-C6A-N6A	-4.32	112.58	123.29
2	H	401	NAD	C5N-C4N-C3N	-4.31	116.13	120.36
2	A	401	NAD	C2A-N3A-C4A	4.29	122.31	111.83
2	G	401	NAD	C3N-C7N-N7N	4.28	123.01	117.74
2	B	401	NAD	N3A-C4A-N9A	4.18	134.28	127.17
2	H	401	NAD	N3A-C2A-N1A	-4.14	122.32	128.58
2	E	401	NAD	O2A-PA-O1A	4.09	131.48	112.44
2	D	401	NAD	N6A-C6A-N1A	4.08	127.46	118.38
2	C	401	NAD	C6A-C5A-C4A	-4.02	111.68	117.18
2	C	401	NAD	O5B-PA-O1A	-4.01	93.05	108.94
2	E	401	NAD	C4A-N9A-C1B	-4.00	117.27	126.63
2	D	401	NAD	O2N-PN-O3	-3.99	96.49	107.27
2	E	401	NAD	O5B-C5B-C4B	-3.98	95.43	108.99
2	B	401	NAD	C4D-O4D-C1D	-3.98	106.28	109.92
2	A	401	NAD	O2A-PA-O3	3.96	117.98	107.27
2	A	401	NAD	C3N-C7N-N7N	3.96	122.61	117.74
2	G	401	NAD	C4A-C5A-N7A	3.95	115.10	110.58
2	B	401	NAD	O4D-C4D-C3D	3.92	112.94	105.15
2	A	401	NAD	O4B-C1B-N9A	3.92	115.62	108.09
2	H	401	NAD	C2A-N1A-C6A	3.91	125.15	118.73
2	H	401	NAD	C4A-N9A-C1B	-3.90	117.51	126.63
2	F	401	NAD	O5B-PA-O1A	-3.90	93.50	108.94
2	B	401	NAD	C2B-C1B-N9A	-3.86	103.70	113.30
2	E	401	NAD	O4B-C4B-C5B	-3.86	96.98	109.33
2	E	401	NAD	O3B-C3B-C4B	-3.85	100.01	111.08
2	B	401	NAD	C5D-C4D-C3D	-3.84	101.38	115.21
2	G	401	NAD	C2B-C1B-N9A	-3.82	103.81	113.30
2	E	401	NAD	C2B-C1B-N9A	-3.81	103.84	113.30
2	B	401	NAD	O2N-PN-O3	-3.79	97.04	107.27
2	A	401	NAD	C6N-N1N-C1D	-3.78	112.31	119.73
2	F	401	NAD	N9A-C8A-N7A	-3.76	108.61	113.94
2	F	401	NAD	C2A-N3A-C4A	3.74	120.97	111.83
2	C	401	NAD	N3A-C2A-N1A	-3.74	122.93	128.58
2	C	401	NAD	O3B-C3B-C2B	-3.71	99.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	C6A-C5A-N7A	3.68	139.18	132.09
2	F	401	NAD	O2N-PN-O3	-3.62	97.48	107.27
2	A	401	NAD	C4A-C5A-N7A	-3.57	106.50	110.58
2	E	401	NAD	O3B-C3B-C2B	-3.53	100.50	111.82
2	F	401	NAD	N3A-C4A-N9A	3.53	133.16	127.17
2	E	401	NAD	O4B-C1B-C2B	-3.49	99.15	106.62
2	F	401	NAD	O4B-C4B-C3B	3.48	112.05	105.15
2	C	401	NAD	PA-O5B-C5B	-3.47	101.49	121.35
2	D	401	NAD	O7N-C7N-N7N	-3.45	117.63	122.62
2	C	401	NAD	C2A-N1A-C6A	3.43	124.37	118.73
2	F	401	NAD	C5A-C4A-N9A	-3.41	102.09	105.81
2	B	401	NAD	C2N-C3N-C4N	-3.39	114.31	118.26
2	G	401	NAD	O2A-PA-O1A	3.38	128.19	112.44
2	E	401	NAD	C5N-C4N-C3N	3.36	123.67	120.36
2	E	401	NAD	C3B-C2B-C1B	-3.34	95.15	101.46
2	G	401	NAD	C5A-N7A-C8A	-3.30	98.27	103.45
2	H	401	NAD	C4B-O4B-C1B	-3.25	102.28	109.47
2	B	401	NAD	O3-PA-O1A	-3.22	101.01	110.70
2	A	401	NAD	C4A-N9A-C8A	3.17	109.06	105.74
2	B	401	NAD	C2D-C3D-C4D	-3.17	96.49	102.61
2	E	401	NAD	N9A-C8A-N7A	-3.16	109.45	113.94
2	F	401	NAD	C3N-C7N-N7N	3.16	121.63	117.74
2	D	401	NAD	C5A-C6A-N6A	-3.14	115.51	123.29
2	G	401	NAD	N3A-C2A-N1A	-3.13	123.85	128.58
2	B	401	NAD	C2A-N3A-C4A	3.07	119.33	111.83
2	G	401	NAD	O5B-C5B-C4B	3.06	119.43	108.99
2	B	401	NAD	C5A-C6A-N6A	-3.06	115.70	123.29
2	E	401	NAD	C6N-C5N-C4N	-3.06	115.04	119.45
2	F	401	NAD	C4D-O4D-C1D	3.06	112.72	109.92
2	G	401	NAD	C4B-O4B-C1B	-3.04	102.76	109.47
2	H	401	NAD	O4B-C1B-C2B	3.02	113.08	106.62
2	H	401	NAD	O3D-C3D-C2D	-3.02	102.14	111.82
2	F	401	NAD	O3B-C3B-C4B	3.01	119.73	111.08
2	F	401	NAD	C3B-C2B-C1B	-3.01	95.78	101.46
2	G	401	NAD	O4B-C4B-C3B	3.00	111.11	105.15
2	D	401	NAD	C4D-O4D-C1D	2.98	112.66	109.92
2	G	401	NAD	C1B-N9A-C8A	2.98	133.71	127.09
2	H	401	NAD	C6N-N1N-C2N	-2.98	119.35	121.88
2	E	401	NAD	C3N-C7N-N7N	2.96	121.39	117.74
2	G	401	NAD	O3D-C3D-C2D	-2.96	102.34	111.82
2	H	401	NAD	C2N-C3N-C4N	2.94	121.67	118.26
2	B	401	NAD	C4B-O4B-C1B	-2.93	102.99	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	O3-PA-O1A	-2.91	101.94	110.70
2	G	401	NAD	N3A-C4A-N9A	2.89	132.09	127.17
2	D	401	NAD	C4A-N9A-C8A	2.89	108.77	105.74
2	D	401	NAD	C6N-N1N-C2N	2.88	124.33	121.88
2	B	401	NAD	C6N-C5N-C4N	2.88	123.59	119.45
2	A	401	NAD	O2B-C2B-C3B	-2.87	102.63	111.82
2	H	401	NAD	C3B-C2B-C1B	-2.86	96.05	101.46
2	F	401	NAD	C5A-C6A-N6A	-2.86	116.21	123.29
2	C	401	NAD	O2B-C2B-C3B	-2.82	102.77	111.82
2	D	401	NAD	C2A-N1A-C6A	2.82	123.37	118.73
2	A	401	NAD	O4D-C4D-C5D	-2.81	100.33	109.33
2	A	401	NAD	O3B-C3B-C2B	-2.79	102.87	111.82
2	F	401	NAD	C1B-N9A-C8A	2.77	133.24	127.09
2	B	401	NAD	N9A-C8A-N7A	-2.75	110.03	113.94
2	G	401	NAD	C5N-C4N-C3N	-2.74	117.67	120.36
2	A	401	NAD	O2N-PN-O1N	-2.73	99.73	112.44
2	D	401	NAD	O3D-C3D-C2D	-2.71	103.13	111.82
2	C	401	NAD	O2N-PN-O1N	2.70	125.00	112.44
2	D	401	NAD	O5B-PA-O1A	-2.67	98.35	108.94
2	B	401	NAD	O3D-C3D-C2D	2.66	120.35	111.82
2	H	401	NAD	N9A-C8A-N7A	-2.65	110.17	113.94
2	B	401	NAD	N3A-C2A-N1A	-2.62	124.62	128.58
2	C	401	NAD	C6A-C5A-N7A	2.61	137.13	132.09
2	B	401	NAD	O7N-C7N-N7N	-2.60	118.85	122.62
2	G	401	NAD	O3-PN-O1N	2.57	118.44	110.70
2	G	401	NAD	C4D-O4D-C1D	2.56	112.27	109.92
2	F	401	NAD	O2A-PA-O1A	2.54	124.26	112.44
2	E	401	NAD	O3D-C3D-C4D	2.53	118.36	111.08
2	D	401	NAD	O4D-C4D-C3D	-2.52	100.15	105.15
2	B	401	NAD	O4B-C4B-C3B	2.52	110.16	105.15
2	C	401	NAD	C6N-N1N-C2N	-2.52	119.73	121.88
2	C	401	NAD	C2N-N1N-C1D	2.51	124.67	119.13
2	H	401	NAD	N3A-C4A-N9A	2.51	131.43	127.17
2	D	401	NAD	O2N-PN-O5D	2.49	118.85	107.57
2	B	401	NAD	O2A-PA-O3	2.48	113.97	107.27
2	C	401	NAD	O4B-C4B-C3B	2.46	110.03	105.15
2	G	401	NAD	O4D-C4D-C3D	-2.45	100.28	105.15
2	B	401	NAD	C5N-C6N-N1N	-2.45	117.04	120.38
2	H	401	NAD	O2A-PA-O3	-2.44	100.68	107.27
2	E	401	NAD	O4D-C4D-C5D	-2.42	101.57	109.33
2	A	401	NAD	C2B-C1B-N9A	-2.42	107.30	113.30
2	B	401	NAD	PN-O5D-C5D	-2.41	107.56	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	NAD	O4B-C1B-C2B	2.40	111.74	106.62
2	D	401	NAD	O7N-C7N-C3N	-2.36	116.72	119.60
2	C	401	NAD	O5D-PN-O1N	-2.36	99.60	108.94
2	H	401	NAD	O2A-PA-O5B	2.35	118.23	107.57
2	C	401	NAD	C5D-C4D-C3D	-2.34	106.78	115.21
2	A	401	NAD	C6N-C5N-C4N	-2.34	116.08	119.45
2	B	401	NAD	O2B-C2B-C3B	-2.34	104.32	111.82
2	B	401	NAD	O4B-C1B-N9A	2.31	112.52	108.09
2	F	401	NAD	C2B-C3B-C4B	-2.29	98.18	102.61
2	F	401	NAD	N6A-C6A-N1A	2.29	123.47	118.38
2	C	401	NAD	O4B-C1B-N9A	2.28	112.46	108.09
2	D	401	NAD	N9A-C8A-N7A	-2.26	110.73	113.94
2	C	401	NAD	O2A-PA-O5B	2.25	117.75	107.57
2	B	401	NAD	O2A-PA-O1A	2.25	122.89	112.44
2	B	401	NAD	C2N-C3N-C7N	2.23	125.91	119.46
2	H	401	NAD	N6A-C6A-N1A	2.23	123.35	118.38
2	D	401	NAD	O4B-C1B-C2B	-2.22	101.87	106.62
2	D	401	NAD	C5A-N7A-C8A	2.21	106.93	103.45
2	E	401	NAD	O2A-PA-O3	2.20	113.22	107.27
2	E	401	NAD	C6A-C5A-C4A	-2.20	114.18	117.18
2	A	401	NAD	N3A-C2A-N1A	-2.17	125.30	128.58
2	B	401	NAD	O4B-C1B-C2B	2.16	111.24	106.62
2	H	401	NAD	O2D-C2D-C3D	-2.14	104.95	111.82
2	G	401	NAD	C2B-C3B-C4B	-2.14	98.48	102.61
2	A	401	NAD	C5A-N7A-C8A	2.14	106.81	103.45
2	C	401	NAD	C3B-C2B-C1B	2.13	105.49	101.46
2	C	401	NAD	C6N-N1N-C1D	-2.12	115.58	119.73
2	A	401	NAD	N9A-C8A-N7A	-2.11	110.94	113.94
2	E	401	NAD	C6N-N1N-C2N	2.10	123.67	121.88
2	H	401	NAD	C2A-N3A-C4A	2.10	116.96	111.83
2	E	401	NAD	C4A-C5A-N7A	2.09	112.97	110.58
2	H	401	NAD	C5A-C4A-N3A	-2.09	123.84	126.72
2	H	401	NAD	O2A-PA-O1A	2.08	122.14	112.44
2	G	401	NAD	O2N-PN-O3	-2.07	101.67	107.27
2	A	401	NAD	C5N-C4N-C3N	2.06	122.39	120.36
2	H	401	NAD	C1B-N9A-C8A	2.06	131.66	127.09
2	H	401	NAD	O5D-C5D-C4D	-2.05	102.02	108.99
2	A	401	NAD	C5A-C6A-N6A	-2.05	118.22	123.29

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C5B-O5B-PA-O1A
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	E	401	NAD	C5B-O5B-PA-O1A
2	E	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	C5B-O5B-PA-O1A
2	H	401	NAD	C5D-O5D-PN-O1N
2	H	401	NAD	C5D-O5D-PN-O2N
2	H	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	C3B-C4B-C5B-O5B
2	H	401	NAD	O4D-C4D-C5D-O5D
2	F	401	NAD	O4D-C4D-C5D-O5D
2	B	401	NAD	O4B-C4B-C5B-O5B
2	H	401	NAD	C3D-C4D-C5D-O5D
2	F	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	C2B-C1B-N9A-C8A
2	H	401	NAD	C2B-C1B-N9A-C8A
2	B	401	NAD	PN-O3-PA-O1A
2	B	401	NAD	PN-O3-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O3
2	E	401	NAD	C5B-O5B-PA-O3
2	H	401	NAD	C5B-O5B-PA-O2A
2	H	401	NAD	C5D-O5D-PN-O3

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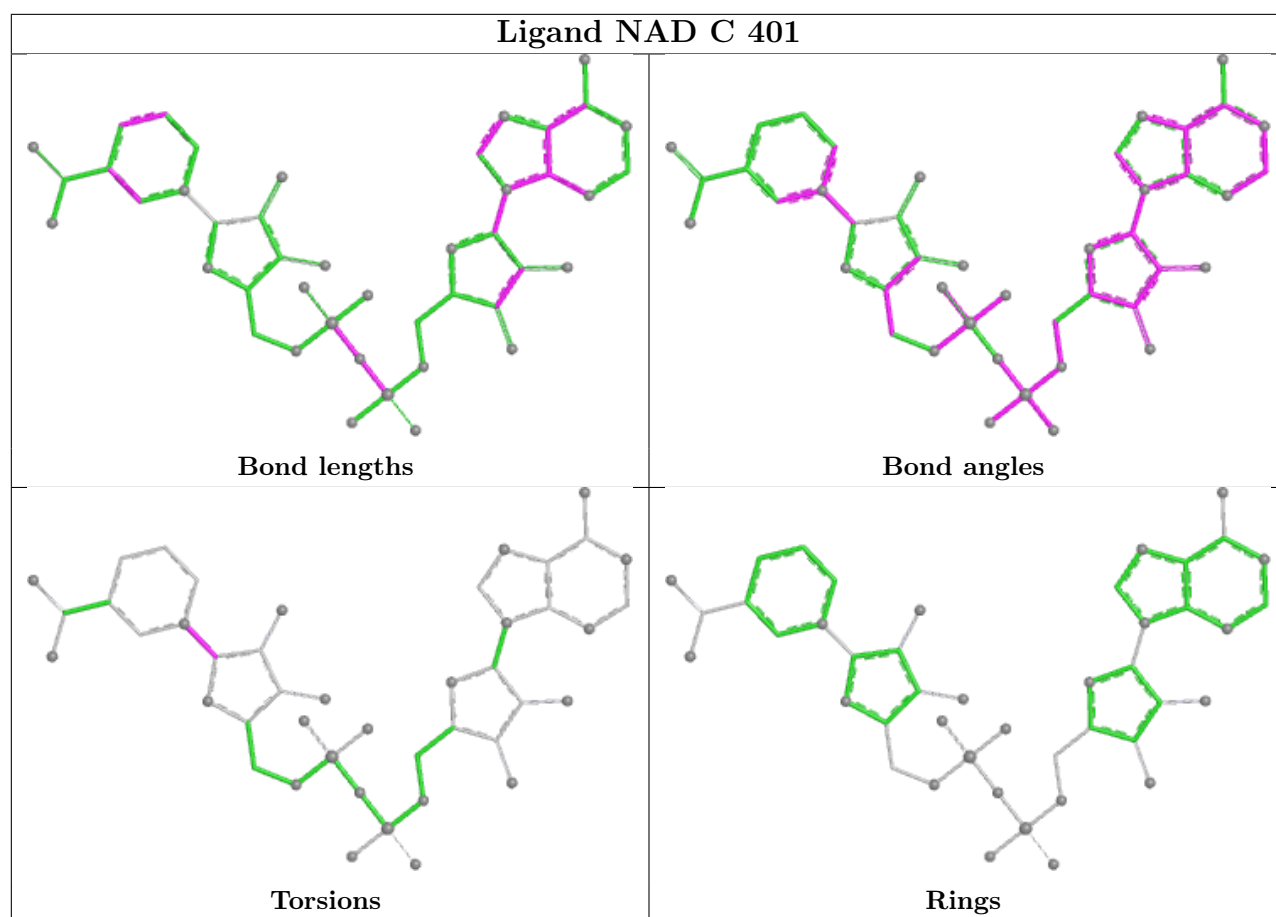
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	PN-O3-PA-O2A
2	G	401	NAD	PN-O3-PA-O1A
2	H	401	NAD	O4B-C1B-N9A-C8A
2	D	401	NAD	PN-O3-PA-O2A
2	G	401	NAD	PN-O3-PA-O2A
2	D	401	NAD	PN-O3-PA-O1A
2	H	401	NAD	PN-O3-PA-O1A

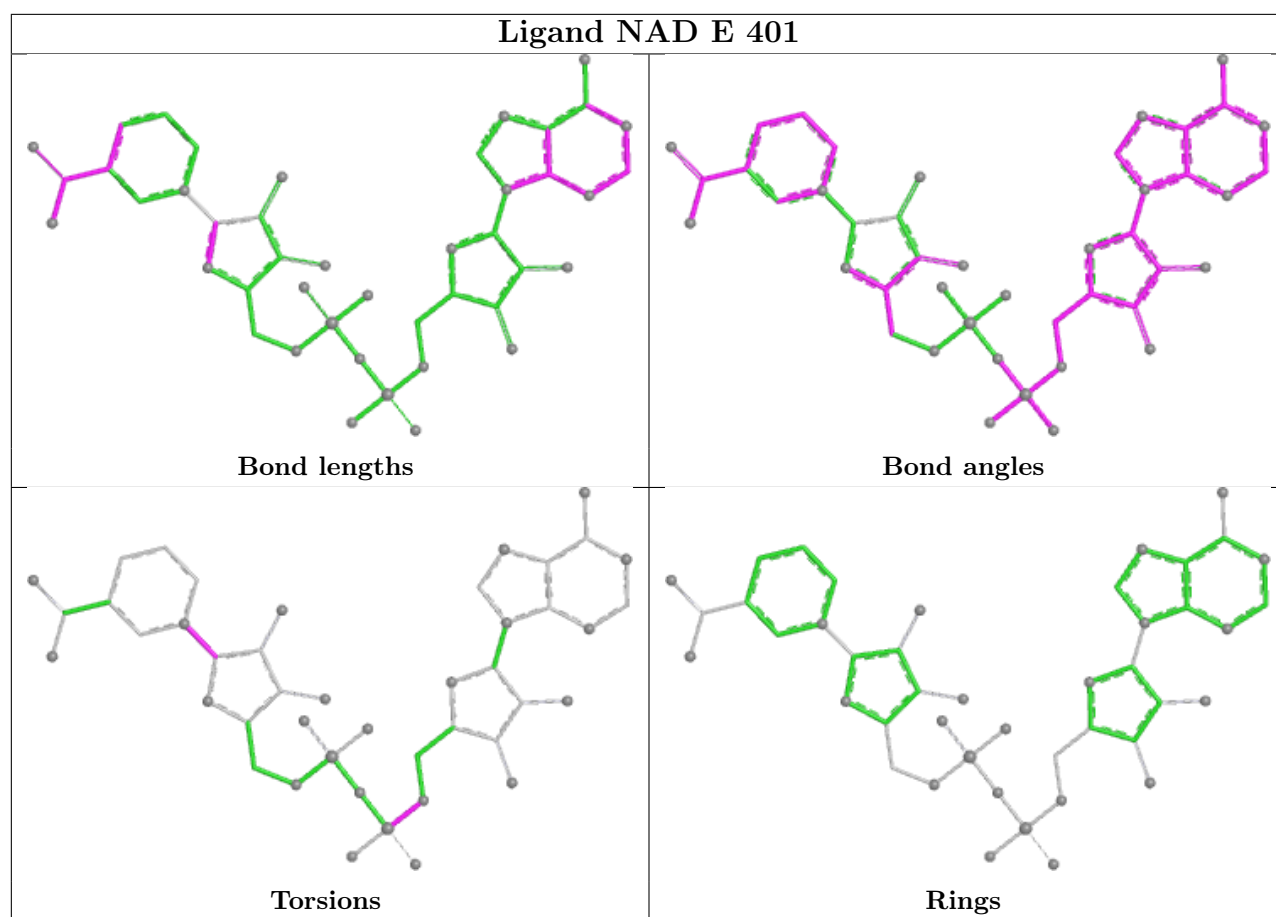
There are no ring outliers.

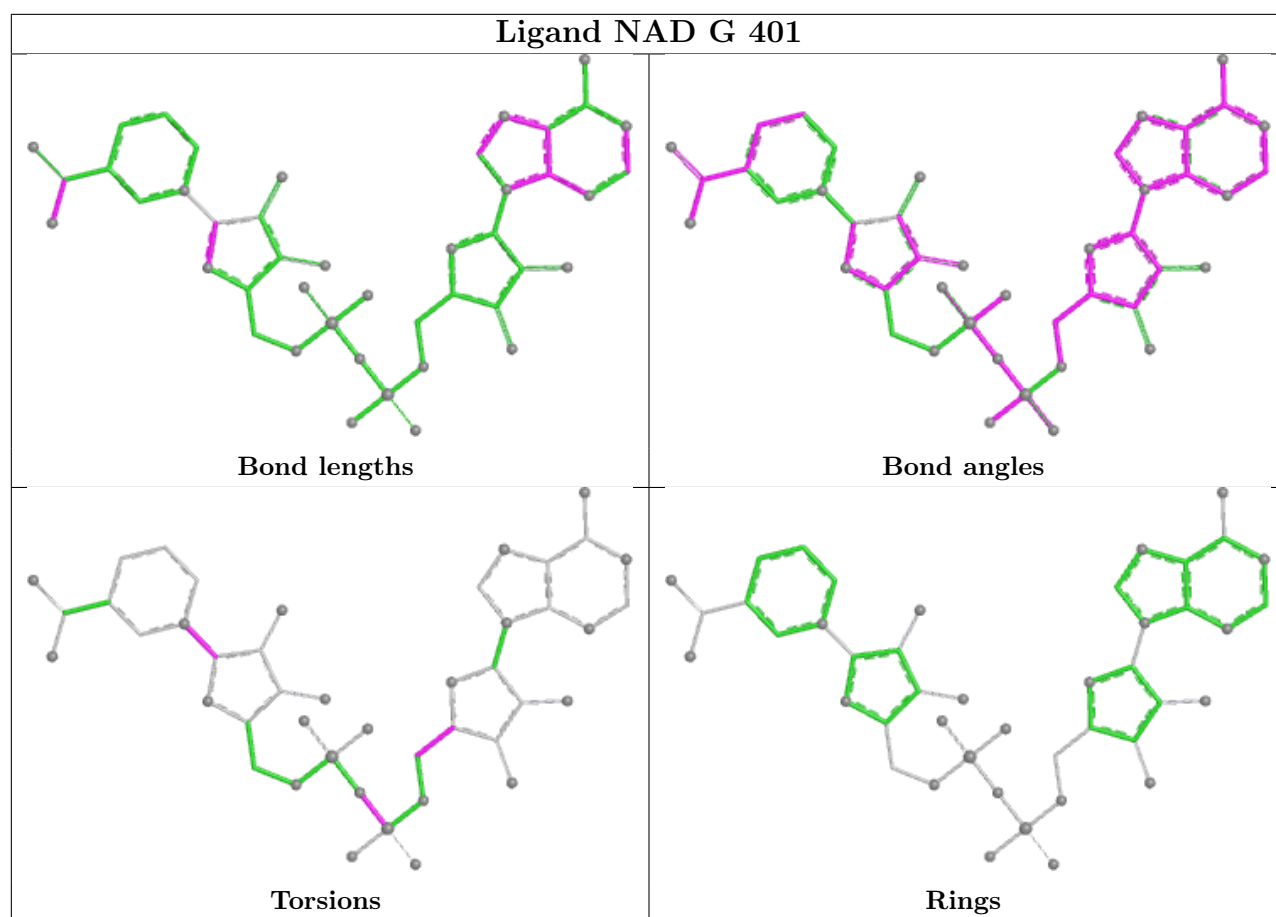
8 monomers are involved in 73 short contacts:

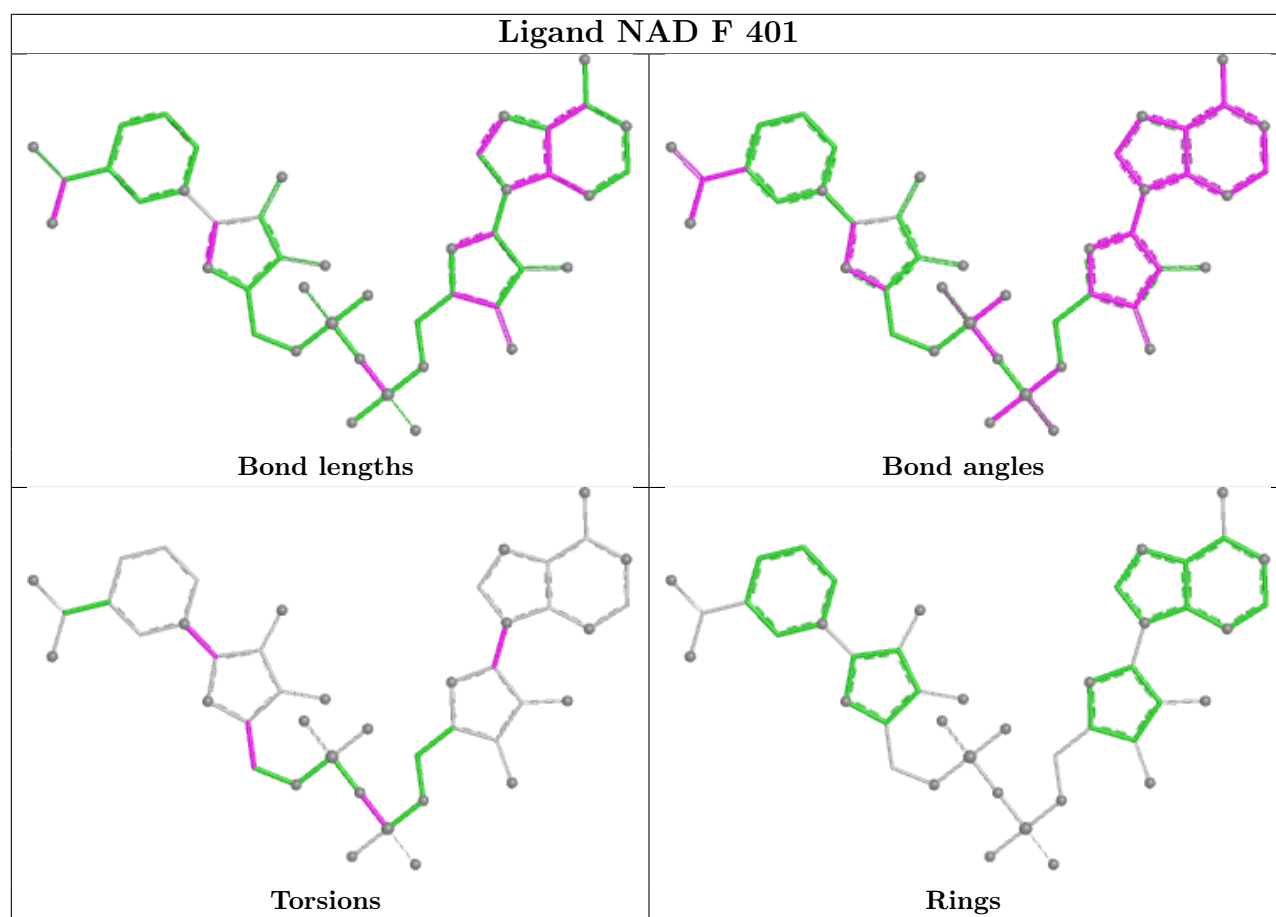
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAD	12	0
2	E	401	NAD	10	0
2	G	401	NAD	7	0
2	F	401	NAD	15	0
2	B	401	NAD	8	0
2	H	401	NAD	8	0
2	D	401	NAD	6	0
2	A	401	NAD	7	0

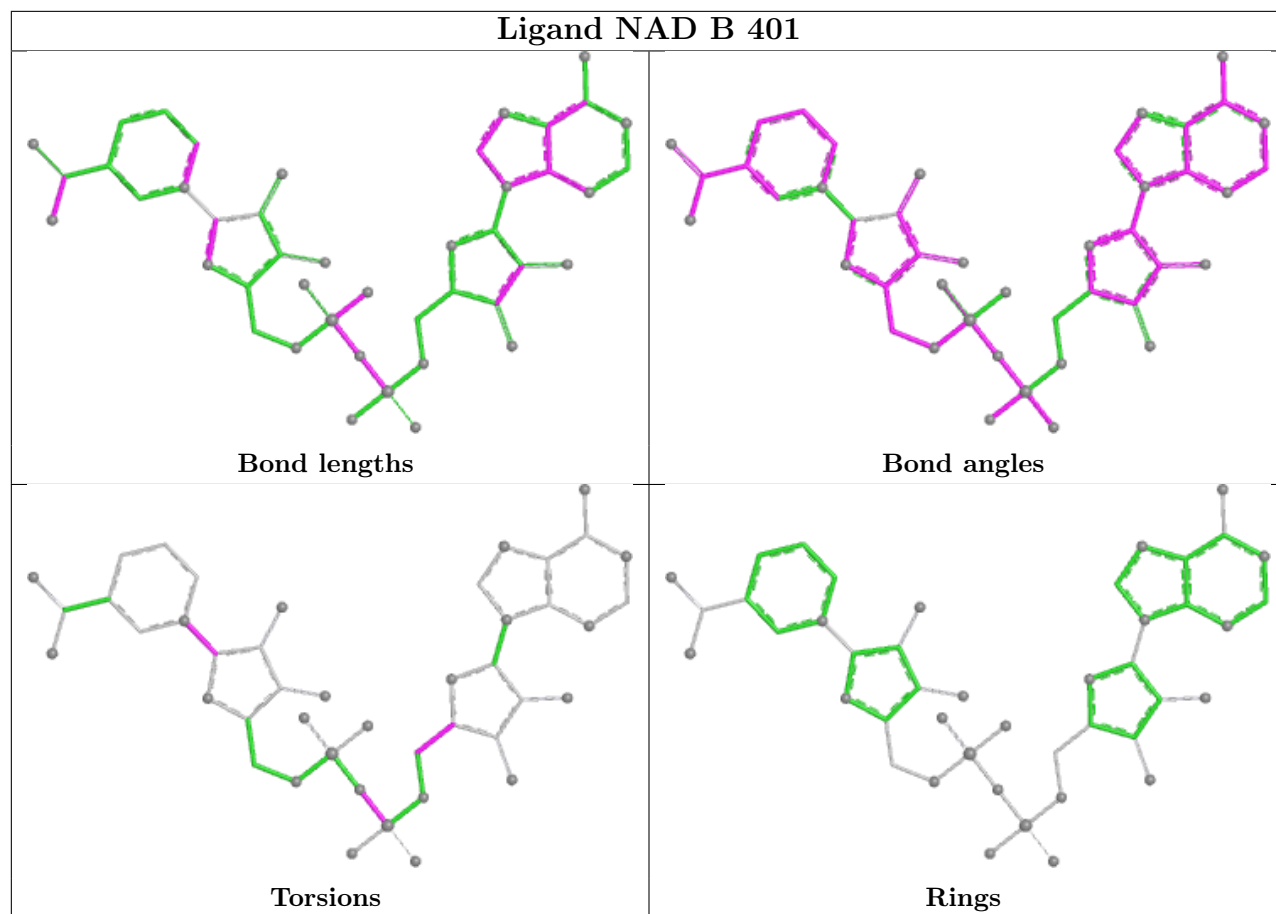
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

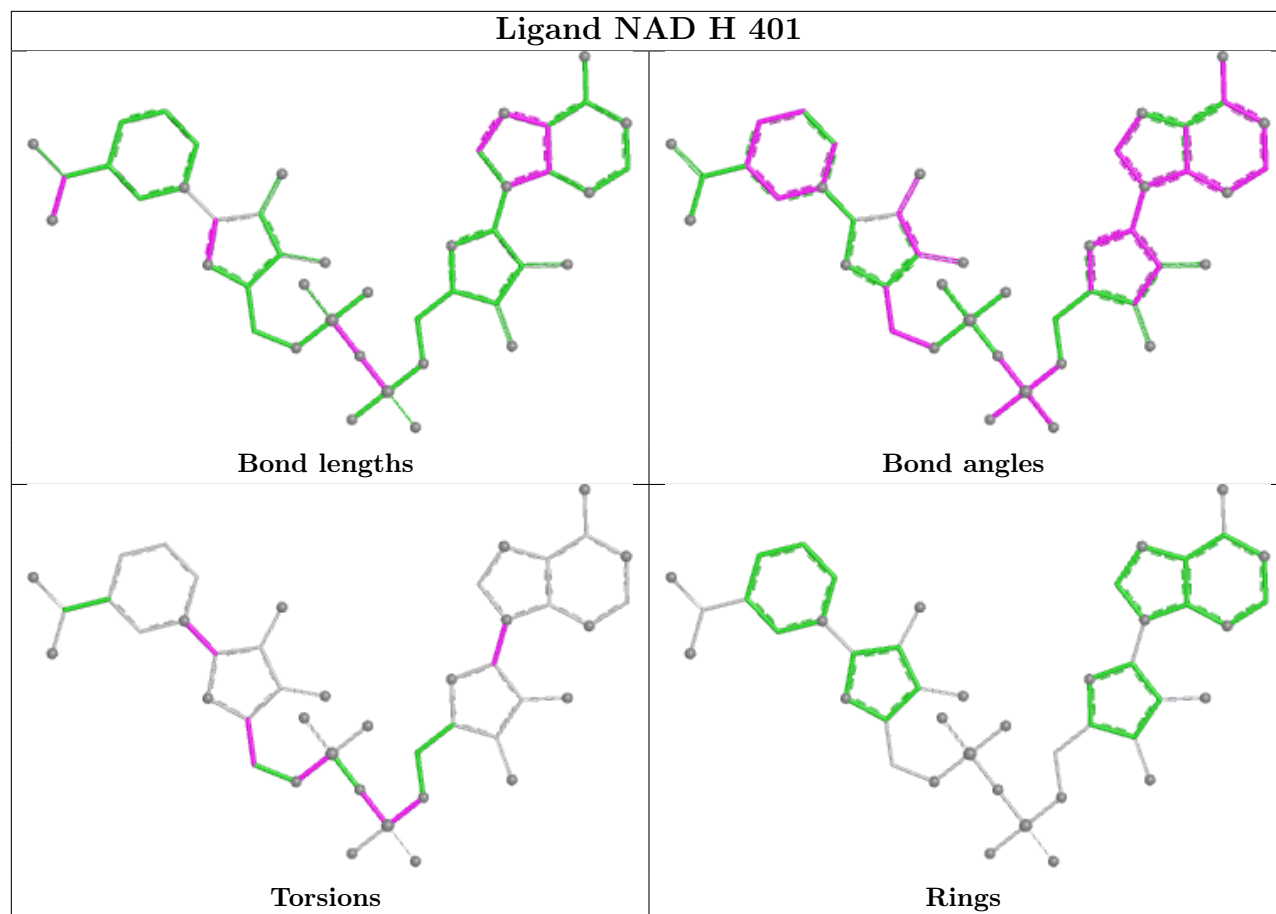


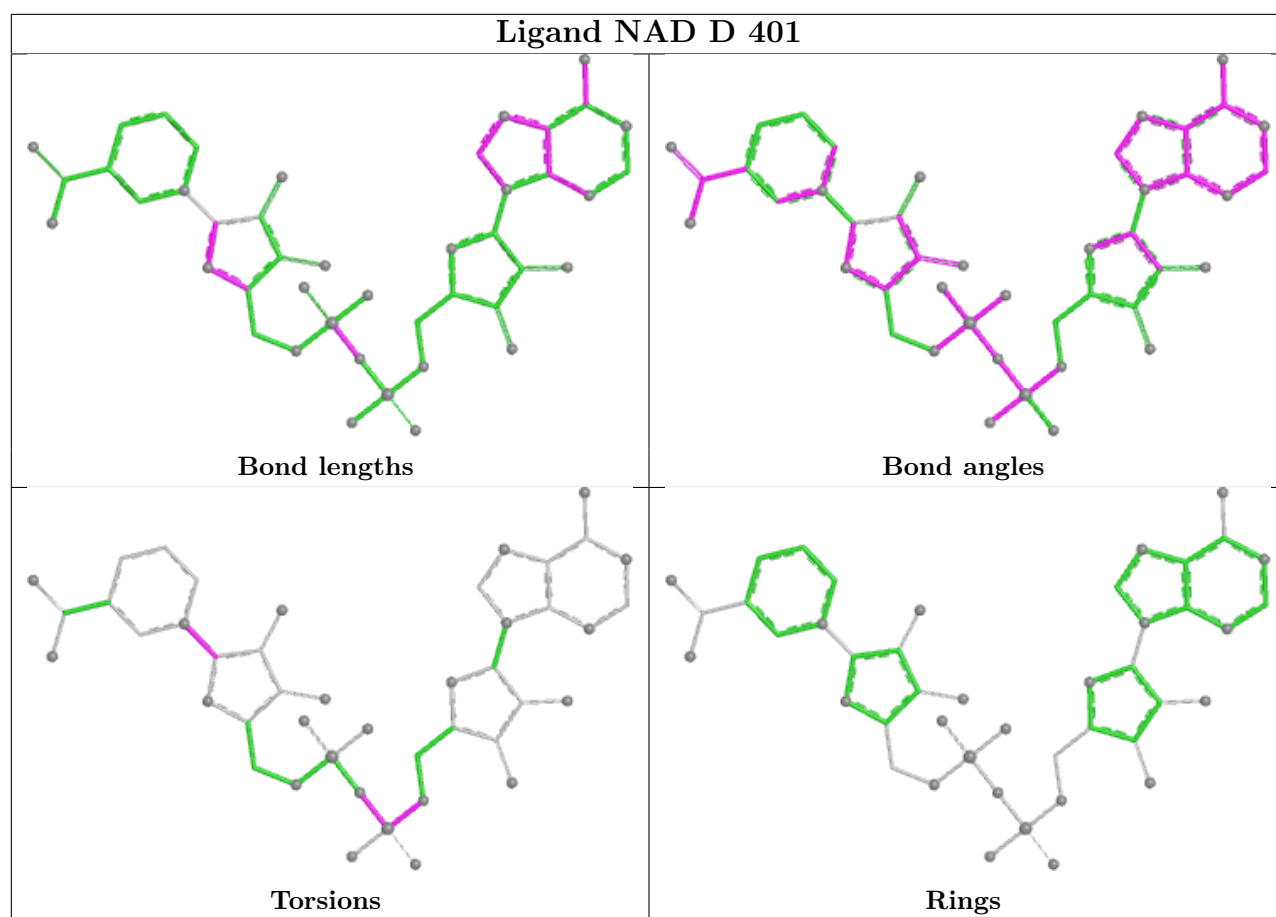


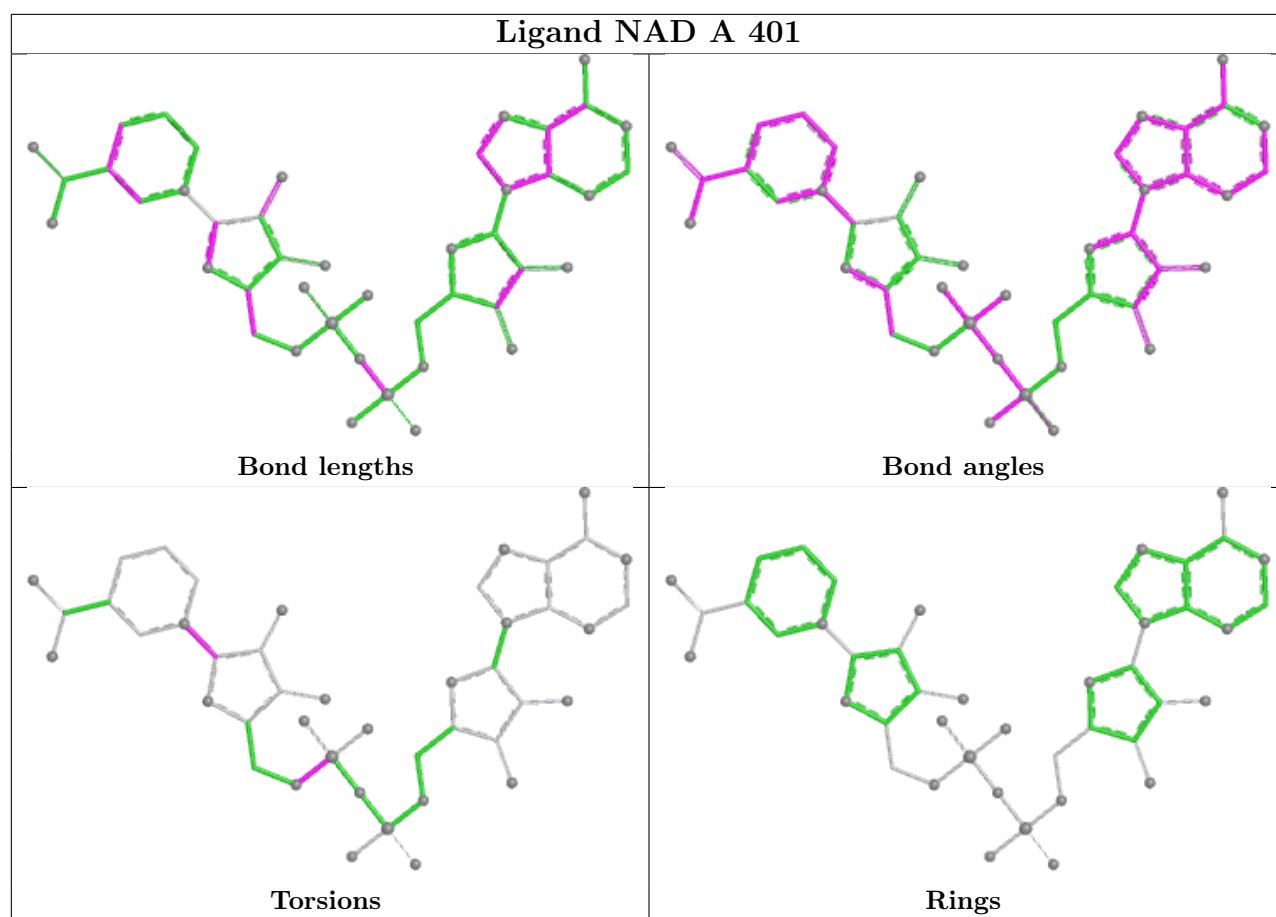












5.7 Other polymers [i](#)

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	299/312 (95%)	0.52	10 (3%)	49	39	20, 44, 70, 88	0
1	B	295/312 (94%)	0.47	8 (2%)	56	46	19, 41, 68, 97	0
1	C	295/312 (94%)	0.60	10 (3%)	48	39	20, 43, 73, 86	0
1	D	293/312 (93%)	0.58	10 (3%)	48	39	20, 44, 69, 83	0
1	E	299/312 (95%)	0.47	7 (2%)	61	51	22, 40, 67, 106	0
1	F	263/312 (84%)	0.93	43 (16%)	4	4	23, 50, 86, 113	0
1	G	298/312 (95%)	0.38	11 (3%)	45	36	20, 39, 67, 93	0
1	H	250/312 (80%)	0.90	33 (13%)	7	6	22, 48, 83, 110	0
All	All	2292/2496 (91%)	0.60	132 (5%)	29	22	19, 43, 75, 113	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	PHE	4.4
1	A	92	SER	4.2
1	D	142	PHE	4.1
1	F	12	GLY	3.9
1	F	110	GLU	3.9
1	G	41	GLU	3.6
1	H	120	GLU	3.5
1	F	13	SER	3.5
1	F	142	PHE	3.4
1	B	310	ASN	3.4
1	F	310	ASN	3.4
1	C	179	ASN	3.4
1	F	158	ALA	3.2
1	H	143	GLY	3.2
1	H	36	VAL	3.1
1	F	263	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	126	ASN	3.1
1	H	166	LYS	3.1
1	F	90	ILE	3.1
1	H	172	LEU	3.0
1	F	118	PRO	3.0
1	H	29	ILE	2.9
1	H	27	LEU	2.9
1	H	118	PRO	2.9
1	E	42	HIS	2.9
1	F	29	ILE	2.9
1	H	173	ASN	2.9
1	B	57	LEU	2.9
1	F	7	GLY	2.9
1	H	19	LEU	2.9
1	G	142	PHE	2.8
1	H	252	GLU	2.8
1	F	116	PHE	2.7
1	H	116	PHE	2.7
1	F	283	ARG	2.7
1	A	128	MET	2.7
1	D	91	GLN	2.7
1	A	142	PHE	2.7
1	H	158	ALA	2.7
1	H	79	LYS	2.7
1	H	32	TRP	2.6
1	F	167	LEU	2.6
1	F	16	GLY	2.6
1	H	144	SER	2.6
1	C	162	LYS	2.6
1	F	93	LEU	2.6
1	G	254	ILE	2.6
1	H	112	ILE	2.6
1	B	1	MET	2.6
1	F	6	ALA	2.6
1	C	247	SER	2.6
1	B	254	ILE	2.6
1	H	174	ALA	2.6
1	F	5	ILE	2.5
1	F	138	GLN	2.5
1	G	247	SER	2.5
1	B	44	LEU	2.5
1	A	46	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	269	HIS	2.5
1	H	117	VAL	2.4
1	F	114	GLU	2.4
1	F	30	ASP	2.4
1	F	89	ASP	2.4
1	A	279	GLY	2.4
1	D	143	GLY	2.4
1	F	85	LYS	2.4
1	D	247	SER	2.4
1	C	145	GLY	2.3
1	G	255	GLY	2.3
1	H	30	ASP	2.3
1	F	37	GLN	2.3
1	F	59	ILE	2.3
1	G	159	ALA	2.3
1	H	110	GLU	2.3
1	H	119	MET	2.3
1	E	38	GLN	2.3
1	F	75	ILE	2.3
1	H	121	ASN	2.3
1	A	152	LEU	2.3
1	E	247	SER	2.3
1	F	18	MET	2.2
1	C	134	GLU	2.2
1	B	19	LEU	2.2
1	C	256	LEU	2.2
1	C	192	GLY	2.2
1	H	7	GLY	2.2
1	F	19	LEU	2.2
1	E	254	ILE	2.2
1	A	98	THR	2.2
1	A	282	SER	2.2
1	F	22	SER	2.2
1	D	155	GLY	2.2
1	F	86	MET	2.2
1	C	142	PHE	2.2
1	H	132	GLY	2.2
1	F	166	LYS	2.2
1	D	243	ALA	2.2
1	F	160	ALA	2.2
1	C	234	ILE	2.2
1	H	310	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	129	TRP	2.2
1	B	56	LYS	2.2
1	D	289	GLY	2.2
1	B	142	PHE	2.2
1	E	59	ILE	2.1
1	G	91	GLN	2.1
1	D	310	ASN	2.1
1	G	49	ASN	2.1
1	F	58	PRO	2.1
1	F	162	LYS	2.1
1	E	54	GLU	2.1
1	C	121	ASN	2.1
1	H	31	GLY	2.1
1	H	13	SER	2.1
1	A	263	GLN	2.1
1	G	263	GLN	2.1
1	F	115	LYS	2.1
1	F	252	GLU	2.1
1	A	38	GLN	2.0
1	G	138	GLN	2.0
1	H	162	LYS	2.0
1	F	8	ALA	2.0
1	F	174	ALA	2.0
1	G	33	ALA	2.0
1	F	286	LYS	2.0
1	D	82	GLN	2.0
1	F	17	LEU	2.0
1	F	57	LEU	2.0
1	H	4	ALA	2.0
1	H	33	ALA	2.0
1	D	134	GLU	2.0
1	H	139	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](#)

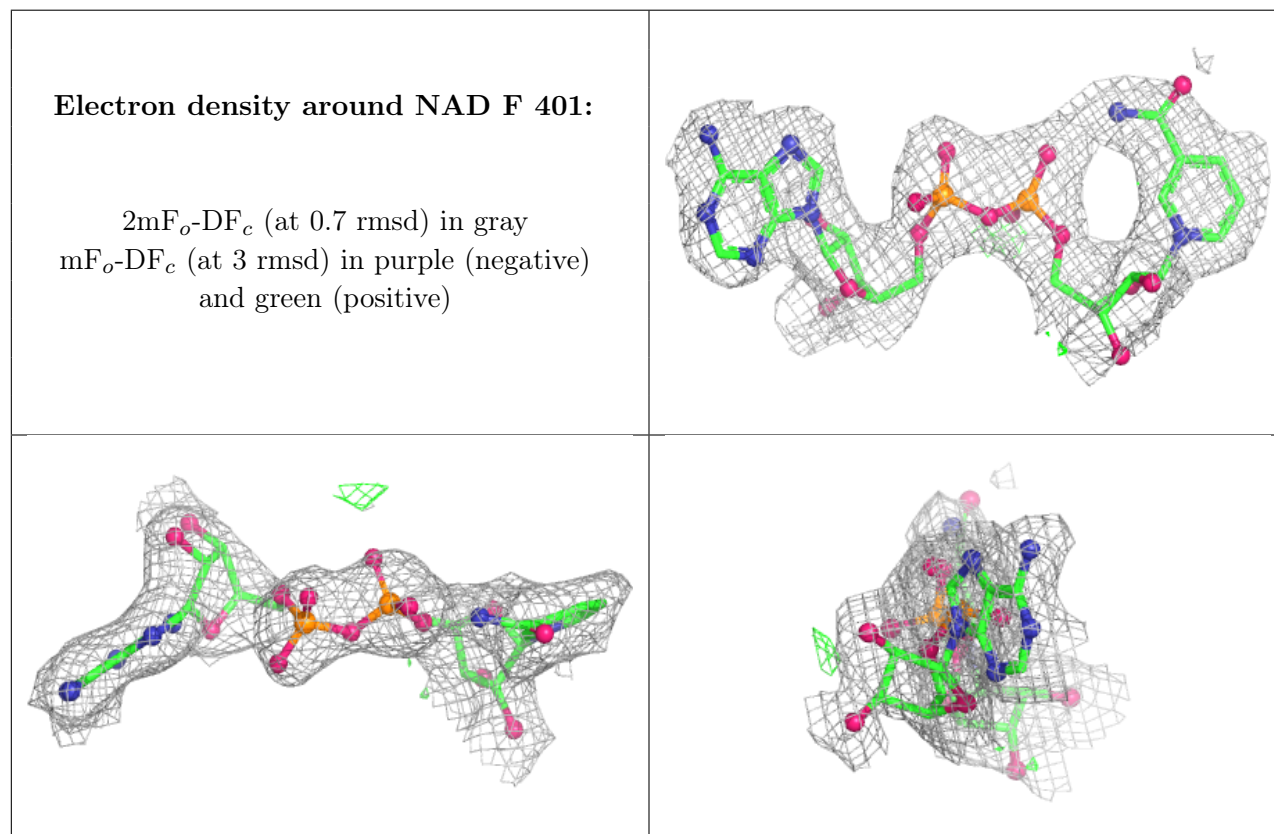
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

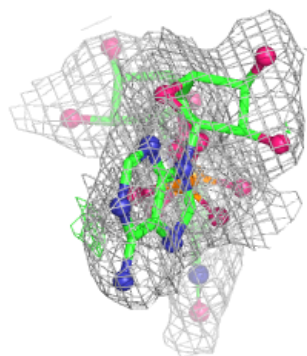
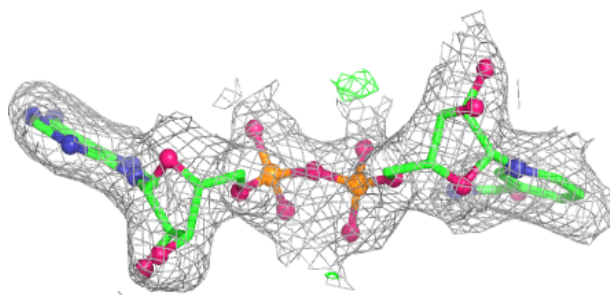
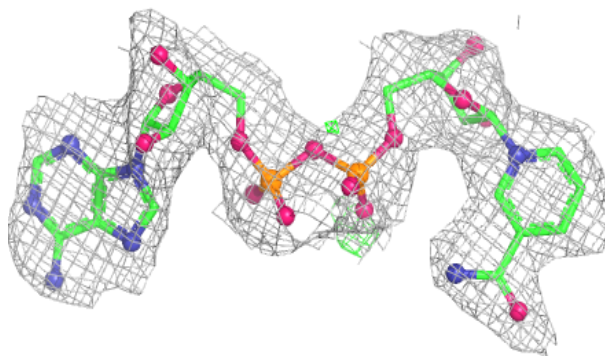
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	F	401	44/44	0.91	0.11	26,38,49,78	0
2	NAD	H	401	44/44	0.92	0.10	19,42,53,56	0
2	NAD	B	401	44/44	0.93	0.10	20,30,38,43	0
2	NAD	E	401	44/44	0.94	0.09	17,25,34,40	0
2	NAD	A	401	44/44	0.94	0.09	22,33,46,54	0
2	NAD	C	401	44/44	0.94	0.09	17,26,31,38	0
2	NAD	G	401	44/44	0.95	0.08	16,24,33,34	0
2	NAD	D	401	44/44	0.96	0.08	18,26,38,51	0

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

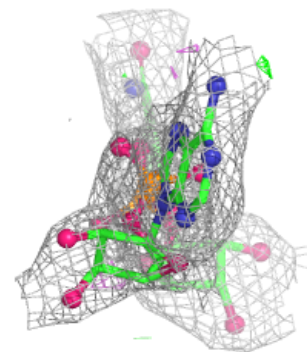
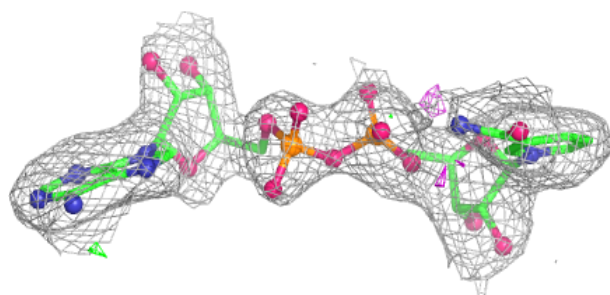
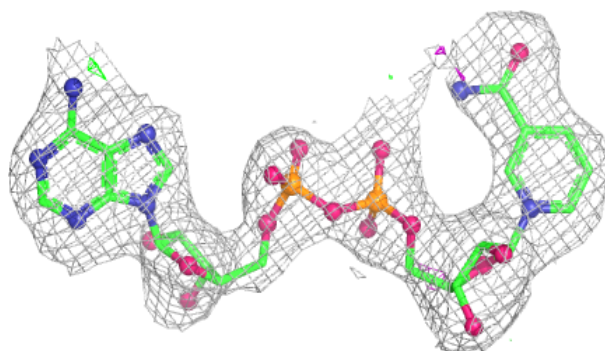


Electron density around NAD H 401:

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

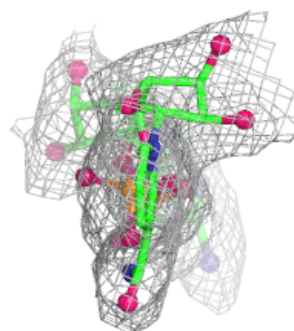
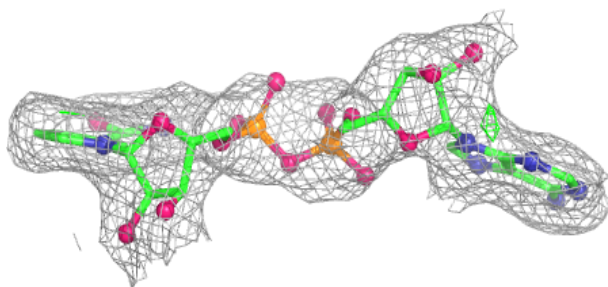
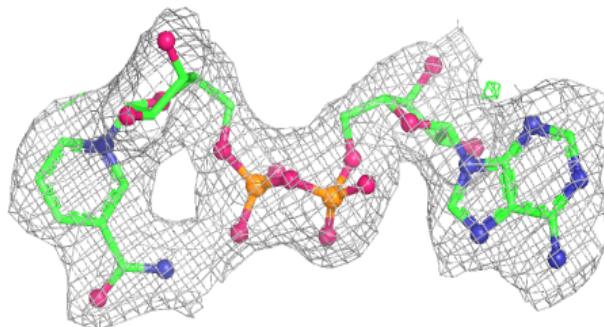
**Electron density around NAD B 401:**

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

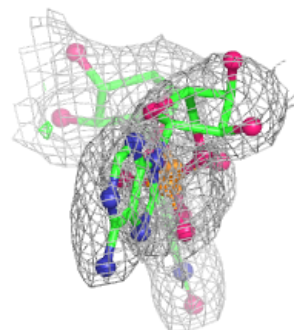
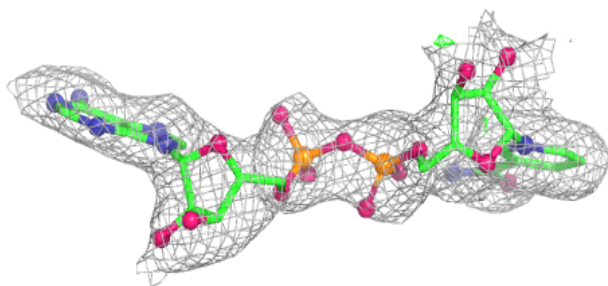
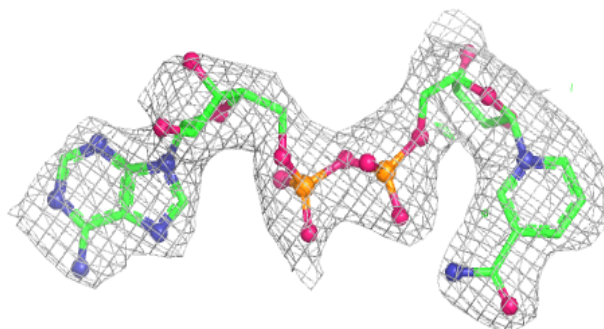


Electron density around NAD E 401:

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

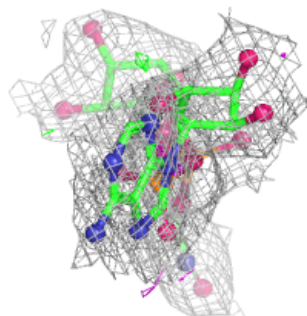
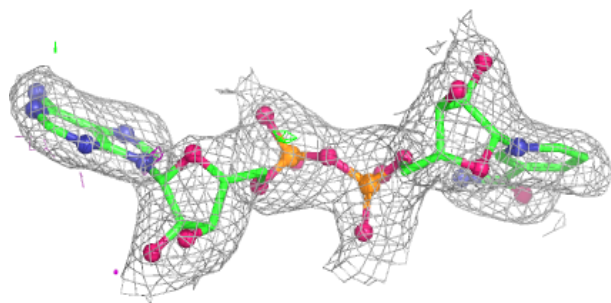
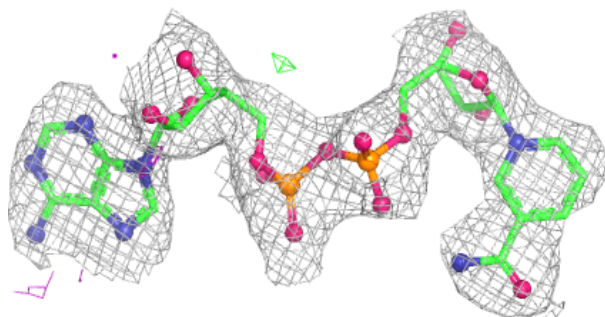
**Electron density around NAD A 401:**

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

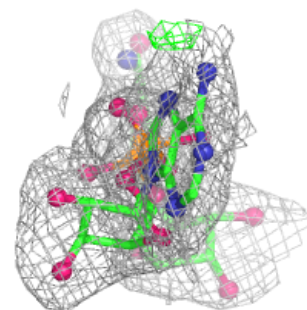
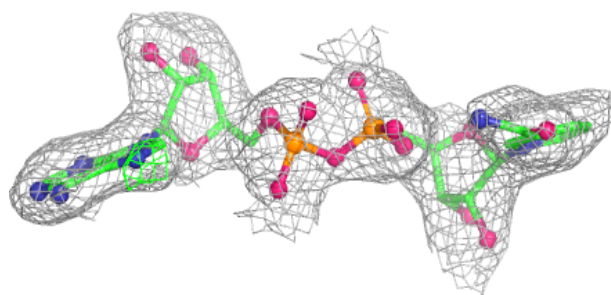
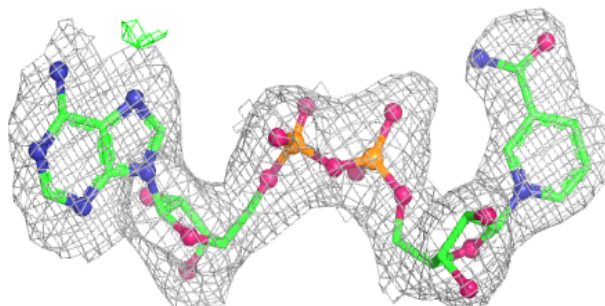


Electron density around NAD C 401:

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

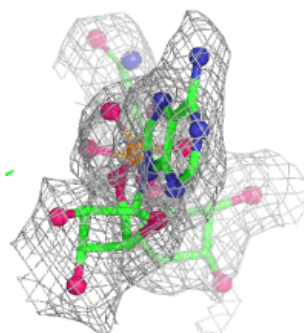
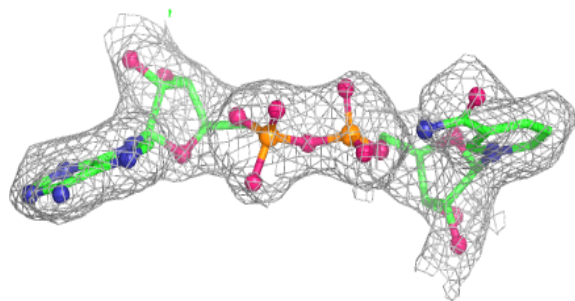
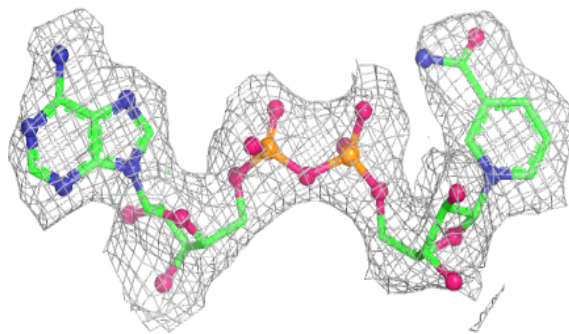
**Electron density around NAD G 401:**

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



Electron density around NAD D 401:

$2mF_o - DF_c$ (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.