



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:08 PM UTC

PDB ID : 4I3X / pdb_00004i3x
Title : Structure of phosphonoacetaldehyde dehydrogenase in complex with phosphonoacetate and cofactor NAD⁺
Authors : Nair, S.K.; Agarwal, V.
Deposited on : 2012-11-26
Resolution : 2.07 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:

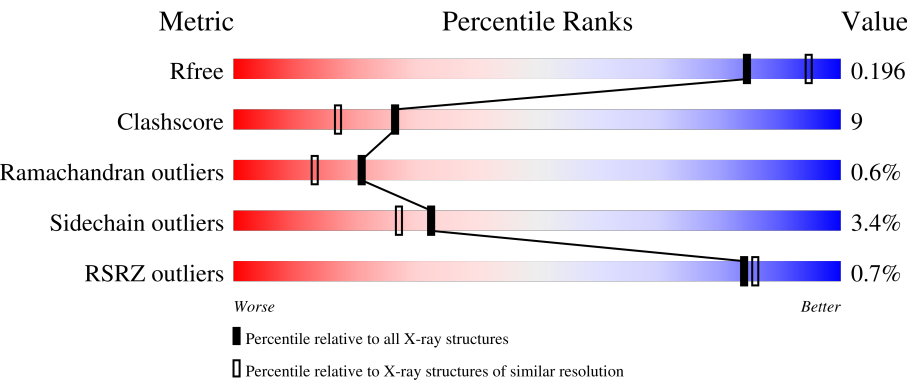
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.07 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.



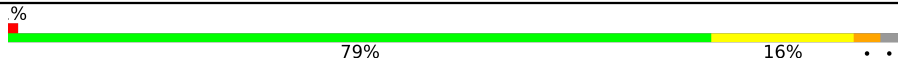
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	488	82%14%..
1	B	488	% 84%12%..
1	C	488	% 82%13%..
1	D	488	% 77%16%...
1	E	488	% 80%15%..

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Mol	Chain	Length	Quality of chain
1	F	488	
1	G	488	
1	H	488	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PAE	C	502	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aldehyde dehydrogenase (NAD+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3651	2310	636	686	19			
1	B	474	Total	C	N	O	S	0	0	0
			3633	2299	631	684	19			
1	C	475	Total	C	N	O	S	0	0	0
			3644	2305	635	685	19			
1	D	476	Total	C	N	O	S	0	0	0
			3651	2310	636	686	19			
1	E	476	Total	C	N	O	S	0	0	0
			3649	2308	636	686	19			
1	F	476	Total	C	N	O	S	0	0	0
			3651	2310	636	686	19			
1	G	474	Total	C	N	O	S	0	0	0
			3633	2299	631	684	19			
1	H	476	Total	C	N	O	S	0	0	0
			3651	2310	636	686	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q92UV7
A	-1	SER	-	expression tag	UNP Q92UV7
A	0	HIS	-	expression tag	UNP Q92UV7
B	-2	GLY	-	expression tag	UNP Q92UV7
B	-1	SER	-	expression tag	UNP Q92UV7
B	0	HIS	-	expression tag	UNP Q92UV7
C	-2	GLY	-	expression tag	UNP Q92UV7
C	-1	SER	-	expression tag	UNP Q92UV7
C	0	HIS	-	expression tag	UNP Q92UV7
D	-2	GLY	-	expression tag	UNP Q92UV7
D	-1	SER	-	expression tag	UNP Q92UV7
D	0	HIS	-	expression tag	UNP Q92UV7
E	-2	GLY	-	expression tag	UNP Q92UV7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q92UV7
E	0	HIS	-	expression tag	UNP Q92UV7
F	-2	GLY	-	expression tag	UNP Q92UV7
F	-1	SER	-	expression tag	UNP Q92UV7
F	0	HIS	-	expression tag	UNP Q92UV7
G	-2	GLY	-	expression tag	UNP Q92UV7
G	-1	SER	-	expression tag	UNP Q92UV7
G	0	HIS	-	expression tag	UNP Q92UV7
H	-2	GLY	-	expression tag	UNP Q92UV7
H	-1	SER	-	expression tag	UNP Q92UV7
H	0	HIS	-	expression tag	UNP Q92UV7

- # NAD

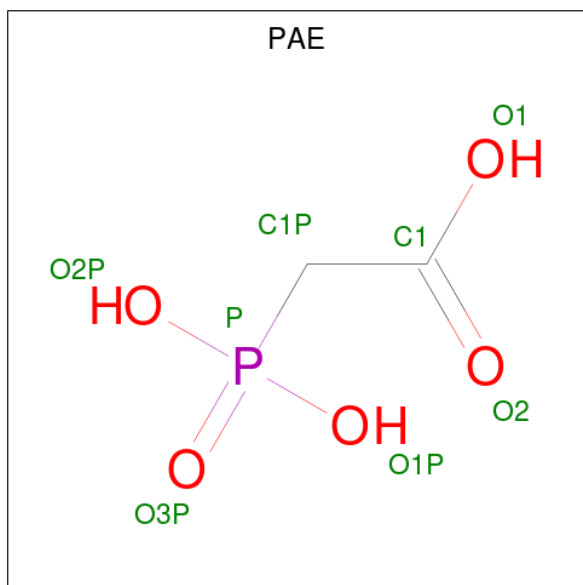
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 PHOSPHONOACETIC ACID (CCD ID: PAE) (formula: $C_2H_5O_5P$).



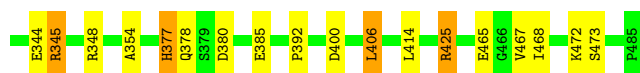
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	2	5	1		
3	B	1	Total	C	O	P	0	0
			8	2	5	1		
3	C	1	Total	C	O	P	0	0
			8	2	5	1		
3	D	1	Total	C	O	P	0	0
			8	2	5	1		
3	E	1	Total	C	O	P	0	0
			8	2	5	1		
3	F	1	Total	C	O	P	0	0
			8	2	5	1		
3	G	1	Total	C	O	P	0	0
			8	2	5	1		
3	H	1	Total	C	O	P	0	0
			8	2	5	1		

- Molecule 4 is water.

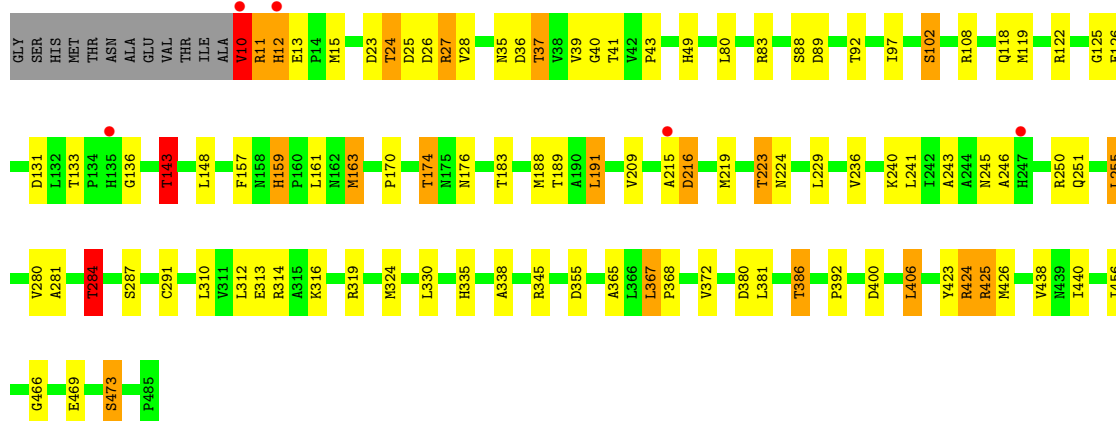
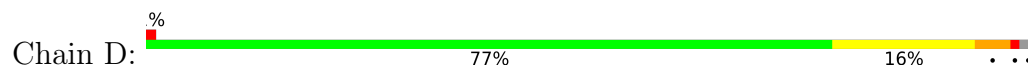
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	497	Total 497	O 497	0	0
4	B	380	Total 380	O 380	0	0
4	C	337	Total 337	O 337	0	0
4	D	302	Total 302	O 302	0	0
4	E	376	Total 376	O 376	0	0
4	F	325	Total 325	O 325	0	0
4	G	358	Total 358	O 358	0	0
4	H	298	Total 298	O 298	0	0

- Molecule 1: Aldehyde dehydrogenase (NAD⁺)

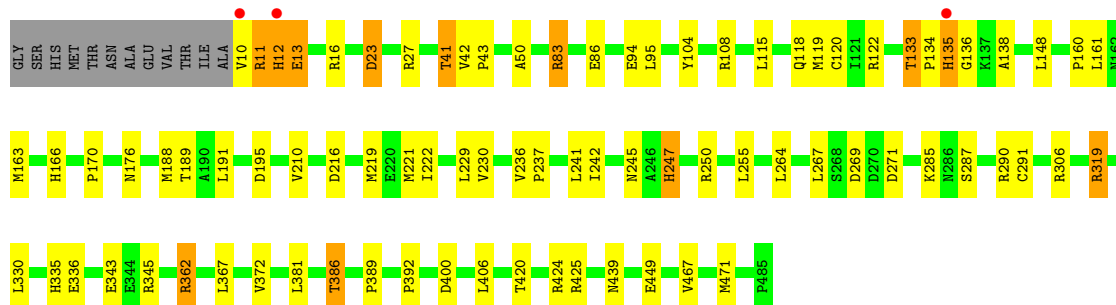
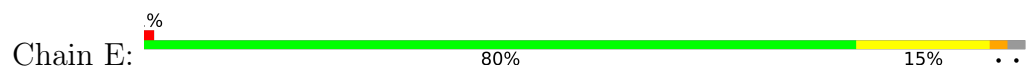




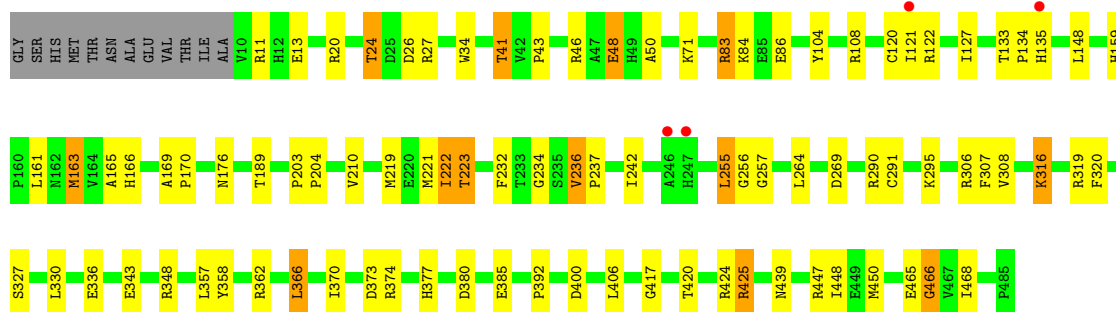
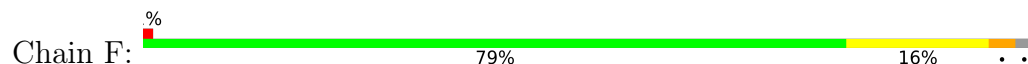
• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

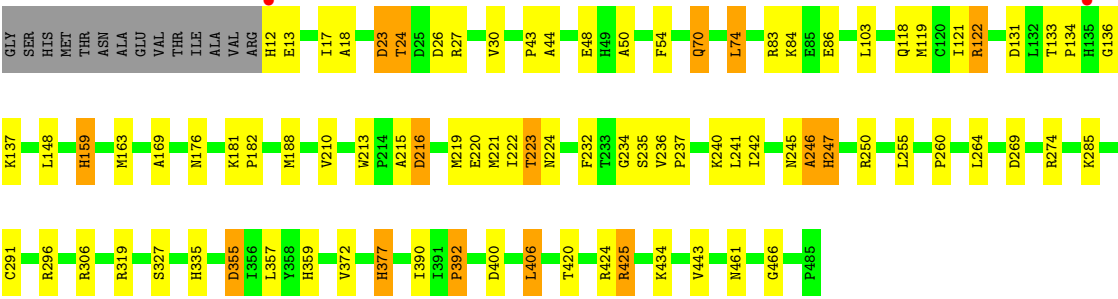


• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

Chain G:

79%

15%

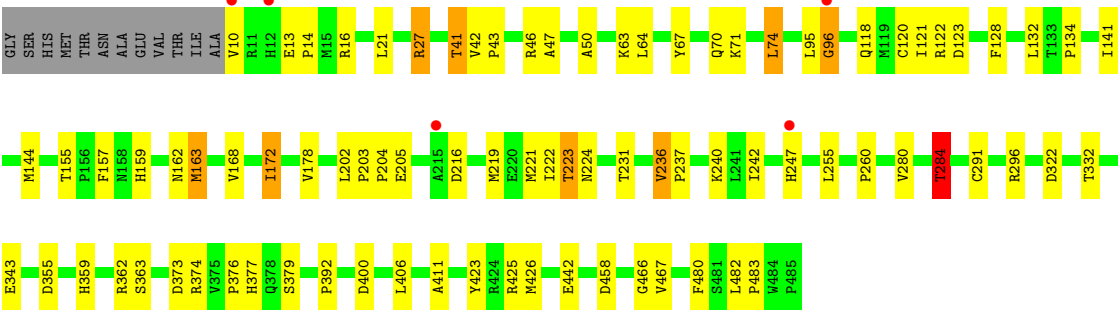


• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

Chain H:

80%

16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.16Å 172.76Å 142.60Å 90.00° 107.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-2.07) 94.0 (50.00-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.217 (Not available) , 0.196	Depositor DCC
R_{free} test set	12509 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32452	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, PAE

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	1.41	13/3724 (0.3%)	1.22	14/5066 (0.3%)
1	B	1.25	4/3706 (0.1%)	1.23	13/5042 (0.3%)
1	C	1.31	9/3717 (0.2%)	1.23	9/5056 (0.2%)
1	D	1.25	7/3724 (0.2%)	1.22	19/5066 (0.4%)
1	E	1.31	10/3722 (0.3%)	1.26	15/5063 (0.3%)
1	F	1.23	6/3724 (0.2%)	1.21	11/5066 (0.2%)
1	G	1.22	9/3706 (0.2%)	1.19	13/5042 (0.3%)
1	H	1.20	5/3724 (0.1%)	1.21	20/5066 (0.4%)
All	All	1.27	63/29747 (0.2%)	1.22	114/40467 (0.3%)

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	F	0	1
1	G	0	1
All	All	0	2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	ARG	CD-NE	-7.08	1.36	1.46
1	G	335	HIS	CG-CD2	7.03	1.43	1.35
1	D	335	HIS	CG-CD2	6.67	1.43	1.35
1	D	159	HIS	CG-CD2	6.61	1.43	1.35
1	G	377	HIS	CG-CD2	6.47	1.43	1.35
1	G	443	VAL	N-CA	-6.46	1.38	1.46
1	D	159	HIS	ND1-CE1	6.28	1.38	1.32
1	C	282	GLY	N-CA	6.21	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	359	HIS	CG-CD2	6.17	1.42	1.35
1	C	308	VAL	CA-C	6.10	1.57	1.52
1	H	377	HIS	CG-CD2	6.08	1.42	1.35
1	F	135	HIS	CG-CD2	6.07	1.42	1.35
1	G	159	HIS	CG-CD2	6.04	1.42	1.35
1	C	135	HIS	CG-CD2	6.04	1.42	1.35
1	A	249	LYS	CA-C	-6.02	1.45	1.52
1	H	203	PRO	CA-C	5.98	1.57	1.52
1	C	31	ARG	CA-C	-5.90	1.45	1.52
1	E	335	HIS	CG-CD2	5.79	1.42	1.35
1	A	330	LEU	C-O	5.79	1.30	1.24
1	H	96	GLY	N-CA	5.76	1.54	1.45
1	F	308	VAL	CA-CB	5.76	1.57	1.53
1	G	335	HIS	ND1-CE1	5.73	1.38	1.32
1	A	186	THR	CA-C	5.70	1.59	1.52
1	A	174	THR	CA-C	5.62	1.59	1.52
1	E	135	HIS	CG-CD2	5.62	1.42	1.35
1	F	166	HIS	CG-CD2	5.59	1.42	1.35
1	A	97	ILE	CA-CB	5.58	1.59	1.54
1	A	236	VAL	CA-CB	5.56	1.56	1.54
1	B	335	HIS	CG-CD2	5.53	1.42	1.35
1	G	159	HIS	ND1-CE1	5.45	1.38	1.32
1	A	151	ILE	C-O	5.43	1.29	1.24
1	E	335	HIS	ND1-CE1	5.43	1.38	1.32
1	E	12	HIS	CG-CD2	5.34	1.41	1.35
1	B	42	VAL	CA-C	5.31	1.57	1.52
1	B	335	HIS	ND1-CE1	5.29	1.37	1.32
1	D	368	PRO	CA-C	5.29	1.57	1.52
1	B	126	GLU	CD-OE1	5.27	1.35	1.25
1	D	12	HIS	CG-CD2	5.27	1.41	1.35
1	C	335	HIS	ND1-CE1	5.26	1.37	1.32
1	C	291	CYS	C-O	-5.25	1.17	1.24
1	E	135	HIS	N-CA	5.25	1.53	1.46
1	H	178	VAL	C-O	5.23	1.29	1.24
1	A	335	HIS	ND1-CE1	5.22	1.37	1.32
1	F	377	HIS	CG-CD2	5.22	1.41	1.35
1	A	290	ARG	N-CA	5.19	1.52	1.46
1	F	165	ALA	CA-C	5.19	1.60	1.52
1	E	104	TYR	CA-C	5.19	1.59	1.52
1	G	70	GLN	N-CA	-5.19	1.40	1.46
1	E	439	ASN	N-CA	5.18	1.52	1.46
1	D	355	ASP	N-CA	-5.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	PRO	CA-C	5.15	1.56	1.52
1	E	230	VAL	N-CA	-5.15	1.40	1.46
1	C	467	VAL	CA-C	5.13	1.59	1.52
1	D	97	ILE	CA-CB	5.12	1.60	1.54
1	F	135	HIS	ND1-CE1	5.12	1.37	1.32
1	A	12	HIS	CE1-NE2	5.06	1.37	1.32
1	C	414	LEU	CA-C	5.06	1.55	1.52
1	G	359	HIS	CG-CD2	5.06	1.41	1.35
1	E	166	HIS	CE1-NE2	5.04	1.37	1.32
1	A	263	ILE	CA-C	5.04	1.59	1.52
1	C	354	ALA	N-CA	5.03	1.52	1.45
1	E	138	ALA	CA-C	5.03	1.59	1.52
1	G	355	ASP	CA-C	5.02	1.59	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	A	466	GLY	N-CA-C	-8.24	102.29	112.68
1	B	245	ASN	CA-C-N	-8.14	110.40	122.86
1	B	245	ASN	C-N-CA	-8.14	110.40	122.86
1	G	425	ARG	NE-CZ-NH2	-8.13	111.88	119.20
1	H	467	VAL	N-CA-C	8.11	118.20	110.42
1	A	174	THR	N-CA-CB	-7.84	99.12	110.80
1	E	133	THR	CA-C-N	-7.66	111.83	119.56
1	E	133	THR	C-N-CA	-7.66	111.83	119.56
1	A	136	GLY	N-CA-C	7.51	130.98	113.18
1	F	120	CYS	CB-CA-C	-7.47	95.96	110.46
1	E	136	GLY	N-CA-C	7.32	120.38	112.33
1	G	466	GLY	N-CA-C	-7.27	103.52	112.68
1	H	236	VAL	CA-C-N	-7.27	111.49	119.19
1	H	236	VAL	C-N-CA	-7.27	111.49	119.19
1	G	236	VAL	CA-C-N	-7.11	111.10	118.85
1	G	236	VAL	C-N-CA	-7.11	111.10	118.85
1	C	163	MET	N-CA-C	-6.85	103.60	112.23
1	H	322	ASP	CA-C-N	6.58	125.81	118.97
1	H	322	ASP	C-N-CA	6.58	125.81	118.97
1	G	247	HIS	N-CA-C	6.57	119.03	111.02
1	C	174	THR	N-CA-CB	-6.54	100.41	111.27
1	A	164	VAL	N-CA-C	-6.54	103.87	111.00
1	D	102	SER	CB-CA-C	-6.47	99.85	110.85
1	E	83	ARG	NE-CZ-NH2	-6.39	113.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASN	N-CA-C	6.37	121.22	113.38
1	G	425	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	A	362	ARG	CG-CD-NE	-6.27	98.20	112.00
1	D	367	LEU	CA-C-N	-6.24	113.95	120.38
1	D	367	LEU	C-N-CA	-6.24	113.95	120.38
1	H	466	GLY	N-CA-C	-6.14	104.94	112.68
1	E	134	PRO	CA-C-N	6.14	130.42	120.60
1	E	134	PRO	C-N-CA	6.14	130.42	120.60
1	H	120	CYS	CB-CA-C	-6.11	97.42	110.32
1	D	10	VAL	CA-C-N	6.11	132.69	121.70
1	D	10	VAL	C-N-CA	6.11	132.69	121.70
1	E	120	CYS	N-CA-C	6.10	119.56	111.75
1	F	308	VAL	CA-C-N	-6.08	112.74	119.19
1	F	308	VAL	C-N-CA	-6.08	112.74	119.19
1	B	245	ASN	CB-CA-C	-6.00	99.67	110.35
1	B	355	ASP	N-CA-CB	-5.99	101.11	110.87
1	D	466	GLY	N-CA-C	-5.97	105.25	112.48
1	E	362	ARG	CG-CD-NE	-5.95	98.92	112.00
1	G	169	ALA	CA-C-N	-5.93	112.91	119.19
1	G	169	ALA	C-N-CA	-5.93	112.91	119.19
1	B	245	ASN	N-CA-C	5.91	122.52	113.19
1	H	96	GLY	N-CA-C	5.86	125.05	115.73
1	G	181	LYS	CA-C-N	-5.85	114.73	120.52
1	G	181	LYS	C-N-CA	-5.85	114.73	120.52
1	E	13	GLU	CA-C-N	-5.82	114.76	120.52
1	E	13	GLU	C-N-CA	-5.82	114.76	120.52
1	C	425	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	D	424	ARG	N-CA-C	-5.77	104.99	111.28
1	D	143	THR	N-CA-CB	-5.75	100.90	111.37
1	H	172	ILE	CB-CA-C	-5.73	104.64	111.97
1	E	42	VAL	CA-C-N	-5.71	114.05	119.76
1	E	42	VAL	C-N-CA	-5.71	114.05	119.76
1	F	307	PHE	N-CA-C	5.69	117.56	111.36
1	D	236	VAL	CB-CA-C	-5.67	108.31	113.70
1	B	216	ASP	N-CA-C	5.67	118.32	111.40
1	D	28	VAL	N-CA-C	-5.65	100.25	108.17
1	G	269	ASP	N-CA-C	5.62	117.08	111.07
1	B	265	ASN	N-CA-C	5.62	119.75	113.01
1	C	345	ARG	CB-CG-CD	5.60	124.17	111.30
1	C	473	SER	CB-CA-C	-5.59	100.29	110.63
1	E	467	VAL	N-CA-C	5.58	116.22	110.36
1	H	95	LEU	CA-C-N	-5.49	106.74	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	95	LEU	C-N-CA	-5.49	106.74	122.06
1	B	308	VAL	CA-C-N	-5.48	113.25	119.28
1	B	308	VAL	C-N-CA	-5.48	113.25	119.28
1	H	95	LEU	N-CA-C	-5.48	101.19	109.85
1	B	466	GLY	N-CA-C	-5.47	104.72	112.81
1	A	372	VAL	CB-CA-C	-5.46	102.36	110.33
1	H	42	VAL	CA-C-N	-5.44	114.32	119.76
1	H	42	VAL	C-N-CA	-5.44	114.32	119.76
1	H	483	PRO	CA-C-N	-5.43	117.31	122.37
1	H	483	PRO	C-N-CA	-5.43	117.31	122.37
1	H	284	THR	N-CA-CB	-5.43	102.77	110.81
1	F	366	LEU	N-CA-C	5.43	117.09	108.67
1	B	83	ARG	CB-CG-CD	-5.43	98.82	111.30
1	F	466	GLY	N-CA-C	-5.43	105.84	112.68
1	A	174	THR	CB-CA-C	5.40	119.39	109.99
1	C	425	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	F	468	ILE	N-CA-C	5.37	115.57	110.42
1	F	370	ILE	N-CA-C	5.36	116.61	109.37
1	D	216	ASP	N-CA-C	5.30	122.10	110.80
1	E	135	HIS	N-CA-C	5.29	118.83	112.38
1	H	162	ASN	N-CA-C	5.29	117.79	111.71
1	A	425	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	D	133	THR	CA-C-N	-5.26	113.62	119.19
1	D	133	THR	C-N-CA	-5.26	113.62	119.19
1	C	236	VAL	CA-C-N	-5.26	113.22	119.05
1	C	236	VAL	C-N-CA	-5.26	113.22	119.05
1	F	83	ARG	CB-CG-CD	-5.25	99.23	111.30
1	B	372	VAL	CB-CA-C	-5.24	102.00	110.28
1	D	284	THR	N-CA-CB	-5.23	101.65	110.49
1	A	450	MET	N-CA-C	5.22	120.30	113.30
1	H	155	THR	CA-C-N	5.22	126.36	119.84
1	H	155	THR	C-N-CA	5.22	126.36	119.84
1	D	80	LEU	N-CA-C	-5.22	105.27	111.69
1	C	468	ILE	N-CA-C	5.20	115.42	110.42
1	E	83	ARG	CB-CG-CD	-5.20	99.34	111.30
1	B	132	LEU	CB-CG-CD1	-5.16	95.21	110.70
1	D	365	ALA	N-CA-C	-5.12	107.03	113.28
1	A	83	ARG	CB-CG-CD	-5.12	99.52	111.30
1	D	338	ALA	N-CA-C	-5.11	105.62	111.14
1	F	257	GLY	N-CA-C	-5.09	103.70	111.14
1	D	143	THR	CA-CB-CG2	5.08	119.14	110.50
1	D	425	ARG	NE-CZ-NH2	-5.08	114.63	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	213	TRP	CA-C-N	5.06	124.72	119.56
1	G	213	TRP	C-N-CA	5.06	124.72	119.56
1	A	259	ASP	N-CA-C	5.05	116.43	110.07
1	A	36	ASP	N-CA-C	5.04	118.55	111.74
1	F	236	VAL	N-CA-CB	5.02	113.89	110.52

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	222	ILE	Peptide
1	G	246	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3651	0	3684	57	0
1	B	3633	0	3662	61	0
1	C	3644	0	3675	81	0
1	D	3651	0	3684	91	0
1	E	3649	0	3677	75	0
1	F	3651	0	3684	77	0
1	G	3633	0	3662	86	0
1	H	3651	0	3684	53	0
2	A	44	0	26	4	0
2	B	44	0	26	2	0
2	C	44	0	26	5	0
2	D	44	0	26	6	0
2	E	44	0	26	3	0
2	F	44	0	26	4	0
2	G	44	0	26	4	0
2	H	44	0	26	3	0
3	A	8	0	2	0	0
3	B	8	0	2	1	0
3	C	8	0	2	5	0
3	D	8	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	8	0	2	2	0
3	F	8	0	2	2	0
3	G	8	0	2	0	0
3	H	8	0	2	0	0
4	A	497	0	0	6	0
4	B	380	0	0	7	0
4	C	337	0	0	12	1
4	D	302	0	0	15	0
4	E	376	0	0	8	2
4	F	325	0	0	10	1
4	G	358	0	0	15	0
4	H	298	0	0	4	0
All	All	32452	0	29636	550	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:HIS:CE1	1:C:27:ARG:NH2	1.82	1.44
1:C:221:MET:SD	4:C:911:HOH:O	2.00	1.18
1:C:12:HIS:CE1	1:C:27:ARG:HH22	1.51	1.16
1:C:291:CYS:SG	2:C:501:NAD:C4N	2.35	1.15
1:C:290:ARG:HE	3:C:502:PAE:H12	1.04	1.11
1:B:246:ALA:HB3	1:B:251:GLN:NE2	1.64	1.10
1:D:11:ARG:HH11	1:D:188:MET:HE1	1.05	1.09
1:D:426:MET:SD	4:D:836:HOH:O	2.10	1.09
1:B:122:ARG:HB2	1:D:122:ARG:HH22	0.92	1.08
1:B:132:LEU:HD12	1:B:132:LEU:N	1.63	1.07
1:B:221:MET:SD	4:B:945:HOH:O	2.12	1.07
1:C:12:HIS:ND1	1:C:27:ARG:NH2	2.03	1.06
1:A:345:ARG:HH11	1:A:386:THR:HG22	1.18	1.05
1:E:122:ARG:HD2	1:G:122:ARG:NE	1.69	1.04
1:E:122:ARG:NH2	4:E:854:HOH:O	1.92	1.02
1:B:246:ALA:HB3	1:B:251:GLN:HE21	1.19	1.01
1:E:122:ARG:HD2	1:G:122:ARG:HE	0.85	1.01
1:D:345:ARG:CZ	4:D:877:HOH:O	2.06	1.00
1:A:291:CYS:SG	2:A:501:NAD:C4N	2.50	1.00
1:B:12:HIS:HE1	1:B:27:ARG:NH2	1.59	0.99
1:E:122:ARG:CD	1:G:122:ARG:HE	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:HIS:CE1	1:B:27:ARG:NH2	2.31	0.99
1:B:122:ARG:HB2	1:D:122:ARG:NH2	1.77	0.98
1:C:319:ARG:HH12	1:E:269:ASP:HB3	1.27	0.97
1:B:122:ARG:CB	1:D:122:ARG:HH22	1.76	0.97
1:B:210:VAL:HG21	1:B:221:MET:HE1	1.45	0.97
1:F:148:LEU:H	1:F:176:ASN:HD21	1.10	0.94
1:D:11:ARG:NH1	1:D:188:MET:HE1	1.82	0.94
1:C:50:ALA:HB1	1:C:221:MET:CE	1.97	0.94
1:B:12:HIS:ND1	1:B:41:THR:HG22	1.84	0.92
1:H:400:ASP:OD2	1:H:425:ARG:HD3	1.69	0.92
1:A:400:ASP:OD2	1:A:425:ARG:HD3	1.70	0.91
1:C:159:HIS:NE2	3:C:502:PAE:H11	1.84	0.91
1:F:221:MET:SD	4:F:645:HOH:O	2.28	0.91
1:B:246:ALA:CB	1:B:251:GLN:HE21	1.82	0.91
1:E:122:ARG:HG2	1:G:122:ARG:HH21	1.35	0.91
1:G:50:ALA:HB1	1:G:221:MET:CE	1.99	0.91
1:A:400:ASP:OD2	1:A:425:ARG:CD	2.19	0.91
1:D:291:CYS:SG	2:D:501:NAD:C4N	2.58	0.90
1:B:132:LEU:HD12	1:B:132:LEU:H	1.34	0.90
1:C:290:ARG:NE	3:C:502:PAE:H12	1.87	0.90
1:A:122:ARG:NH2	1:H:122:ARG:HB2	1.86	0.90
1:F:27:ARG:HD3	1:F:41:THR:HG21	1.53	0.89
1:G:221:MET:SD	4:G:889:HOH:O	2.29	0.89
1:C:174:THR:CG2	1:C:176:ASN:OD1	2.22	0.88
1:F:319:ARG:CD	4:F:849:HOH:O	2.21	0.88
1:H:291:CYS:SG	2:H:501:NAD:C4N	2.61	0.88
1:G:291:CYS:SG	2:G:501:NAD:C4N	2.62	0.88
1:B:291:CYS:SG	2:B:501:NAD:C4N	2.61	0.88
1:E:119:MET:HE3	1:G:121:ILE:HD11	1.57	0.86
1:A:27:ARG:HE	1:A:41:THR:CG2	1.89	0.85
1:F:319:ARG:HD3	4:F:849:HOH:O	1.75	0.85
1:D:345:ARG:NE	4:D:877:HOH:O	2.07	0.84
1:G:148:LEU:H	1:G:176:ASN:HD21	1.25	0.83
1:A:345:ARG:NH1	1:A:386:THR:HG22	1.92	0.83
1:A:27:ARG:HH21	1:A:41:THR:HG22	1.40	0.83
1:C:50:ALA:HB1	1:C:221:MET:HE3	1.60	0.83
1:A:148:LEU:H	1:A:176:ASN:HD21	1.28	0.82
1:G:23:ASP:OD1	1:G:27:ARG:NH1	2.13	0.82
1:C:122:ARG:HE	1:F:122:ARG:NH2	1.78	0.82
1:G:221:MET:HA	1:G:221:MET:HE2	1.62	0.81
1:F:319:ARG:NE	4:F:849:HOH:O	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG21	1:B:221:MET:CE	2.10	0.81
1:E:148:LEU:H	1:E:176:ASN:HD21	1.26	0.81
1:E:50:ALA:HB1	1:E:221:MET:HE2	1.61	0.81
1:C:174:THR:HG23	1:C:176:ASN:OD1	1.79	0.81
1:E:291:CYS:SG	2:E:501:NAD:C4N	2.69	0.81
1:C:291:CYS:SG	2:C:501:NAD:C3N	2.69	0.80
1:F:159:HIS:HB2	1:F:163:MET:HG2	1.64	0.80
1:C:148:LEU:H	1:C:176:ASN:HD21	1.29	0.80
1:C:221:MET:HE2	1:C:221:MET:HA	1.64	0.80
1:G:133:THR:O	4:G:822:HOH:O	2.00	0.80
1:C:11:ARG:N	4:C:752:HOH:O	2.15	0.79
1:F:291:CYS:SG	2:F:501:NAD:C4N	2.71	0.79
1:E:381:LEU:O	1:E:386:THR:HG23	1.83	0.78
1:B:246:ALA:CB	1:B:251:GLN:NE2	2.40	0.78
1:G:27:ARG:NH2	4:G:868:HOH:O	2.12	0.78
1:F:50:ALA:HB2	1:F:221:MET:CE	2.14	0.77
1:G:50:ALA:HB1	1:G:221:MET:HE3	1.65	0.77
1:G:159:HIS:HB2	1:G:163:MET:HG2	1.66	0.77
1:D:174:THR:CG2	1:D:176:ASN:OD1	2.32	0.77
1:D:148:LEU:H	1:D:176:ASN:HD21	1.29	0.77
1:F:50:ALA:HB2	1:F:221:MET:HE2	1.66	0.77
1:C:12:HIS:HE1	1:C:27:ARG:HH22	0.83	0.76
1:D:88:SER:HB2	1:D:102:SER:HB2	1.66	0.76
1:F:27:ARG:HH11	1:F:41:THR:HG21	1.50	0.76
1:B:84:LYS:HD2	4:B:764:HOH:O	1.85	0.76
1:B:159:HIS:HB2	1:B:163:MET:HG2	1.67	0.76
1:G:50:ALA:CB	1:G:221:MET:HE3	2.17	0.75
1:A:174:THR:HG23	1:A:176:ASN:OD1	1.85	0.75
1:C:50:ALA:CB	1:C:221:MET:HE3	2.16	0.74
1:F:50:ALA:CB	1:F:221:MET:HE2	2.18	0.74
1:H:96:GLY:HA3	1:H:332:THR:OG1	1.87	0.74
1:C:12:HIS:HE1	1:C:27:ARG:NH2	1.45	0.74
1:D:280:VAL:O	1:D:284:THR:HB	1.87	0.74
1:B:135:HIS:NE2	4:B:946:HOH:O	2.18	0.73
1:H:219:MET:O	1:H:223:THR:HB	1.88	0.73
1:G:216:ASP:N	1:G:216:ASP:OD2	2.20	0.73
1:A:27:ARG:HE	1:A:41:THR:HG23	1.51	0.73
1:G:54:PHE:HE2	1:G:221:MET:CE	2.02	0.73
1:H:280:VAL:O	1:H:284:THR:HB	1.88	0.73
1:B:210:VAL:CG2	1:B:221:MET:HE1	2.16	0.72
1:C:319:ARG:NH1	1:E:269:ASP:HB3	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ALA:HB1	1:G:221:MET:HE1	1.70	0.72
1:F:148:LEU:H	1:F:176:ASN:ND2	1.85	0.72
1:B:291:CYS:SG	2:B:501:NAD:C3N	2.77	0.72
1:C:12:HIS:CE1	1:C:27:ARG:CZ	2.72	0.72
1:C:50:ALA:HB1	1:C:221:MET:HE1	1.72	0.71
1:D:406:LEU:HD13	4:D:661:HOH:O	1.90	0.71
1:F:27:ARG:HH11	1:F:41:THR:CG2	2.03	0.71
1:D:12:HIS:HB3	1:D:27:ARG:HH21	1.54	0.71
1:H:13:GLU:HG3	1:H:16:ARG:HH12	1.55	0.71
1:H:291:CYS:SG	2:H:501:NAD:C3N	2.79	0.70
1:C:277:ASP:OD1	4:C:877:HOH:O	2.08	0.70
1:H:163:MET:HE2	1:H:163:MET:HA	1.73	0.70
1:A:400:ASP:OD2	1:A:425:ARG:HD2	1.90	0.70
1:G:319:ARG:NH2	1:G:327:SER:HB2	2.06	0.70
1:G:222:ILE:CD1	1:G:242:ILE:HG12	2.22	0.70
1:C:400:ASP:OD2	1:C:425:ARG:HD3	1.92	0.69
1:F:219:MET:O	1:F:223:THR:HB	1.92	0.69
1:E:381:LEU:O	1:E:386:THR:CG2	2.41	0.69
1:B:132:LEU:N	1:B:132:LEU:CD1	2.49	0.69
1:B:12:HIS:CE1	1:B:27:ARG:CZ	2.75	0.69
1:D:125:GLY:HA2	1:D:143:THR:HG22	1.74	0.69
1:E:163:MET:HE2	1:E:163:MET:HA	1.74	0.68
1:B:210:VAL:CG2	1:B:221:MET:CE	2.71	0.68
1:C:182:PRO:HD2	1:C:210:VAL:O	1.93	0.68
1:C:291:CYS:SG	2:C:501:NAD:H4N	2.31	0.68
1:G:122:ARG:HH11	1:G:122:ARG:HB2	1.58	0.68
1:H:50:ALA:HB1	1:H:221:MET:CE	2.24	0.68
1:E:12:HIS:HB3	4:E:769:HOH:O	1.93	0.68
1:G:131:ASP:OD2	4:G:931:HOH:O	2.11	0.67
1:A:244:ALA:HA	1:B:247:HIS:ND1	2.09	0.67
1:F:400:ASP:OD2	1:F:425:ARG:HD3	1.94	0.67
1:G:223:THR:HG22	4:G:740:HOH:O	1.92	0.67
1:E:247:HIS:N	4:E:853:HOH:O	2.26	0.67
1:D:174:THR:HG23	1:D:176:ASN:OD1	1.95	0.67
1:D:291:CYS:SG	2:D:501:NAD:C3N	2.83	0.67
1:E:319:ARG:HB3	1:E:319:ARG:HH11	1.60	0.67
1:A:174:THR:CG2	1:A:176:ASN:OD1	2.43	0.66
1:B:129:SER:O	1:B:132:LEU:HD11	1.95	0.66
1:D:131:ASP:OD2	4:D:797:HOH:O	2.12	0.66
1:G:54:PHE:HE2	1:G:221:MET:HE2	1.59	0.66
1:H:163:MET:HA	1:H:163:MET:CE	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HH21	1:C:41:THR:HG22	1.61	0.66
1:E:345:ARG:HH11	1:E:386:THR:HG22	1.61	0.66
1:A:119:MET:HE1	1:A:122:ARG:NH1	2.11	0.65
1:G:274:ARG:NH1	4:G:856:HOH:O	2.29	0.65
1:D:400:ASP:OD2	1:D:425:ARG:CD	2.44	0.65
1:G:24:THR:HB	1:G:43:PRO:HB3	1.79	0.65
1:C:170:PRO:O	1:C:174:THR:HB	1.97	0.65
1:E:119:MET:HE2	1:E:119:MET:HA	1.78	0.64
1:A:27:ARG:HH21	1:A:41:THR:CG2	2.10	0.64
1:F:83:ARG:HD3	1:F:86:GLU:OE1	1.98	0.64
1:G:70:GLN:HG2	1:G:74:LEU:HD22	1.79	0.64
1:D:345:ARG:NH2	4:D:877:HOH:O	2.25	0.64
1:D:381:LEU:O	1:D:386:THR:CG2	2.45	0.64
1:A:170:PRO:O	1:A:174:THR:HB	1.97	0.64
1:E:122:ARG:CG	1:G:122:ARG:HH21	2.09	0.64
1:G:222:ILE:HD12	1:G:242:ILE:HG12	1.79	0.64
1:C:345:ARG:HD3	4:C:910:HOH:O	1.97	0.64
1:G:182:PRO:HD2	1:G:210:VAL:O	1.98	0.64
1:F:210:VAL:HG21	1:F:221:MET:HE1	1.80	0.63
1:D:345:ARG:HH11	1:D:380:ASP:HB3	1.63	0.63
1:D:400:ASP:OD2	1:D:425:ARG:HD3	1.99	0.63
1:E:269:ASP:OD1	1:E:306:ARG:HD2	1.97	0.63
1:A:130:CYS:O	1:A:136:GLY:O	2.17	0.63
1:B:400:ASP:OD2	1:B:425:ARG:HD2	1.99	0.63
1:C:54:PHE:HE2	1:C:221:MET:HE2	1.64	0.63
1:D:424:ARG:NH2	4:D:685:HOH:O	2.31	0.63
1:D:35:ASN:OD1	1:D:37:THR:HG23	1.99	0.63
1:C:290:ARG:HE	3:C:502:PAE:C1P	1.97	0.63
1:A:291:CYS:SG	2:A:501:NAD:C3N	2.87	0.62
1:E:291:CYS:SG	2:E:501:NAD:C3N	2.87	0.62
1:B:30:VAL:HG11	1:B:188:MET:HE2	1.81	0.62
1:B:135:HIS:CE1	4:B:946:HOH:O	2.52	0.62
1:G:24:THR:CG2	1:G:26:ASP:O	2.48	0.62
1:F:27:ARG:HD3	1:F:41:THR:CG2	2.28	0.62
1:F:400:ASP:OD2	1:F:425:ARG:CD	2.46	0.62
1:E:237:PRO:O	1:E:241:LEU:HD13	2.00	0.62
1:G:54:PHE:CE2	1:G:221:MET:HE1	2.35	0.62
1:A:159:HIS:HB2	1:A:163:MET:HG2	1.82	0.61
1:D:35:ASN:CG	1:D:37:THR:HG23	2.25	0.61
1:F:319:ARG:NH2	1:F:327:SER:OG	2.32	0.61
1:A:381:LEU:O	1:A:386:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:PHE:CE2	1:G:221:MET:CE	2.83	0.61
1:H:400:ASP:OD2	1:H:425:ARG:CD	2.47	0.61
1:A:244:ALA:HA	1:B:247:HIS:HD1	1.65	0.61
1:G:119:MET:SD	1:G:122:ARG:NH1	2.71	0.61
1:C:400:ASP:OD2	1:C:425:ARG:CD	2.49	0.61
1:G:148:LEU:H	1:G:176:ASN:ND2	1.95	0.61
1:G:219:MET:HE1	1:G:245:ASN:HB3	1.83	0.61
1:F:348:ARG:NH1	1:F:380:ASP:OD2	2.34	0.61
1:E:27:ARG:HE	1:E:41:THR:HG23	1.65	0.60
1:G:221:MET:HE2	1:G:221:MET:CA	2.29	0.60
1:F:222:ILE:CD1	1:F:242:ILE:HG12	2.31	0.60
1:B:400:ASP:OD2	1:B:425:ARG:CD	2.50	0.60
1:A:122:ARG:HH22	1:H:122:ARG:HB2	1.65	0.60
1:D:13:GLU:O	1:D:43:PRO:HD3	2.02	0.60
1:E:50:ALA:CB	1:E:221:MET:HE2	2.32	0.59
1:E:219:MET:HE1	1:E:245:ASN:OD1	2.02	0.59
1:F:11:ARG:NH1	4:F:855:HOH:O	2.36	0.59
1:A:10:VAL:N	4:A:957:HOH:O	2.35	0.59
1:F:163:MET:HE3	1:F:163:MET:HA	1.82	0.59
1:E:122:ARG:NH1	1:E:122:ARG:HB3	2.16	0.59
1:A:119:MET:HE1	1:A:122:ARG:CZ	2.33	0.59
1:E:424:ARG:HB3	4:E:955:HOH:O	2.03	0.59
1:H:172:ILE:HD12	1:H:202:LEU:CD1	2.33	0.59
1:F:24:THR:HG22	1:F:26:ASP:O	2.03	0.59
1:G:222:ILE:HG23	1:G:246:ALA:HB2	1.85	0.59
1:D:426:MET:HE1	1:H:482:LEU:HD22	1.83	0.58
1:F:316:LYS:HD3	1:F:358:TYR:CD1	2.37	0.58
1:G:50:ALA:CB	1:G:221:MET:CE	2.75	0.58
1:F:222:ILE:HD12	1:F:242:ILE:HG23	1.84	0.58
1:A:20:ARG:HD3	4:A:1067:HOH:O	2.03	0.58
1:F:27:ARG:NH1	1:F:41:THR:HG21	2.17	0.58
1:C:84:LYS:NZ	4:C:836:HOH:O	2.36	0.58
1:D:88:SER:HB2	1:D:102:SER:CB	2.34	0.58
1:B:108:ARG:HD2	1:B:449:GLU:OE1	2.03	0.58
1:D:12:HIS:HB3	1:D:27:ARG:NH2	2.18	0.58
1:D:23:ASP:OD1	1:D:27:ARG:NH1	2.36	0.58
1:E:10:VAL:O	1:E:11:ARG:HB2	2.03	0.58
1:E:381:LEU:HD12	1:E:386:THR:HG21	1.87	0.57
1:F:50:ALA:CB	1:F:221:MET:CE	2.78	0.57
1:E:13:GLU:O	1:E:43:PRO:HD3	2.05	0.57
1:G:188:MET:CE	4:G:928:HOH:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ARG:HH12	3:D:502:PAE:P	2.28	0.57
1:E:23:ASP:OD1	1:E:27:ARG:NH1	2.38	0.57
1:A:343:GLU:OE1	1:A:362:ARG:HD3	2.04	0.57
1:C:119:MET:HE1	1:F:122:ARG:HD2	1.86	0.57
1:D:161:LEU:HB2	1:D:189:THR:HG21	1.86	0.57
1:F:210:VAL:HG21	1:F:221:MET:CE	2.35	0.56
1:F:236:VAL:HB	1:F:237:PRO:HD3	1.87	0.56
1:G:400:ASP:OD2	1:G:425:ARG:CD	2.53	0.56
1:D:119:MET:HE1	1:D:122:ARG:NH1	2.21	0.56
1:C:27:ARG:HB3	1:C:41:THR:HG23	1.87	0.56
1:B:122:ARG:CB	1:D:122:ARG:NH2	2.52	0.56
1:B:121:ILE:HD11	1:D:119:MET:CE	2.35	0.56
1:C:83:ARG:HD3	1:C:86:GLU:OE1	2.06	0.56
1:D:400:ASP:OD2	1:D:425:ARG:HD2	2.05	0.56
1:D:10:VAL:HG12	1:D:11:ARG:HE	1.71	0.55
1:B:132:LEU:H	1:B:132:LEU:CD1	2.15	0.55
1:C:118:GLN:O	1:C:121:ILE:HG12	2.07	0.55
1:E:27:ARG:HH21	1:E:41:THR:HG23	1.71	0.55
1:F:222:ILE:HD12	1:F:242:ILE:HG12	1.87	0.55
1:D:92:THR:OG1	1:D:102:SER:OG	2.24	0.55
1:F:424:ARG:NH2	4:F:819:HOH:O	2.30	0.55
1:C:54:PHE:CE2	1:C:221:MET:CE	2.90	0.55
1:D:381:LEU:O	1:D:386:THR:HG23	2.07	0.55
1:A:291:CYS:HB3	2:A:501:NAD:C2N	2.36	0.55
1:A:345:ARG:HH11	1:A:386:THR:CG2	2.07	0.55
1:H:50:ALA:CB	1:H:221:MET:CE	2.85	0.55
1:C:64:LEU:HD13	4:C:889:HOH:O	2.07	0.55
1:G:133:THR:HB	1:G:134:PRO:HD2	1.88	0.55
1:C:250:ARG:NH1	4:C:754:HOH:O	2.41	0.54
1:E:50:ALA:HB1	1:E:221:MET:CE	2.35	0.54
1:D:24:THR:HB	1:D:43:PRO:HB3	1.88	0.54
1:G:24:THR:HG22	1:G:26:ASP:O	2.07	0.54
1:H:172:ILE:HD12	1:H:202:LEU:HD13	1.88	0.54
1:G:136:GLY:HA2	4:G:815:HOH:O	2.08	0.54
1:E:290:ARG:HH21	3:E:502:PAE:P	2.31	0.54
1:H:118:GLN:O	1:H:121:ILE:HG12	2.08	0.54
1:E:16:ARG:NH2	1:E:195:ASP:OD2	2.28	0.53
1:D:170:PRO:O	1:D:174:THR:HB	2.08	0.53
1:E:291:CYS:HB3	2:E:501:NAD:C2N	2.36	0.53
1:E:267:LEU:HD22	1:E:271:ASP:HB3	1.90	0.53
1:G:54:PHE:HE2	1:G:221:MET:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:PRO:HG2	1:H:21:LEU:HD22	1.91	0.53
1:C:54:PHE:HE2	1:C:221:MET:CE	2.21	0.53
1:C:269:ASP:OD1	1:C:306:ARG:HD2	2.09	0.53
1:G:222:ILE:HD11	1:G:242:ILE:HG12	1.90	0.53
1:G:306:ARG:HG3	1:G:306:ARG:HH11	1.74	0.53
1:D:312:LEU:HG	1:D:316:LYS:HE3	1.91	0.53
1:D:426:MET:HE3	1:D:440:ILE:HG13	1.90	0.53
1:F:13:GLU:O	1:F:43:PRO:HD3	2.08	0.53
1:C:122:ARG:HE	1:F:122:ARG:HH22	1.52	0.52
1:G:13:GLU:O	1:G:43:PRO:HD3	2.09	0.52
1:A:264:LEU:HD12	1:A:420:THR:HB	1.92	0.52
1:H:222:ILE:HD12	1:H:242:ILE:HG23	1.90	0.52
1:G:424:ARG:NE	4:G:792:HOH:O	2.42	0.52
1:F:24:THR:CG2	1:F:26:ASP:O	2.58	0.52
1:A:291:CYS:SG	2:A:501:NAD:H4N	2.48	0.52
1:E:222:ILE:CD1	1:E:242:ILE:HG12	2.40	0.52
1:C:465:GLU:HB2	4:C:703:HOH:O	2.10	0.52
1:D:291:CYS:HB3	2:D:501:NAD:C2N	2.40	0.52
1:G:400:ASP:OD2	1:G:425:ARG:HD2	2.10	0.52
1:A:234:GLY:O	1:A:255:LEU:HA	2.11	0.51
1:G:24:THR:HG21	1:G:44:ALA:H	1.73	0.51
1:E:400:ASP:OD2	1:E:425:ARG:CD	2.58	0.51
1:G:255:LEU:O	2:G:501:NAD:H2N	2.10	0.51
1:A:133:THR:HB	1:A:134:PRO:HD2	1.92	0.51
1:B:130:CYS:C	1:B:132:LEU:CD1	2.84	0.51
1:F:269:ASP:OD1	1:F:306:ARG:HD2	2.10	0.51
1:D:219:MET:HE1	1:D:245:ASN:ND2	2.26	0.51
1:D:406:LEU:HD12	4:D:771:HOH:O	2.11	0.51
1:E:229:LEU:HD23	1:E:229:LEU:C	2.36	0.51
1:C:163:MET:HA	1:C:163:MET:HE3	1.93	0.51
1:C:377:HIS:CD2	1:C:406:LEU:HD11	2.45	0.51
1:C:159:HIS:HB2	1:C:163:MET:HG2	1.93	0.51
1:C:378:GLN:NE2	4:C:773:HOH:O	2.22	0.51
1:E:122:ARG:HB3	1:E:122:ARG:CZ	2.42	0.50
2:D:501:NAD:H5N	3:D:502:PAE:O2	2.11	0.50
1:F:291:CYS:SG	2:F:501:NAD:C3N	2.99	0.50
1:B:330:LEU:HD23	1:B:369:PRO:HD3	1.93	0.50
1:G:12:HIS:HB3	4:G:868:HOH:O	2.11	0.50
1:G:222:ILE:CG2	1:G:246:ALA:HB2	2.42	0.50
1:C:122:ARG:HD3	1:C:123:ASP:N	2.27	0.50
1:C:221:MET:HE2	1:C:221:MET:CA	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:HE2	1:B:385:GLU:HG3	1.94	0.50
1:D:11:ARG:N	4:D:842:HOH:O	2.45	0.50
1:D:83:ARG:NH2	4:D:834:HOH:O	2.41	0.50
1:H:291:CYS:HB3	2:H:501:NAD:C2N	2.42	0.50
1:B:447:ARG:HD2	4:B:607:HOH:O	2.12	0.49
1:D:255:LEU:O	2:D:501:NAD:H2N	2.12	0.49
1:B:12:HIS:CE1	1:B:27:ARG:HH22	2.24	0.49
1:C:122:ARG:HD3	1:C:123:ASP:H	1.76	0.49
1:G:291:CYS:SG	2:G:501:NAD:C3N	3.00	0.49
1:H:50:ALA:HB1	1:H:221:MET:HE2	1.91	0.49
1:E:115:LEU:HD12	1:E:449:GLU:HB2	1.93	0.49
1:F:161:LEU:HB2	1:F:189:THR:HG21	1.94	0.49
1:A:381:LEU:HD11	1:A:390:ILE:HG21	1.93	0.49
1:A:51:ARG:HD2	4:A:1076:HOH:O	2.12	0.49
1:C:291:CYS:HB3	2:C:501:NAD:C2N	2.42	0.49
1:E:119:MET:HE1	1:G:122:ARG:CD	2.42	0.49
1:G:219:MET:O	1:G:223:THR:HB	2.12	0.49
1:A:183:THR:HG23	1:A:186:THR:H	1.77	0.49
1:D:250:ARG:NH1	4:D:757:HOH:O	2.45	0.49
1:D:10:VAL:HG12	1:D:11:ARG:NE	2.27	0.49
1:E:319:ARG:HH11	1:E:319:ARG:CB	2.25	0.49
1:E:367:LEU:HD23	1:E:389:PRO:HD2	1.94	0.49
1:C:27:ARG:HE	1:C:41:THR:CG2	2.26	0.48
1:D:126:GLU:H	1:D:143:THR:HG22	1.78	0.48
1:F:83:ARG:NH2	4:F:816:HOH:O	2.45	0.48
1:G:24:THR:HG21	1:G:44:ALA:N	2.28	0.48
1:E:287:SER:HA	1:E:330:LEU:CD1	2.43	0.48
1:E:400:ASP:OD2	1:E:425:ARG:HD3	2.13	0.48
1:G:400:ASP:OD2	1:G:425:ARG:HD3	2.12	0.48
1:C:54:PHE:CE2	1:C:221:MET:HE1	2.48	0.48
1:D:219:MET:O	1:D:223:THR:HB	2.14	0.48
1:E:424:ARG:HD2	4:E:955:HOH:O	2.12	0.48
1:F:343:GLU:OE1	1:F:362:ARG:HD3	2.12	0.48
1:A:27:ARG:NE	1:A:41:THR:HG23	2.25	0.48
1:D:281:ALA:HB3	4:D:838:HOH:O	2.12	0.48
1:F:320:PHE:HA	1:F:330:LEU:O	2.13	0.48
1:F:316:LYS:HD3	1:F:358:TYR:CE1	2.47	0.48
1:C:148:LEU:H	1:C:176:ASN:ND2	2.05	0.48
1:D:11:ARG:O	1:D:40:GLY:HA2	2.14	0.48
1:D:126:GLU:H	1:D:143:THR:CG2	2.25	0.48
1:D:159:HIS:HB2	1:D:163:MET:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:LEU:HD12	1:E:420:THR:HB	1.96	0.48
1:E:50:ALA:CB	1:E:221:MET:CE	2.92	0.48
1:F:169:ALA:HB3	1:F:170:PRO:HD3	1.95	0.48
1:H:236:VAL:O	1:H:240:LYS:HG2	2.14	0.48
1:E:119:MET:HE1	1:G:122:ARG:NE	2.28	0.48
1:H:411:ALA:O	1:H:458:ASP:HB2	2.14	0.48
1:A:27:ARG:HE	1:A:41:THR:HG21	1.74	0.48
1:H:122:ARG:NH2	4:H:879:HOH:O	2.46	0.48
1:A:381:LEU:O	1:A:386:THR:CG2	2.62	0.47
1:D:125:GLY:CA	1:D:143:THR:HG22	2.41	0.47
1:A:343:GLU:O	1:A:347:MET:HG2	2.14	0.47
1:H:204:PRO:HD2	1:H:205:GLU:OE1	2.15	0.47
1:B:108:ARG:HH22	3:B:502:PAE:P	2.37	0.47
1:A:163:MET:HA	1:A:163:MET:HE2	1.96	0.47
1:C:108:ARG:HH12	3:C:502:PAE:P	2.38	0.47
1:D:246:ALA:HB3	1:D:251:GLN:NE2	2.29	0.47
1:D:319:ARG:HD3	4:D:839:HOH:O	2.14	0.47
1:E:27:ARG:NH2	4:E:769:HOH:O	2.47	0.47
1:G:119:MET:HE1	1:G:122:ARG:HH22	1.79	0.47
1:E:119:MET:HE3	1:G:121:ILE:CD1	2.39	0.47
1:E:94:GLU:HB3	1:E:188:MET:HE2	1.95	0.47
1:F:163:MET:HE3	1:F:163:MET:CA	2.44	0.47
1:G:188:MET:HE3	4:G:928:HOH:O	2.13	0.47
1:H:168:VAL:O	1:H:172:ILE:HG12	2.15	0.47
1:H:423:TYR:CD1	1:H:426:MET:HE2	2.50	0.47
1:E:319:ARG:HH11	1:E:319:ARG:CG	2.28	0.46
1:F:108:ARG:HH12	3:F:502:PAE:P	2.38	0.46
1:B:229:LEU:C	1:B:229:LEU:HD23	2.40	0.46
1:E:236:VAL:HB	1:E:237:PRO:HD3	1.96	0.46
1:C:50:ALA:CB	1:C:221:MET:CE	2.77	0.46
1:E:12:HIS:HA	1:E:41:THR:HG22	1.97	0.46
1:G:235:SER:HB2	1:G:237:PRO:HD2	1.97	0.46
1:E:148:LEU:H	1:E:176:ASN:ND2	2.04	0.46
1:H:159:HIS:HB2	1:H:163:MET:HG2	1.97	0.46
1:E:343:GLU:OE1	1:E:362:ARG:HD3	2.16	0.46
1:F:121:ILE:HG13	1:F:122:ARG:HG3	1.97	0.46
1:G:50:ALA:HB3	1:G:220:GLU:HG2	1.97	0.46
1:A:27:ARG:NE	1:A:41:THR:CG2	2.69	0.46
4:A:814:HOH:O	1:B:247:HIS:HB3	2.16	0.46
1:H:237:PRO:HG2	4:H:718:HOH:O	2.15	0.46
1:H:343:GLU:OE1	1:H:362:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:SER:HA	1:C:330:LEU:CD1	2.46	0.45
1:D:191:LEU:HD13	1:D:209:VAL:CG1	2.46	0.45
1:C:122:ARG:HE	1:F:122:ARG:HH21	1.58	0.45
1:C:348:ARG:NH1	1:C:380:ASP:OD2	2.48	0.45
1:G:188:MET:HE1	4:G:928:HOH:O	2.14	0.45
1:H:157:PHE:CD1	1:H:157:PHE:C	2.94	0.45
1:A:241:LEU:C	1:A:241:LEU:HD23	2.40	0.45
1:A:336:GLU:OE2	1:A:362:ARG:NH2	2.45	0.45
1:F:222:ILE:HD11	1:F:242:ILE:HG12	1.98	0.45
1:D:10:VAL:HA	1:D:11:ARG:HB3	1.98	0.45
1:D:89:ASP:OD1	1:D:324:MET:HE1	2.17	0.45
1:F:34:TRP:HZ3	1:F:366:LEU:HD22	1.81	0.45
1:F:264:LEU:HD12	1:F:420:THR:HB	1.98	0.45
1:F:400:ASP:OD2	1:F:425:ARG:HD2	2.15	0.45
1:G:50:ALA:HB2	1:G:221:MET:HE3	1.96	0.45
1:G:390:ILE:O	1:G:392:PRO:HD3	2.17	0.45
1:F:71:LYS:HD2	4:F:833:HOH:O	2.17	0.45
1:B:130:CYS:C	1:B:132:LEU:HD12	2.41	0.45
1:E:133:THR:OG1	1:E:135:HIS:HB2	2.16	0.45
1:E:210:VAL:HG21	1:E:221:MET:HE3	1.99	0.45
1:B:181:LYS:HB2	1:B:221:MET:HE3	1.99	0.45
1:E:83:ARG:HD3	1:E:86:GLU:OE1	2.17	0.45
1:F:290:ARG:HH21	3:F:502:PAE:P	2.40	0.45
1:H:70:GLN:HG3	1:H:74:LEU:HD22	1.98	0.45
1:C:345:ARG:HD2	1:C:380:ASP:HB3	1.98	0.44
1:G:247:HIS:N	4:G:748:HOH:O	2.49	0.44
1:H:63:LYS:O	1:H:64:LEU:C	2.60	0.44
1:C:13:GLU:O	1:C:43:PRO:HD3	2.17	0.44
1:H:260:PRO:HA	1:H:296:ARG:O	2.17	0.44
1:B:241:LEU:C	1:B:241:LEU:HD23	2.42	0.44
1:B:400:ASP:OD2	1:B:425:ARG:HD3	2.16	0.44
1:A:11:ARG:HG3	4:A:904:HOH:O	2.18	0.44
1:F:104:TYR:HE2	1:F:108:ARG:HD2	1.82	0.44
1:G:291:CYS:HB3	2:G:501:NAD:C2N	2.47	0.44
1:A:426:MET:HE1	1:D:423:TYR:HB3	1.99	0.44
1:F:373:ASP:OD1	1:F:374:ARG:N	2.45	0.44
1:G:83:ARG:HD2	1:G:86:GLU:OE1	2.17	0.44
1:D:10:VAL:HG12	1:D:11:ARG:HH21	1.81	0.44
1:B:210:VAL:CG2	1:B:221:MET:HE3	2.47	0.44
1:C:303:VAL:HG12	1:C:306:ARG:NH2	2.32	0.44
1:D:243:ALA:HA	1:D:251:GLN:HE22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:THR:HB	1:F:134:PRO:HD2	2.00	0.44
1:A:14:PRO:HG3	1:A:21:LEU:HB3	1.99	0.44
1:D:386:THR:HA	4:D:657:HOH:O	2.17	0.44
1:F:46:ARG:NH1	1:F:48:GLU:OE1	2.51	0.44
1:G:232:PHE:CZ	1:G:234:GLY:HA3	2.51	0.44
1:G:306:ARG:NH1	4:G:692:HOH:O	2.51	0.44
1:G:434:LYS:HD2	4:G:709:HOH:O	2.18	0.44
1:B:336:GLU:HG3	1:B:364:GLY:HA2	1.99	0.43
1:C:122:ARG:NE	1:F:122:ARG:NH2	2.57	0.43
1:C:157:PHE:CD1	1:C:157:PHE:C	2.96	0.43
1:D:469:GLU:O	1:D:473:SER:HB2	2.18	0.43
1:E:400:ASP:OD2	1:E:425:ARG:HD2	2.18	0.43
1:E:83:ARG:CD	1:E:86:GLU:OE1	2.66	0.43
1:B:84:LYS:HB3	1:B:84:LYS:HE2	1.73	0.43
1:F:203:PRO:HA	1:F:204:PRO:HD3	1.80	0.43
1:F:465:GLU:HB3	1:F:466:GLY:H	1.58	0.43
2:C:501:NAD:H51A	2:C:501:NAD:H2B	1.56	0.43
1:H:27:ARG:HG3	1:H:41:THR:HG21	1.99	0.43
1:C:31:ARG:HD3	1:C:36:ASP:OD1	2.18	0.43
1:D:223:THR:O	1:D:224:ASN:C	2.58	0.43
1:D:12:HIS:HD1	1:D:41:THR:HG1	1.67	0.43
1:E:10:VAL:O	1:E:11:ARG:CB	2.66	0.43
1:G:30:VAL:HG11	1:G:188:MET:HE2	2.00	0.43
1:H:13:GLU:O	1:H:43:PRO:HD3	2.19	0.43
1:D:24:THR:CG2	1:D:26:ASP:O	2.67	0.43
1:D:219:MET:HE1	1:D:245:ASN:HD22	1.83	0.43
1:E:27:ARG:NH1	4:E:769:HOH:O	2.51	0.43
1:B:163:MET:HE1	1:B:233:THR:HG21	2.01	0.43
1:C:295:LYS:HE2	1:C:385:GLU:HG3	2.00	0.43
1:D:10:VAL:HG12	1:D:11:ARG:NH2	2.34	0.42
1:H:426:MET:HE2	1:H:426:MET:HB2	1.87	0.42
1:A:170:PRO:HB3	1:A:471:MET:HG3	2.00	0.42
1:D:35:ASN:O	1:D:37:THR:CG2	2.67	0.42
1:E:27:ARG:HE	1:E:41:THR:CG2	2.30	0.42
1:F:84:LYS:HE2	1:F:84:LYS:HB3	1.80	0.42
1:D:24:THR:HG22	1:D:26:ASP:O	2.19	0.42
1:F:50:ALA:HB2	1:F:221:MET:HE1	1.99	0.42
1:G:148:LEU:HD21	1:G:250:ARG:HH22	1.84	0.42
1:H:13:GLU:HG3	1:H:16:ARG:NH1	2.29	0.42
1:A:12:HIS:ND1	1:A:41:THR:HB	2.35	0.42
1:C:11:ARG:N	4:C:728:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:NE	1:F:122:ARG:HH22	2.14	0.42
1:C:122:ARG:HH22	1:F:450:MET:HE3	1.85	0.42
1:C:153:ALA:HB1	1:C:167:LYS:HG2	2.01	0.42
1:F:417:GLY:HA2	1:F:439:ASN:O	2.19	0.42
2:F:501:NAD:H2B	4:F:800:HOH:O	2.18	0.42
1:G:355:ASP:OD2	1:G:357:LEU:HD21	2.20	0.42
1:H:362:ARG:HG2	1:H:363:SER:N	2.34	0.42
1:B:121:ILE:HD13	1:D:118:GLN:OE1	2.19	0.42
1:B:340:ALA:O	1:B:344:GLU:HG3	2.19	0.42
1:E:108:ARG:HH12	3:E:502:PAE:P	2.43	0.42
1:F:295:LYS:HE2	1:F:385:GLU:HG3	2.02	0.42
1:F:357:LEU:HD22	4:F:917:HOH:O	2.18	0.42
1:A:144:MET:HE1	4:D:648:HOH:O	2.20	0.42
1:C:123:ASP:OD1	4:C:867:HOH:O	2.21	0.42
1:D:287:SER:HA	1:D:330:LEU:CD1	2.49	0.42
1:F:163:MET:HE2	1:F:163:MET:HB3	1.72	0.42
1:H:67:TYR:OH	1:H:71:LYS:HE2	2.19	0.42
1:H:223:THR:O	1:H:224:ASN:C	2.62	0.42
1:C:260:PRO:HA	1:C:296:ARG:O	2.19	0.42
1:E:170:PRO:HB3	1:E:471:MET:HG3	2.00	0.42
1:G:84:LYS:HE2	1:G:103:LEU:HD22	2.01	0.42
1:E:95:LEU:HD22	1:E:160:PRO:HD3	2.02	0.42
1:H:376:PRO:HG2	1:H:379:SER:HB3	2.02	0.42
1:C:54:PHE:CE1	1:C:179:VAL:HB	2.54	0.41
1:F:24:THR:HB	1:F:43:PRO:HB3	2.01	0.41
1:H:122:ARG:HG2	1:H:123:ASP:N	2.35	0.41
1:A:13:GLU:O	1:A:43:PRO:HD3	2.19	0.41
1:A:118:GLN:HG2	1:H:118:GLN:HG2	2.02	0.41
1:D:246:ALA:CB	1:D:251:GLN:NE2	2.83	0.41
1:G:377:HIS:CG	1:G:406:LEU:HD11	2.54	0.41
1:F:232:PHE:CZ	1:F:234:GLY:HA3	2.55	0.41
1:G:260:PRO:HA	1:G:296:ARG:O	2.20	0.41
1:H:128:PHE:HB2	1:H:141:ILE:HB	2.03	0.41
1:B:83:ARG:HD3	1:B:86:GLU:OE1	2.20	0.41
1:D:426:MET:CE	1:H:482:LEU:HD22	2.50	0.41
1:E:11:ARG:NH1	4:E:874:HOH:O	2.53	0.41
1:B:465:GLU:HB3	1:B:466:GLY:H	1.59	0.41
1:D:157:PHE:CD1	1:D:157:PHE:C	2.98	0.41
1:G:70:GLN:CG	1:G:74:LEU:HD22	2.48	0.41
1:A:182:PRO:HD2	1:A:210:VAL:O	2.20	0.41
1:A:264:LEU:HD12	1:A:420:THR:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HE	1:C:41:THR:HG21	1.85	0.41
1:B:163:MET:HE3	1:B:163:MET:HB3	1.81	0.41
1:D:310:LEU:O	1:D:314:ARG:HD2	2.21	0.41
1:D:438:VAL:O	1:H:480:PHE:HA	2.20	0.41
1:E:118:GLN:HG2	1:G:118:GLN:HG2	2.02	0.41
1:H:355:ASP:HB2	4:H:808:HOH:O	2.19	0.41
1:A:83:ARG:CD	1:A:86:GLU:OE1	2.68	0.41
1:B:67:TYR:CZ	1:H:134:PRO:HG3	2.56	0.41
1:D:157:PHE:HA	1:D:183:THR:HG21	2.03	0.41
1:D:174:THR:HG22	1:D:176:ASN:OD1	2.19	0.41
1:G:17:ILE:O	1:G:18:ALA:C	2.64	0.41
1:H:46:ARG:NH2	4:H:870:HOH:O	2.45	0.41
1:H:373:ASP:OD1	1:H:374:ARG:N	2.44	0.41
1:A:163:MET:HE1	4:A:723:HOH:O	2.20	0.41
4:B:667:HOH:O	1:H:144:MET:HE1	2.20	0.41
1:D:125:GLY:HA2	1:D:143:THR:CG2	2.45	0.41
1:E:163:MET:HA	1:E:163:MET:CE	2.46	0.40
1:F:127:ILE:HD13	1:F:127:ILE:HG21	1.89	0.40
1:G:264:LEU:HD12	1:G:420:THR:HB	2.01	0.40
1:D:36:ASP:CG	1:D:36:ASP:O	2.63	0.40
1:E:161:LEU:HB2	1:E:189:THR:HG21	2.03	0.40
1:F:234:GLY:O	1:F:255:LEU:HA	2.21	0.40
1:F:256:GLY:HA2	2:F:501:NAD:O2D	2.21	0.40
1:G:223:THR:O	1:G:224:ASN:C	2.64	0.40
1:B:157:PHE:CD1	1:B:157:PHE:C	2.98	0.40
1:B:169:ALA:HB3	1:B:170:PRO:HD3	2.02	0.40
1:B:348:ARG:NH2	1:B:380:ASP:OD2	2.41	0.40
1:C:234:GLY:O	1:C:255:LEU:HA	2.21	0.40
1:D:15:MET:HE1	1:D:49:HIS:CG	2.57	0.40
1:A:169:ALA:HB3	1:A:170:PRO:HD3	2.03	0.40
1:C:186:THR:N	1:C:187:PRO:HD3	2.36	0.40
1:D:229:LEU:C	1:D:229:LEU:HD23	2.46	0.40
2:D:501:NAD:C5N	3:D:502:PAE:O2	2.70	0.40
1:B:319:ARG:HD2	4:B:682:HOH:O	2.21	0.40
1:C:70:GLN:O	1:C:74:LEU:HD22	2.22	0.40
1:C:472:LYS:HE3	4:C:787:HOH:O	2.20	0.40
1:D:35:ASN:OD1	1:D:35:ASN:C	2.64	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:937:HOH:O	4:F:895:HOH:O[2_555]	2.04	0.16
4:C:895:HOH:O	4:E:904:HOH:O[2_545]	2.14	0.06

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	474/488 (97%)	460 (97%)	11 (2%)	3 (1%)	21	13
1	B	472/488 (97%)	454 (96%)	16 (3%)	2 (0%)	30	23
1	C	473/488 (97%)	454 (96%)	17 (4%)	2 (0%)	30	23
1	D	474/488 (97%)	450 (95%)	20 (4%)	4 (1%)	16	8
1	E	474/488 (97%)	451 (95%)	20 (4%)	3 (1%)	21	13
1	F	474/488 (97%)	453 (96%)	20 (4%)	1 (0%)	43	38
1	G	472/488 (97%)	449 (95%)	20 (4%)	3 (1%)	21	13
1	H	474/488 (97%)	448 (94%)	23 (5%)	3 (1%)	21	13
All	All	3787/3904 (97%)	3619 (96%)	147 (4%)	21 (1%)	21	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLY
1	C	247	HIS
1	D	136	GLY
1	D	215	ALA
1	E	11	ARG
1	E	247	HIS
1	G	215	ALA
1	B	247	HIS
1	A	137	LYS
1	C	392	PRO
1	E	392	PRO

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Mol	Chain	Res	Type
1	H	247	HIS
1	D	216	ASP
1	G	461	ASN
1	A	392	PRO
1	D	392	PRO
1	H	47	ALA
1	H	392	PRO
1	B	392	PRO
1	F	392	PRO
1	G	392	PRO

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	392/401 (98%)	381 (97%)	11 (3%)	38	34
1	B	390/401 (97%)	378 (97%)	12 (3%)	35	30
1	C	391/401 (98%)	383 (98%)	8 (2%)	48	47
1	D	392/401 (98%)	369 (94%)	23 (6%)	18	10
1	E	391/401 (98%)	379 (97%)	12 (3%)	35	30
1	F	392/401 (98%)	379 (97%)	13 (3%)	33	28
1	G	390/401 (97%)	377 (97%)	13 (3%)	33	28
1	H	392/401 (98%)	379 (97%)	13 (3%)	33	28
All	All	3130/3208 (98%)	3025 (97%)	105 (3%)	32	27

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	GLU
1	A	74	LEU
1	A	84	LYS
1	A	174	THR

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Mol	Chain	Res	Type
1	A	240	LYS
1	A	255	LEU
1	A	285	LYS
1	A	359	HIS
1	A	378	GLN
1	A	386	THR
1	B	27	ARG
1	B	41	THR
1	B	71	LYS
1	B	74	LEU
1	B	92	THR
1	B	132	LEU
1	B	219	MET
1	B	250	ARG
1	B	255	LEU
1	B	337	LYS
1	B	372	VAL
1	B	406	LEU
1	C	41	THR
1	C	64	LEU
1	C	74	LEU
1	C	167	LYS
1	C	174	THR
1	C	344	GLU
1	C	377	HIS
1	C	406	LEU
1	D	10	VAL
1	D	11	ARG
1	D	24	THR
1	D	25	ASP
1	D	27	ARG
1	D	37	THR
1	D	39	VAL
1	D	143	THR
1	D	163	MET
1	D	174	THR
1	D	191	LEU
1	D	223	THR
1	D	240	LYS
1	D	241	LEU
1	D	255	LEU
1	D	284	THR

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Mol	Chain	Res	Type
1	D	313	GLU
1	D	367	LEU
1	D	372	VAL
1	D	386	THR
1	D	406	LEU
1	D	456	ILE
1	D	473	SER
1	E	23	ASP
1	E	41	THR
1	E	191	LEU
1	E	216	ASP
1	E	250	ARG
1	E	255	LEU
1	E	285	LYS
1	E	319	ARG
1	E	336	GLU
1	E	372	VAL
1	E	386	THR
1	E	406	LEU
1	F	20	ARG
1	F	24	THR
1	F	41	THR
1	F	48	GLU
1	F	163	MET
1	F	223	THR
1	F	255	LEU
1	F	316	LYS
1	F	336	GLU
1	F	406	LEU
1	F	425	ARG
1	F	447	ARG
1	F	448	ILE
1	G	23	ASP
1	G	24	THR
1	G	48	GLU
1	G	74	LEU
1	G	122	ARG
1	G	137	LYS
1	G	216	ASP
1	G	223	THR
1	G	240	LYS
1	G	241	LEU

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Mol	Chain	Res	Type
1	G	285	LYS
1	G	372	VAL
1	G	406	LEU
1	H	10	VAL
1	H	27	ARG
1	H	41	THR
1	H	74	LEU
1	H	132	LEU
1	H	163	MET
1	H	216	ASP
1	H	223	THR
1	H	231	THR
1	H	255	LEU
1	H	284	THR
1	H	406	LEU
1	H	442	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	HIS
1	B	12	HIS
1	C	70	GLN
1	C	245	ASN
1	D	251	GLN
1	E	176	ASN
1	F	118	GLN
1	F	176	ASN
1	G	176	ASN
1	H	245	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	H	501	-	46,48,48	1.61	8 (17%)	64,73,73	1.77	13 (20%)
2	NAD	G	501	-	46,48,48	1.33	7 (15%)	64,73,73	1.97	18 (28%)
2	NAD	A	501	-	46,48,48	1.38	7 (15%)	64,73,73	1.81	14 (21%)
2	NAD	D	501	-	46,48,48	1.58	8 (17%)	64,73,73	1.82	16 (25%)
3	PAE	H	502	-	7,7,7	1.68	1 (14%)	9,10,10	2.03	3 (33%)
2	NAD	C	501	-	46,48,48	1.59	7 (15%)	64,73,73	2.20	21 (32%)
3	PAE	A	502	-	7,7,7	1.70	2 (28%)	9,10,10	1.95	4 (44%)
3	PAE	C	502	-	7,7,7	1.50	1 (14%)	9,10,10	2.63	2 (22%)
2	NAD	B	501	-	46,48,48	1.48	7 (15%)	64,73,73	1.79	12 (18%)
3	PAE	E	502	-	7,7,7	1.30	1 (14%)	9,10,10	1.73	2 (22%)
3	PAE	B	502	-	7,7,7	1.85	2 (28%)	9,10,10	2.02	2 (22%)
2	NAD	F	501	-	46,48,48	1.53	7 (15%)	64,73,73	1.87	19 (29%)
2	NAD	E	501	-	46,48,48	1.51	9 (19%)	64,73,73	2.15	18 (28%)
3	PAE	D	502	-	7,7,7	1.47	1 (14%)	9,10,10	1.14	0
3	PAE	G	502	-	7,7,7	1.41	0	9,10,10	2.04	4 (44%)
3	PAE	F	502	-	7,7,7	1.31	1 (14%)	9,10,10	2.06	3 (33%)

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	H	501	-	-	3/30/62/62	0/5/5/5
2	NAD	G	501	-	-	1/30/62/62	0/5/5/5
2	NAD	A	501	-	-	2/30/62/62	0/5/5/5
2	NAD	D	501	-	-	3/30/62/62	0/5/5/5
3	PAE	H	502	-	-	0/5/5/5	-
2	NAD	C	501	-	-	5/30/62/62	0/5/5/5
3	PAE	A	502	-	-	0/5/5/5	-
3	PAE	C	502	-	-	3/5/5/5	-
2	NAD	B	501	-	-	3/30/62/62	0/5/5/5
3	PAE	E	502	-	-	0/5/5/5	-
3	PAE	B	502	-	-	0/5/5/5	-
2	NAD	F	501	-	-	4/30/62/62	0/5/5/5
2	NAD	E	501	-	-	5/30/62/62	0/5/5/5
3	PAE	D	502	-	-	3/5/5/5	-
3	PAE	G	502	-	-	0/5/5/5	-
3	PAE	F	502	-	-	0/5/5/5	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	PN-O3	5.90	1.65	1.59
2	D	501	NAD	C5A-C4A	5.38	1.48	1.39
2	H	501	NAD	C5A-C4A	5.19	1.48	1.39
2	B	501	NAD	C5A-C4A	4.75	1.47	1.39
2	H	501	NAD	PN-O3	4.58	1.64	1.59
2	F	501	NAD	C5A-C4A	4.57	1.47	1.39
2	F	501	NAD	PN-O3	4.26	1.64	1.59
2	G	501	NAD	C5A-C4A	4.13	1.46	1.39
2	E	501	NAD	C5A-C4A	4.08	1.46	1.39
2	C	501	NAD	O4D-C1D	3.93	1.46	1.40
2	D	501	NAD	O4D-C1D	3.92	1.46	1.40
2	H	501	NAD	PA-O3	3.88	1.63	1.59
2	A	501	NAD	C5A-C4A	3.73	1.45	1.39
2	B	501	NAD	PA-O3	3.73	1.63	1.59
2	F	501	NAD	PA-O3	3.68	1.63	1.59
2	E	501	NAD	PA-O3	3.66	1.63	1.59
2	G	501	NAD	O4D-C1D	3.64	1.45	1.40
2	A	501	NAD	C5A-N7A	-3.54	1.32	1.39
2	B	501	NAD	PN-O3	3.46	1.63	1.59
2	D	501	NAD	PA-O3	3.31	1.63	1.59
3	H	502	PAE	C1P-C1	-3.27	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	PA-O3	3.26	1.63	1.59
2	F	501	NAD	O4D-C1D	3.22	1.45	1.40
3	B	502	PAE	C1P-C1	-3.14	1.47	1.51
2	H	501	NAD	C8A-N7A	3.13	1.37	1.31
2	B	501	NAD	C5A-C6A	3.08	1.49	1.41
3	B	502	PAE	P-O3P	3.08	1.56	1.50
2	C	501	NAD	C5A-C4A	3.04	1.44	1.39
3	A	502	PAE	C1P-C1	-3.02	1.47	1.51
2	E	501	NAD	C5A-C6A	2.96	1.49	1.41
2	E	501	NAD	C4N-C3N	2.90	1.43	1.39
2	D	501	NAD	C5A-N7A	-2.89	1.33	1.39
2	A	501	NAD	O4D-C1D	2.88	1.44	1.40
2	B	501	NAD	C5A-N7A	-2.84	1.33	1.39
2	D	501	NAD	C8A-N7A	2.81	1.37	1.31
2	E	501	NAD	PN-O3	2.80	1.62	1.59
3	D	502	PAE	O1-C1	-2.77	1.21	1.30
3	A	502	PAE	O1-C1	-2.75	1.21	1.30
2	G	501	NAD	C5A-C6A	2.75	1.48	1.41
2	E	501	NAD	O5B-C5B	-2.70	1.34	1.44
2	D	501	NAD	C4N-C3N	2.70	1.43	1.39
2	E	501	NAD	C5N-C4N	2.66	1.43	1.38
2	H	501	NAD	C4N-C3N	2.64	1.43	1.39
2	C	501	NAD	O5B-C5B	-2.62	1.34	1.44
2	G	501	NAD	PN-O3	2.57	1.62	1.59
2	D	501	NAD	C5A-C6A	2.54	1.48	1.41
2	G	501	NAD	C4A-N9A	-2.53	1.32	1.37
2	H	501	NAD	C5A-C6A	2.49	1.47	1.41
2	C	501	NAD	C5A-N7A	-2.44	1.34	1.39
2	B	501	NAD	O4D-C1D	2.40	1.44	1.40
2	E	501	NAD	C8A-N7A	2.39	1.36	1.31
2	G	501	NAD	C8A-N7A	2.38	1.36	1.31
3	C	502	PAE	O1-C1	-2.36	1.23	1.30
2	H	501	NAD	C3N-C7N	2.35	1.54	1.50
2	H	501	NAD	C5A-N7A	-2.33	1.34	1.39
3	E	502	PAE	O1-C1	-2.32	1.23	1.30
3	F	502	PAE	C1P-C1	-2.31	1.48	1.51
2	B	501	NAD	C8A-N7A	2.31	1.36	1.31
2	D	501	NAD	C4A-N9A	-2.31	1.32	1.37
2	A	501	NAD	C8A-N7A	2.28	1.36	1.31
2	C	501	NAD	C8A-N7A	2.28	1.36	1.31
2	F	501	NAD	C4A-N9A	-2.27	1.33	1.37
2	F	501	NAD	C5A-C6A	2.25	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	NAD	C5A-N7A	-2.24	1.35	1.39
2	A	501	NAD	C5A-C6A	2.24	1.47	1.41
2	F	501	NAD	C8A-N7A	2.22	1.35	1.31
2	C	501	NAD	C4N-C3N	2.19	1.42	1.39
2	A	501	NAD	C4A-N9A	-2.07	1.33	1.37
2	E	501	NAD	C5A-N7A	-2.04	1.35	1.39

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	PAE	O3P-P-C1P	-6.52	96.02	111.10
2	C	501	NAD	C5B-C4B-C3B	-6.47	91.91	115.21
2	B	501	NAD	C5A-C4A-N3A	-5.89	118.61	126.72
2	C	501	NAD	C5A-C4A-N3A	-5.78	118.76	126.72
2	E	501	NAD	C5B-C4B-C3B	-5.73	94.58	115.21
2	C	501	NAD	N3A-C4A-N9A	5.40	136.36	127.17
2	H	501	NAD	C5A-C4A-N3A	-5.37	119.32	126.72
2	G	501	NAD	C3N-C7N-N7N	5.29	124.25	117.74
2	G	501	NAD	N3A-C2A-N1A	-5.27	120.60	128.58
2	F	501	NAD	C4A-N9A-C8A	5.23	111.23	105.74
2	A	501	NAD	C5A-C4A-N3A	-5.18	119.59	126.72
2	E	501	NAD	C5A-C4A-N3A	-5.04	119.78	126.72
2	A	501	NAD	N3A-C4A-N9A	5.03	135.72	127.17
2	E	501	NAD	C3N-C7N-N7N	-4.95	111.64	117.74
2	C	501	NAD	O4B-C4B-C5B	-4.87	93.73	109.33
3	B	502	PAE	O3P-P-C1P	-4.70	100.22	111.10
2	H	501	NAD	N3A-C4A-N9A	4.70	135.16	127.17
2	D	501	NAD	C5A-C4A-N3A	-4.68	120.28	126.72
2	H	501	NAD	N3A-C2A-N1A	-4.63	121.57	128.58
2	E	501	NAD	O7N-C7N-C3N	4.63	125.26	119.60
2	D	501	NAD	C3N-C7N-N7N	4.59	123.39	117.74
2	B	501	NAD	N3A-C4A-N9A	4.56	134.91	127.17
2	C	501	NAD	C4A-N9A-C8A	4.53	110.49	105.74
2	D	501	NAD	N3A-C2A-N1A	-4.41	121.90	128.58
2	D	501	NAD	N3A-C4A-N9A	4.36	134.59	127.17
2	F	501	NAD	N3A-C2A-N1A	-4.31	122.06	128.58
2	E	501	NAD	O4B-C4B-C5B	-4.30	95.55	109.33
2	G	501	NAD	C2A-N3A-C4A	4.29	122.30	111.83
2	G	501	NAD	C5A-C4A-N3A	-4.27	120.83	126.72
2	C	501	NAD	N9A-C8A-N7A	-4.14	108.06	113.94
2	H	501	NAD	C2A-N3A-C4A	4.09	121.83	111.83
2	E	501	NAD	C2A-N3A-C4A	4.08	121.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	NAD	N3A-C2A-N1A	-4.06	122.43	128.58
2	A	501	NAD	O7N-C7N-C3N	4.02	124.52	119.60
2	B	501	NAD	C2A-N3A-C4A	4.01	121.63	111.83
2	E	501	NAD	N3A-C4A-N9A	3.99	133.95	127.17
2	F	501	NAD	N3A-C4A-N9A	3.94	133.87	127.17
2	C	501	NAD	N3A-C2A-N1A	-3.88	122.71	128.58
2	A	501	NAD	C4A-N9A-C8A	3.86	109.79	105.74
3	G	502	PAE	O2P-P-C1P	-3.84	98.78	106.84
2	F	501	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	B	501	NAD	C4A-C5A-N7A	-3.80	106.24	110.58
2	D	501	NAD	C2A-N3A-C4A	3.75	120.98	111.83
2	A	501	NAD	N3A-C2A-N1A	-3.72	122.95	128.58
2	C	501	NAD	C2A-N3A-C4A	3.69	120.84	111.83
2	B	501	NAD	N3A-C2A-N1A	-3.68	123.01	128.58
3	H	502	PAE	O3P-P-C1P	-3.67	102.61	111.10
2	B	501	NAD	C5A-N7A-C8A	3.62	109.14	103.45
2	G	501	NAD	C4A-N9A-C8A	3.54	109.46	105.74
2	F	501	NAD	C5A-C4A-N3A	-3.50	121.90	126.72
3	F	502	PAE	O3P-P-C1P	-3.50	103.01	111.10
3	E	502	PAE	O1P-P-C1P	3.46	114.11	106.84
2	G	501	NAD	C6A-C5A-N7A	3.46	138.76	132.09
2	A	501	NAD	C2A-N3A-C4A	3.45	120.25	111.83
2	C	501	NAD	C5A-N7A-C8A	3.43	108.83	103.45
2	G	501	NAD	N3A-C4A-N9A	3.42	132.99	127.17
2	G	501	NAD	C4A-N9A-C1B	-3.36	118.76	126.63
3	C	502	PAE	O2P-P-O1P	3.32	117.43	107.96
2	G	501	NAD	O7N-C7N-C3N	-3.30	115.57	119.60
2	B	501	NAD	O3-PA-O1A	-3.29	100.81	110.70
2	D	501	NAD	C4A-N9A-C8A	3.28	109.19	105.74
2	F	501	NAD	C4A-N9A-C1B	-3.24	119.06	126.63
2	D	501	NAD	O7N-C7N-C3N	-3.23	115.65	119.60
3	F	502	PAE	O2P-P-O1P	3.21	117.11	107.96
2	G	501	NAD	N9A-C8A-N7A	-3.20	109.39	113.94
2	H	501	NAD	O7N-C7N-C3N	3.16	123.46	119.60
3	E	502	PAE	O3P-P-C1P	-3.14	103.83	111.10
2	F	501	NAD	C2A-N3A-C4A	3.11	119.42	111.83
2	B	501	NAD	N9A-C8A-N7A	-3.09	109.56	113.94
2	F	501	NAD	O3-PA-O1A	-3.07	101.47	110.70
2	E	501	NAD	C4A-C5A-N7A	-3.03	107.11	110.58
2	H	501	NAD	C4A-N9A-C8A	3.02	108.90	105.74
3	A	502	PAE	O1-C1-C1P	3.00	121.41	113.84
2	G	501	NAD	C4A-C5A-N7A	-3.00	107.15	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	NAD	O3-PA-O1A	-2.91	101.95	110.70
2	F	501	NAD	O2N-PN-O1N	2.87	125.81	112.44
2	A	501	NAD	N9A-C8A-N7A	-2.87	109.87	113.94
2	F	501	NAD	C5A-N7A-C8A	2.84	107.92	103.45
2	G	501	NAD	O3-PA-O1A	-2.84	102.17	110.70
2	C	501	NAD	O2A-PA-O3	2.83	114.93	107.27
2	F	501	NAD	C2A-N1A-C6A	2.82	123.37	118.73
2	E	501	NAD	O2A-PA-O5B	2.82	120.37	107.57
3	H	502	PAE	O2P-P-O1P	2.82	116.00	107.96
2	D	501	NAD	O3-PN-O1N	-2.82	102.23	110.70
2	A	501	NAD	O3-PA-O1A	-2.79	102.32	110.70
2	E	501	NAD	C4A-N9A-C8A	2.78	108.66	105.74
2	G	501	NAD	C5A-N7A-C8A	2.78	107.82	103.45
3	A	502	PAE	O3P-P-C1P	-2.77	104.69	111.10
2	B	501	NAD	C6A-C5A-N7A	2.77	137.43	132.09
2	F	501	NAD	O3-PN-O1N	-2.71	102.54	110.70
2	B	501	NAD	C4A-N9A-C8A	2.70	108.58	105.74
2	E	501	NAD	C5A-N7A-C8A	2.68	107.67	103.45
3	H	502	PAE	O2-C1-C1P	-2.67	116.33	122.53
2	A	501	NAD	O2N-PN-O3	2.64	114.41	107.27
2	E	501	NAD	O3-PA-O1A	-2.64	102.76	110.70
3	G	502	PAE	O2-C1-C1P	-2.63	116.42	122.53
2	G	501	NAD	C4D-O4D-C1D	-2.62	107.53	109.92
2	C	501	NAD	C5A-C6A-N6A	-2.59	116.88	123.29
2	D	501	NAD	O2D-C2D-C3D	2.58	120.08	111.82
2	B	501	NAD	O7N-C7N-C3N	2.57	122.74	119.60
2	E	501	NAD	N9A-C8A-N7A	-2.57	110.29	113.94
2	G	501	NAD	C2A-N1A-C6A	2.57	122.94	118.73
2	D	501	NAD	O2N-PN-O1N	2.56	124.36	112.44
2	E	501	NAD	O5B-C5B-C4B	-2.55	100.32	108.99
2	F	501	NAD	O2A-PA-O1A	2.54	124.27	112.44
2	A	501	NAD	C5A-C6A-N6A	-2.53	117.02	123.29
2	D	501	NAD	N9A-C8A-N7A	-2.53	110.35	113.94
2	E	501	NAD	C6A-C5A-N7A	2.51	136.93	132.09
2	C	501	NAD	C4A-C5A-N7A	-2.47	107.76	110.58
2	H	501	NAD	C4A-C5A-N7A	-2.46	107.76	110.58
2	F	501	NAD	N6A-C6A-N1A	2.46	123.85	118.38
2	D	501	NAD	C2A-N1A-C6A	2.45	122.75	118.73
2	C	501	NAD	O4B-C1B-N9A	2.45	112.79	108.09
2	A	501	NAD	C5A-N7A-C8A	2.43	107.27	103.45
2	E	501	NAD	C2B-C3B-C4B	-2.42	97.94	102.61
2	C	501	NAD	O7N-C7N-C3N	2.38	122.51	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	NAD	C2A-N1A-C6A	2.36	122.60	118.73
2	B	501	NAD	O3B-C3B-C2B	-2.36	104.26	111.82
2	C	501	NAD	O5B-PA-O1A	2.35	118.24	108.94
2	D	501	NAD	C4A-N9A-C1B	-2.34	121.16	126.63
2	A	501	NAD	N6A-C6A-N1A	2.34	123.58	118.38
2	C	501	NAD	C4D-O4D-C1D	-2.32	107.80	109.92
3	G	502	PAE	O1-C1-C1P	2.29	119.63	113.84
2	H	501	NAD	C6A-C5A-N7A	2.29	136.50	132.09
2	F	501	NAD	C6A-C5A-N7A	2.28	136.49	132.09
2	C	501	NAD	O2B-C2B-C3B	2.28	119.13	111.82
2	E	501	NAD	O4B-C1B-N9A	2.28	112.46	108.09
2	G	501	NAD	C6A-C5A-C4A	-2.26	114.09	117.18
2	H	501	NAD	C5A-N7A-C8A	2.26	107.00	103.45
2	C	501	NAD	O2D-C2D-C3D	2.25	119.04	111.82
2	C	501	NAD	N6A-C6A-N1A	2.25	123.39	118.38
2	F	501	NAD	O7N-C7N-C3N	-2.23	116.88	119.60
2	D	501	NAD	C6A-C5A-N7A	2.22	136.38	132.09
2	F	501	NAD	O3B-C3B-C4B	-2.22	104.70	111.08
3	B	502	PAE	O1-C1-C1P	2.22	119.44	113.84
2	H	501	NAD	N9A-C8A-N7A	-2.21	110.80	113.94
2	G	501	NAD	O4B-C4B-C3B	2.20	109.53	105.15
2	C	501	NAD	C3B-C2B-C1B	-2.20	97.30	101.46
2	F	501	NAD	C4A-C5A-N7A	-2.17	108.10	110.58
3	F	502	PAE	O2P-P-C1P	-2.17	102.28	106.84
3	A	502	PAE	O2P-P-C1P	-2.16	102.32	106.84
3	A	502	PAE	O2-C1-C1P	-2.14	117.55	122.53
2	D	501	NAD	C5A-N7A-C8A	2.13	106.80	103.45
2	G	501	NAD	C1B-N9A-C8A	2.11	131.77	127.09
2	A	501	NAD	O2D-C2D-C3D	2.07	118.44	111.82
3	G	502	PAE	O3P-P-C1P	-2.07	106.32	111.10
2	A	501	NAD	O3-PN-O1N	-2.06	104.50	110.70
2	C	501	NAD	O2N-PN-O3	-2.05	101.75	107.27
2	F	501	NAD	C5A-C6A-N6A	-2.02	118.30	123.29
2	D	501	NAD	C5A-C6A-N6A	-2.01	118.30	123.29
2	H	501	NAD	O2A-PA-O3	2.01	112.70	107.27

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C5D-O5D-PN-O2N
2	C	501	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	501	NAD	C5D-O5D-PN-O1N
2	E	501	NAD	C5B-O5B-PA-O3
3	C	502	PAE	C1-C1P-P-O1P
3	C	502	PAE	C1-C1P-P-O2P
3	C	502	PAE	C1-C1P-P-O3P
2	C	501	NAD	C3B-C4B-C5B-O5B
2	E	501	NAD	C3B-C4B-C5B-O5B
2	E	501	NAD	O4B-C4B-C5B-O5B
2	E	501	NAD	C4D-C5D-O5D-PN
2	B	501	NAD	PN-O3-PA-O5B
2	F	501	NAD	PN-O3-PA-O5B
2	H	501	NAD	PN-O3-PA-O5B
2	C	501	NAD	C4D-C5D-O5D-PN
2	H	501	NAD	C2B-C1B-N9A-C8A
2	D	501	NAD	C4D-C5D-O5D-PN
2	F	501	NAD	C4D-C5D-O5D-PN
3	D	502	PAE	C1-C1P-P-O2P
3	D	502	PAE	C1-C1P-P-O3P
2	C	501	NAD	C5B-O5B-PA-O2A
2	E	501	NAD	C5B-O5B-PA-O1A
2	F	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C4D-C5D-O5D-PN
2	G	501	NAD	C4D-C5D-O5D-PN
2	H	501	NAD	C4D-C5D-O5D-PN
2	B	501	NAD	C4D-C5D-O5D-PN
2	A	501	NAD	C2B-C1B-N9A-C8A
2	D	501	NAD	C2B-C1B-N9A-C8A
2	F	501	NAD	C2B-C1B-N9A-C8A
2	C	501	NAD	C2B-C1B-N9A-C8A
3	D	502	PAE	C1-C1P-P-O1P

There are no ring outliers.

13 monomers are involved in 42 short contacts:

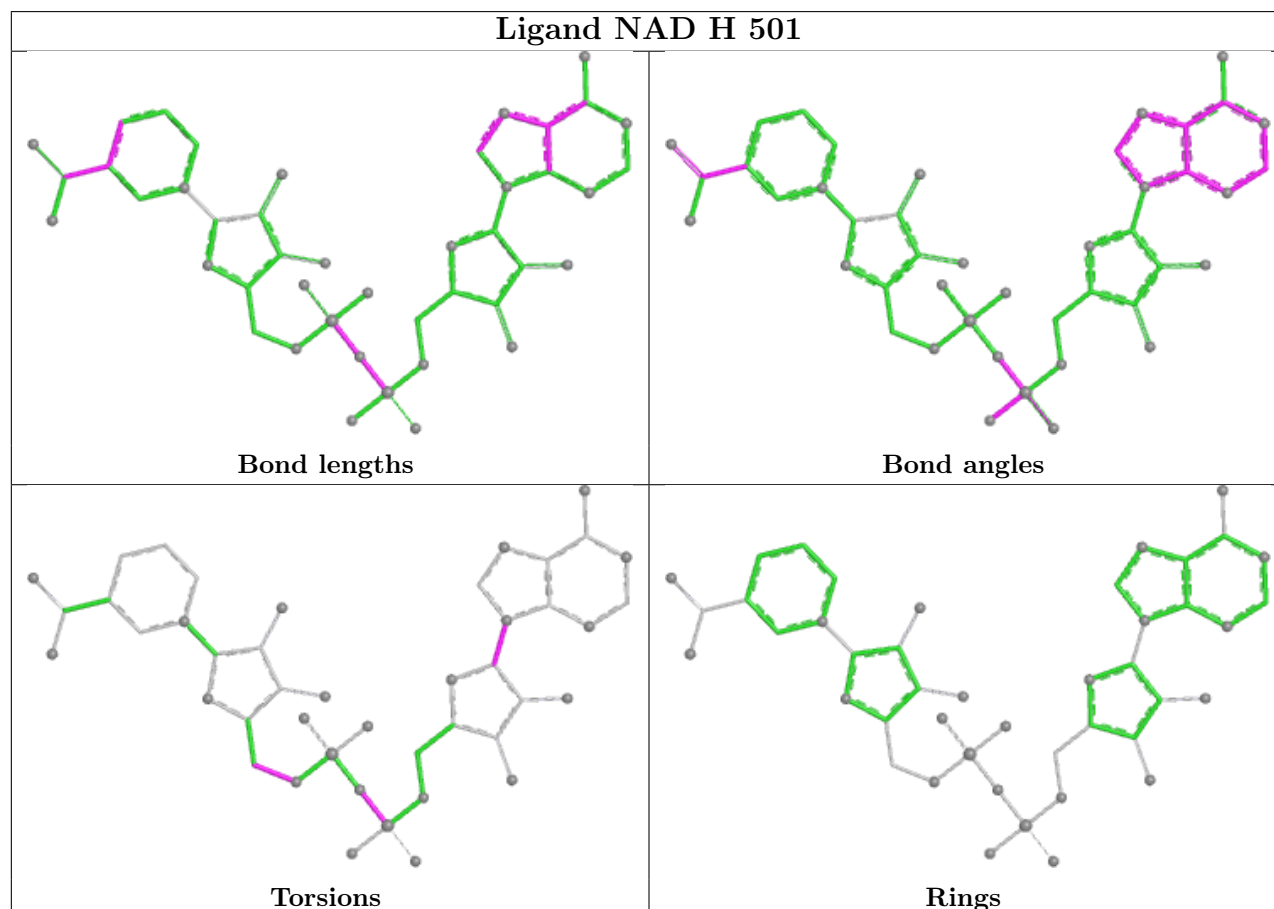
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	NAD	3	0
2	G	501	NAD	4	0
2	A	501	NAD	4	0
2	D	501	NAD	6	0
2	C	501	NAD	5	0
3	C	502	PAE	5	0
2	B	501	NAD	2	0

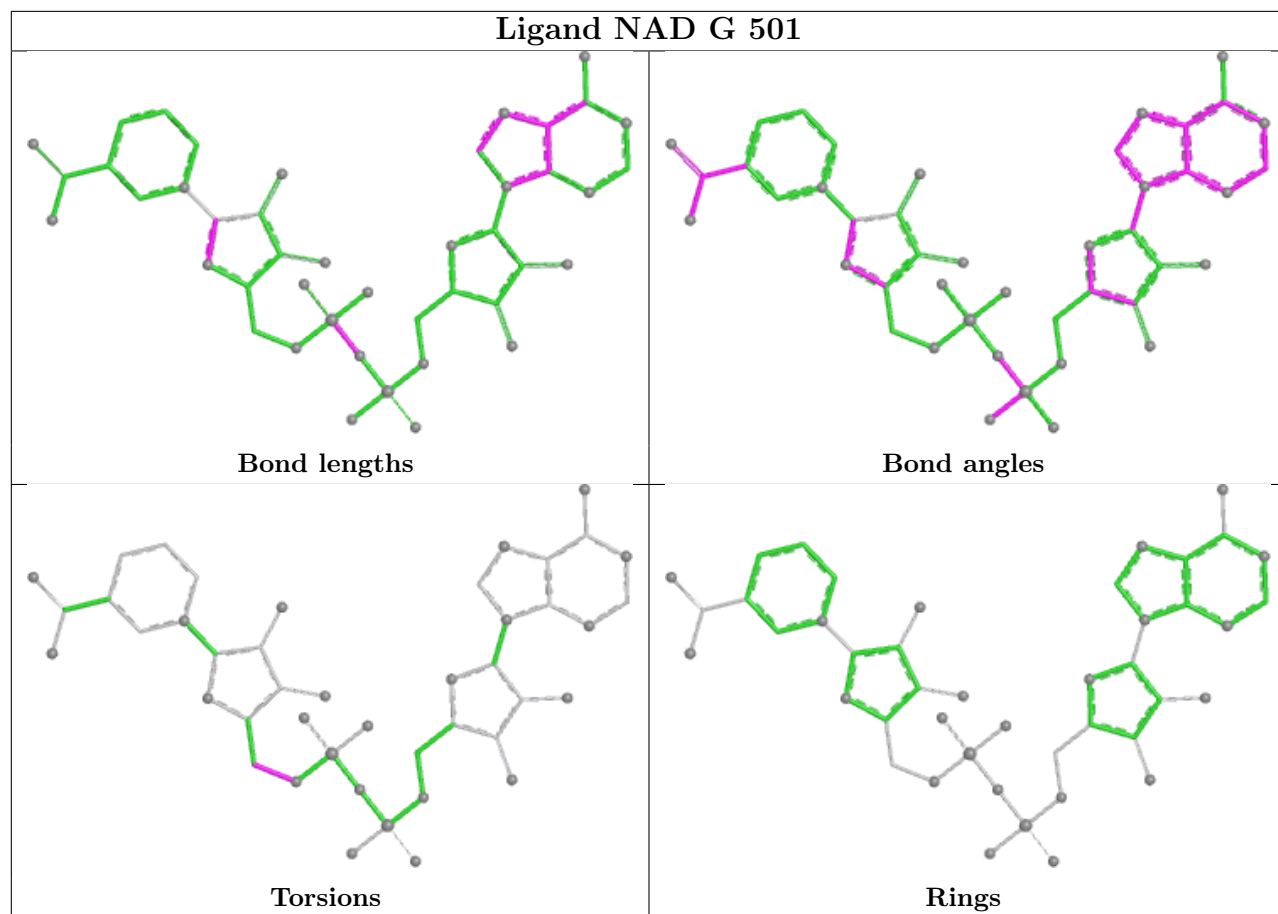
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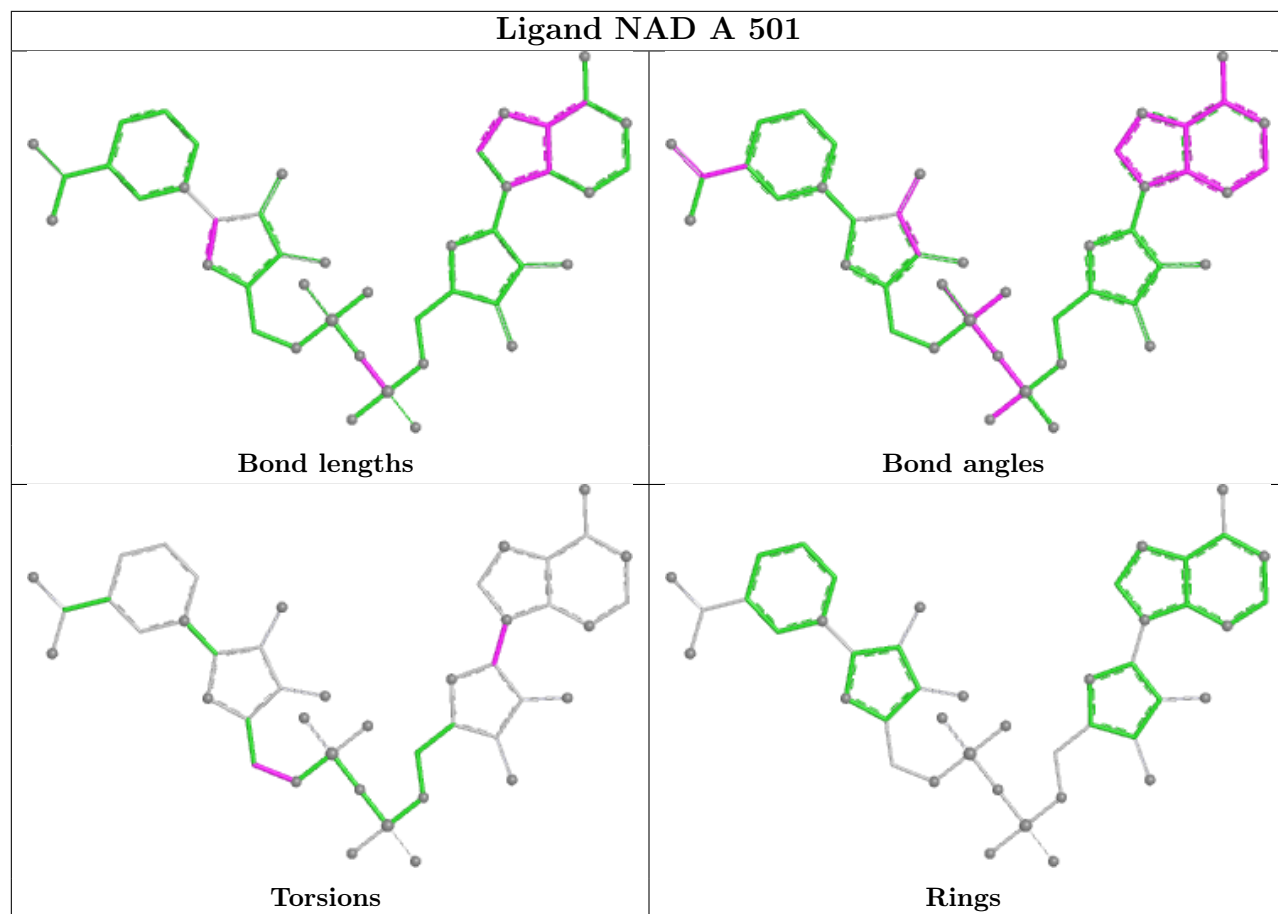
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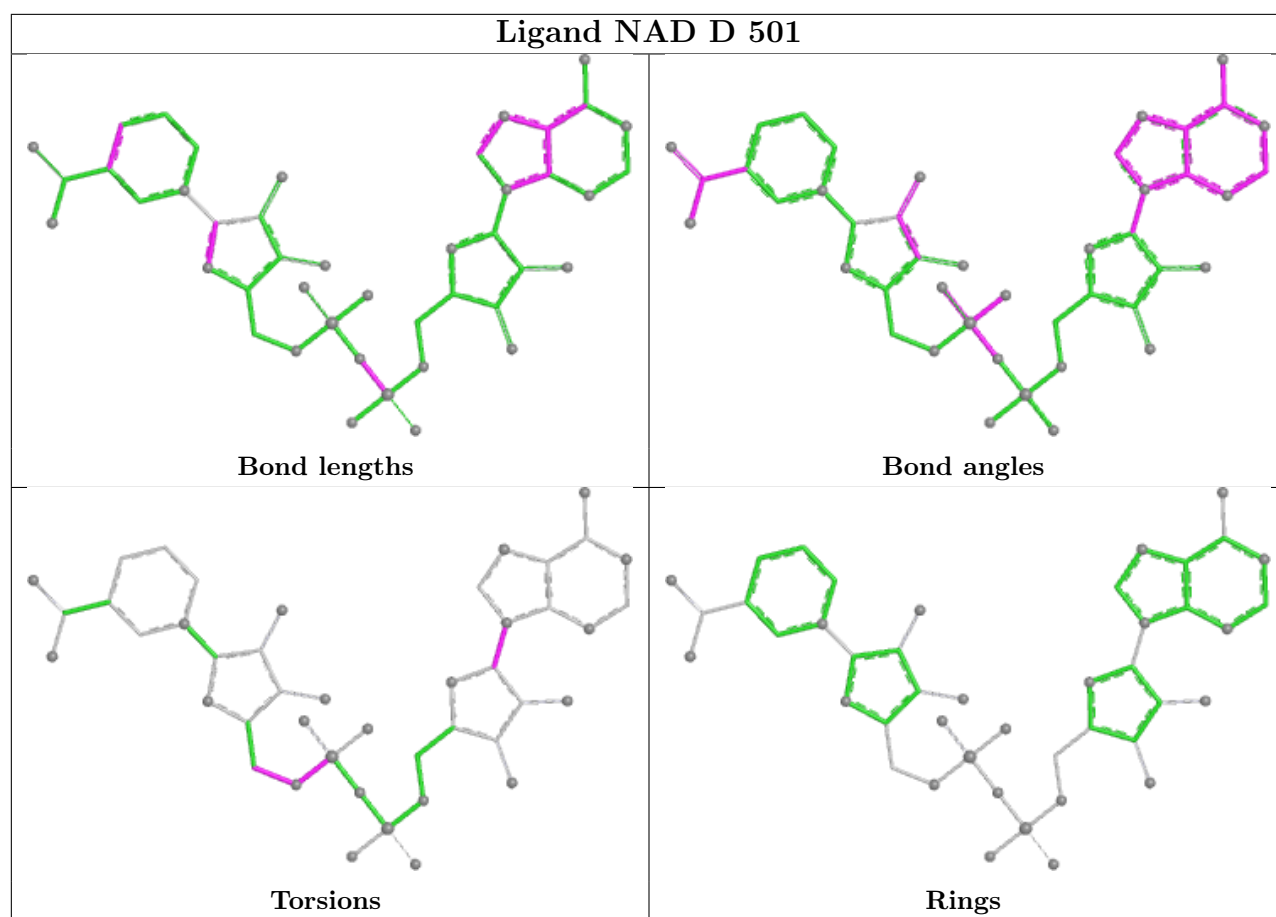
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	PAE	2	0
3	B	502	PAE	1	0
2	F	501	NAD	4	0
2	E	501	NAD	3	0
3	D	502	PAE	3	0
3	F	502	PAE	2	0

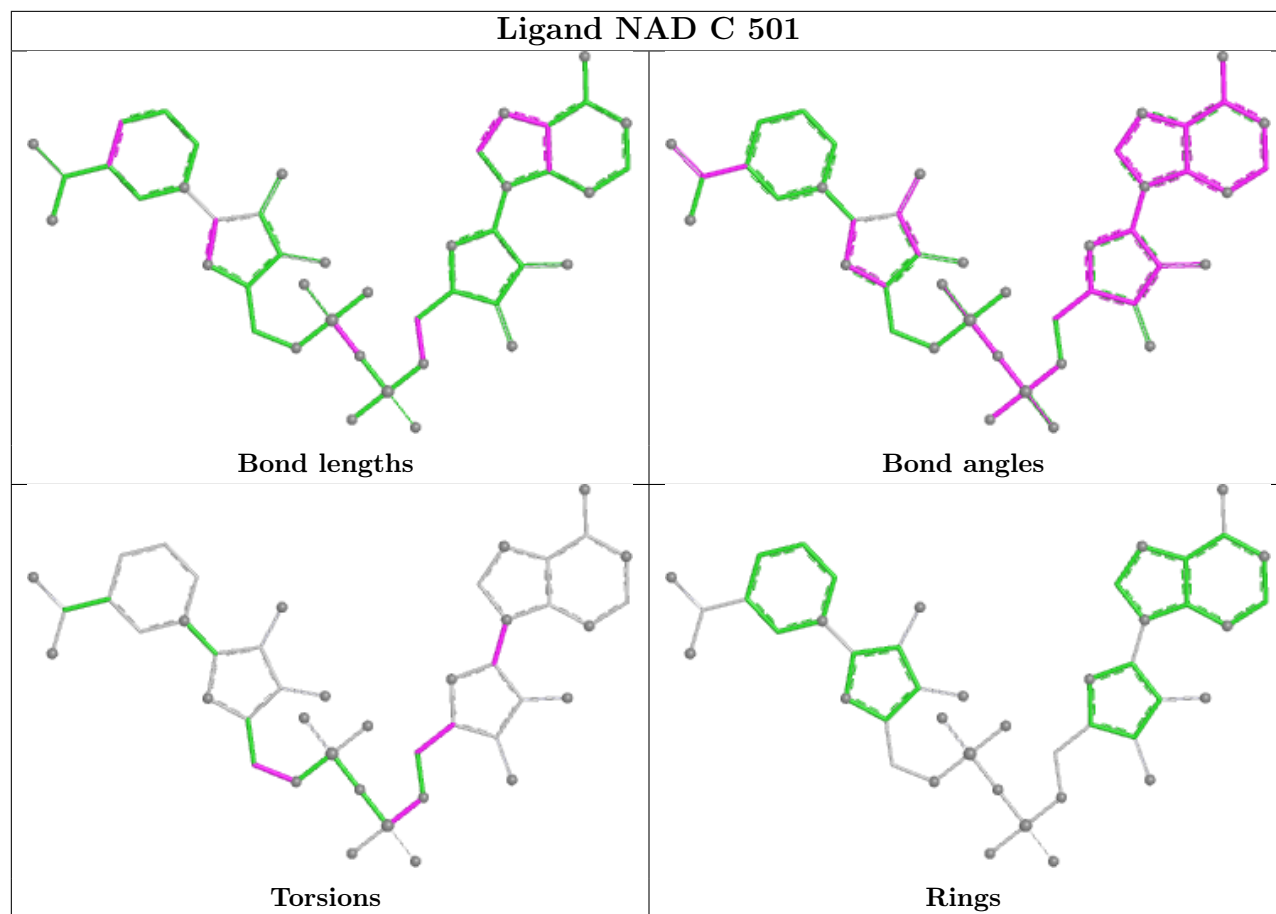
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

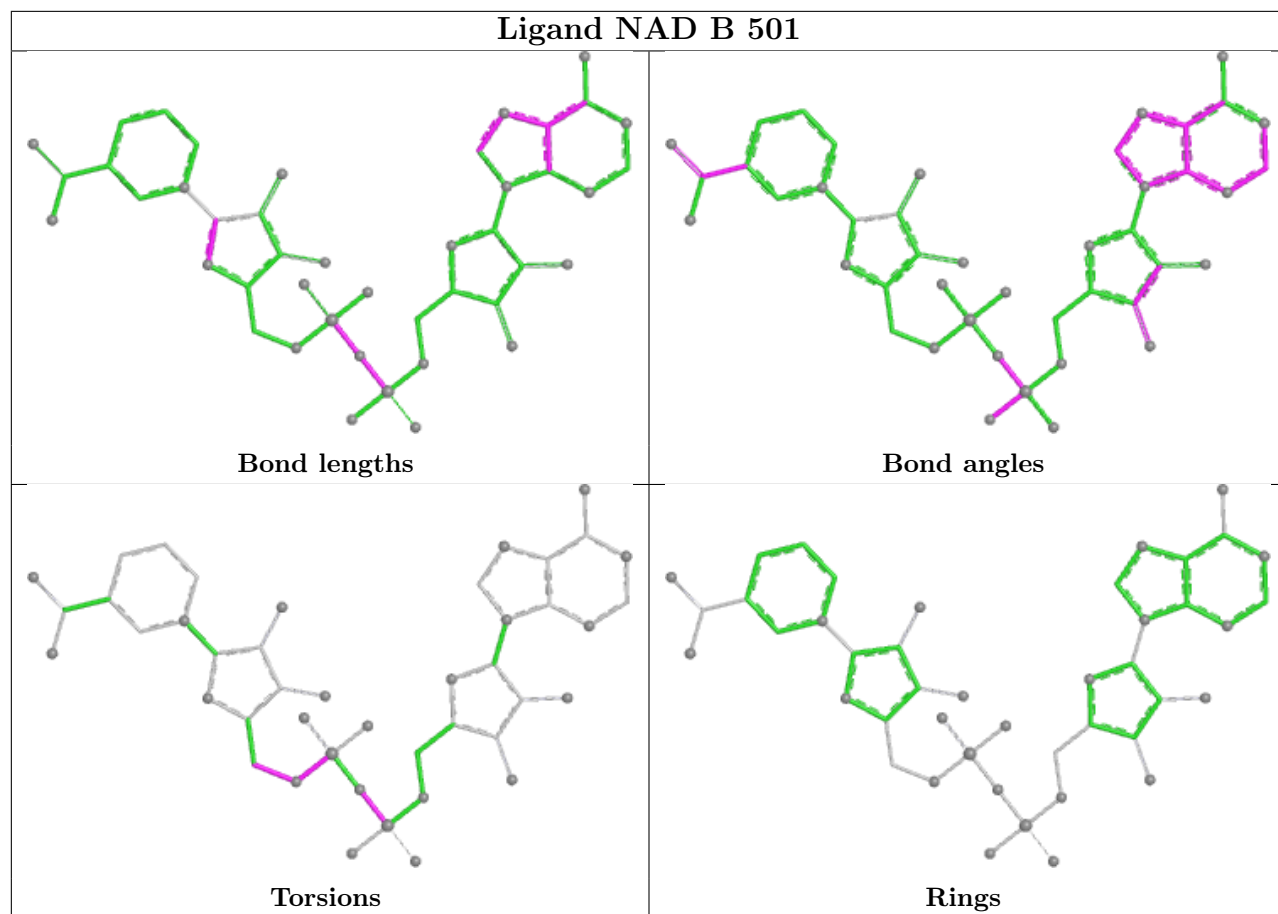


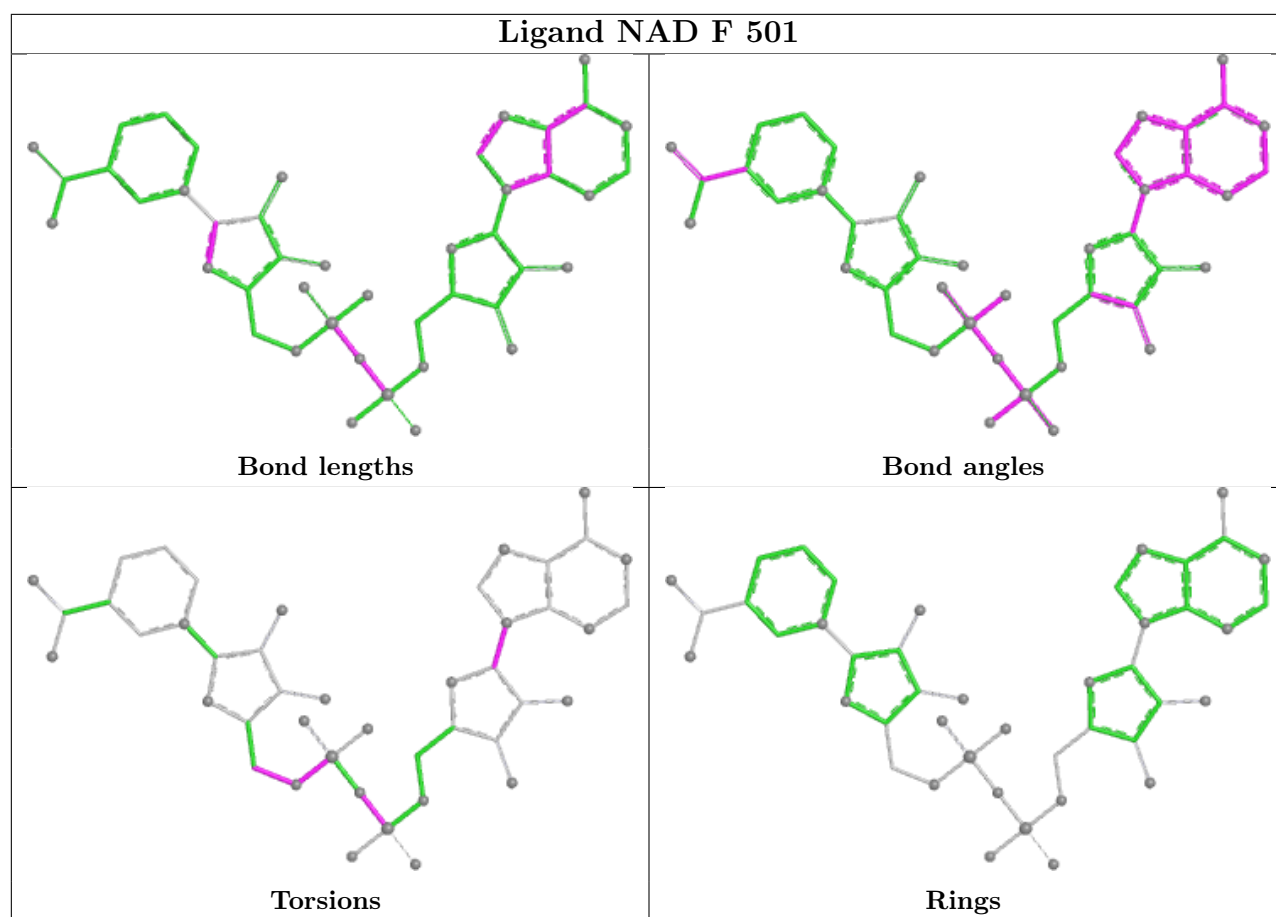


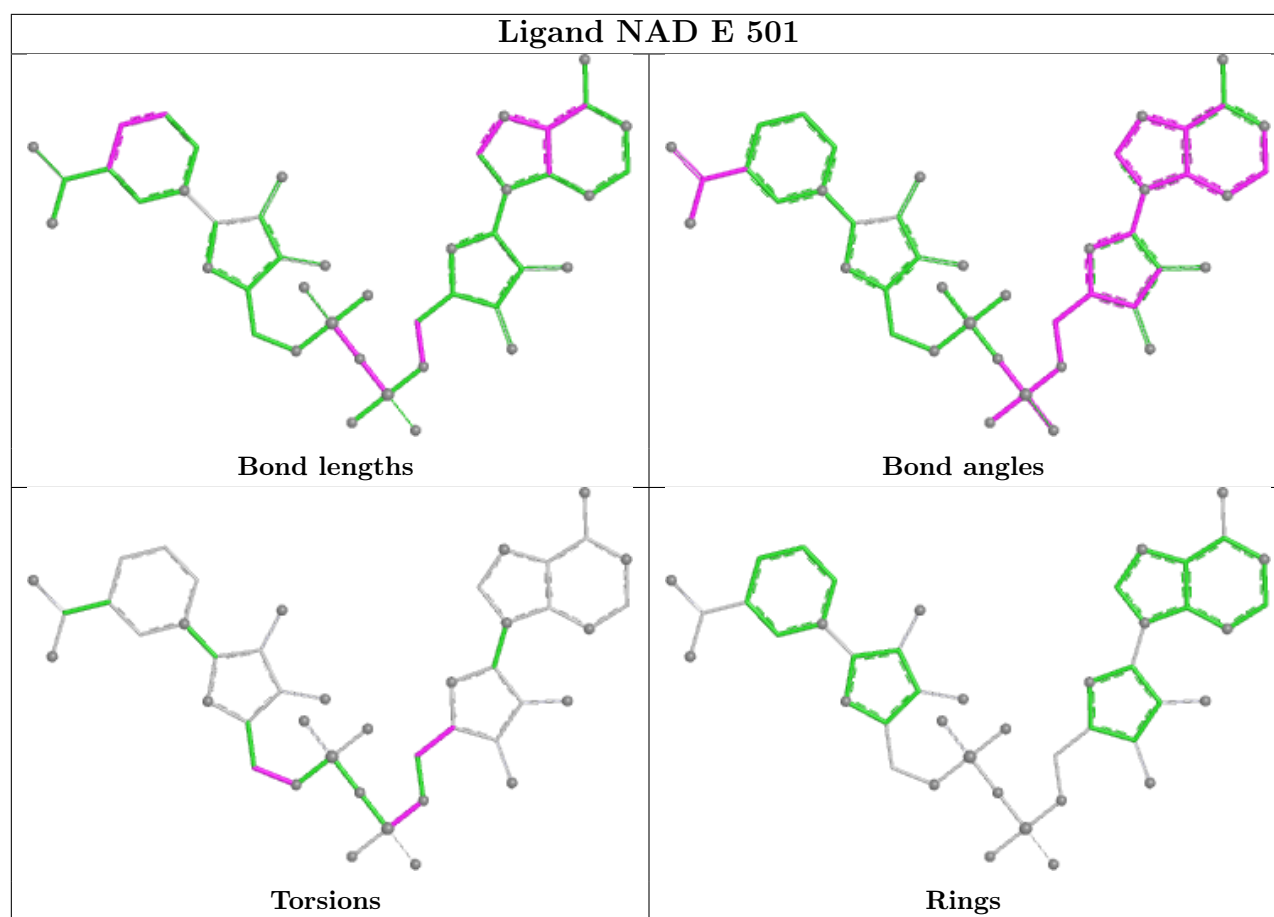












5.7 Other polymers [i](#)

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	476/488 (97%)	-0.84	0 100 100	11, 18, 32, 69	0
1	B	474/488 (97%)	-0.63	3 (0%) 85 88	13, 23, 42, 87	0
1	C	475/488 (97%)	-0.51	6 (1%) 75 77	13, 25, 42, 68	0
1	D	476/488 (97%)	-0.50	5 (1%) 78 80	14, 26, 47, 76	0
1	E	476/488 (97%)	-0.68	3 (0%) 85 88	11, 21, 40, 65	0
1	F	476/488 (97%)	-0.47	4 (0%) 82 84	14, 26, 46, 67	0
1	G	474/488 (97%)	-0.57	2 (0%) 88 90	15, 24, 45, 67	0
1	H	476/488 (97%)	-0.38	5 (1%) 78 80	14, 29, 48, 73	0
All	All	3803/3904 (97%)	-0.57	28 (0%) 84 86	11, 24, 43, 87	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	VAL	3.6
1	B	246	ALA	3.5
1	B	135	HIS	3.4
1	G	135	HIS	3.1
1	G	12	HIS	3.0
1	B	247	HIS	3.0
1	E	135	HIS	2.8
1	C	121	ILE	2.7
1	D	10	VAL	2.7
1	D	247	HIS	2.7
1	D	135	HIS	2.6
1	F	121	ILE	2.6
1	H	96	GLY	2.6
1	C	247	HIS	2.6
1	H	10	VAL	2.5
1	H	215	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	215	ALA	2.4
1	F	135	HIS	2.4
1	H	12	HIS	2.4
1	D	12	HIS	2.3
1	C	120	CYS	2.3
1	F	247	HIS	2.3
1	C	135	HIS	2.2
1	C	122	ARG	2.2
1	E	12	HIS	2.2
1	H	247	HIS	2.1
1	C	248	TYR	2.1
1	F	246	ALA	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.

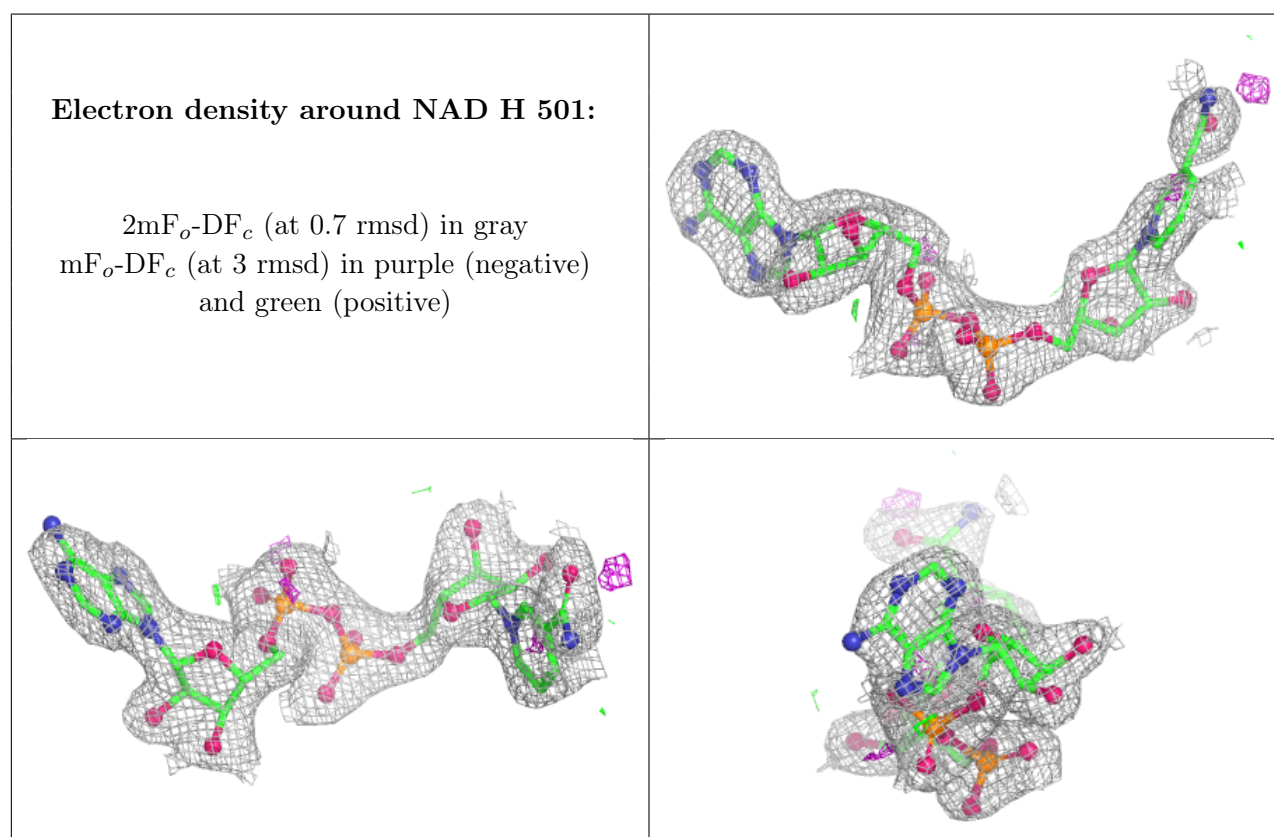
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PAE	C	502	8/8	0.89	0.12	35,44,54,56	0
3	PAE	F	502	8/8	0.90	0.11	39,44,53,55	0
3	PAE	D	502	8/8	0.92	0.10	37,41,45,46	0
3	PAE	E	502	8/8	0.92	0.10	31,39,44,44	0
3	PAE	A	502	8/8	0.92	0.12	29,36,42,48	0
3	PAE	H	502	8/8	0.92	0.11	39,49,56,57	0
3	PAE	B	502	8/8	0.93	0.10	29,32,38,40	0
2	NAD	H	501	44/44	0.95	0.08	26,42,54,58	0
2	NAD	C	501	44/44	0.96	0.06	19,29,37,44	0
2	NAD	D	501	44/44	0.96	0.06	27,34,43,44	0
2	NAD	E	501	44/44	0.96	0.07	17,30,40,46	0

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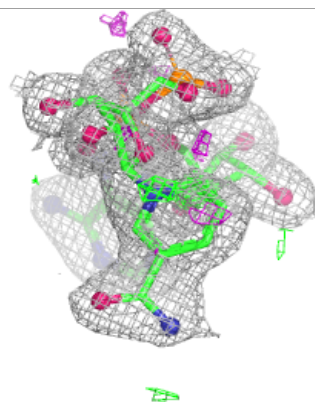
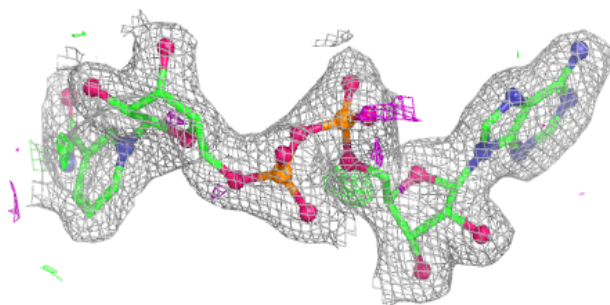
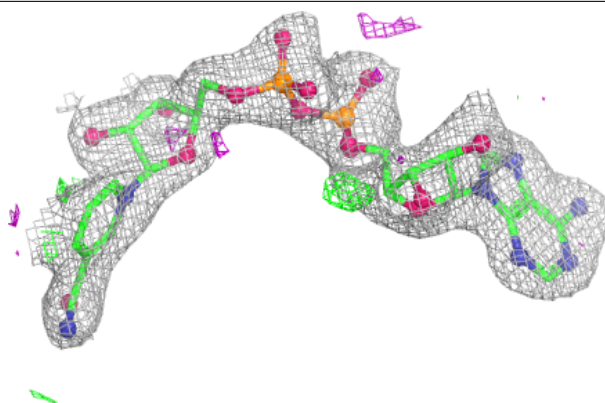
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PAE	G	502	8/8	0.96	0.07	36,40,43,45	0
2	NAD	F	501	44/44	0.96	0.07	28,38,48,56	0
2	NAD	A	501	44/44	0.97	0.05	17,22,31,36	0
2	NAD	B	501	44/44	0.97	0.06	20,32,36,37	0
2	NAD	G	501	44/44	0.97	0.06	27,34,41,50	0

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.

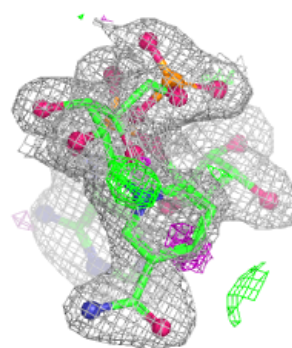
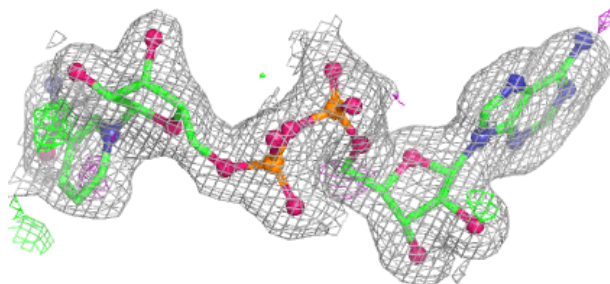
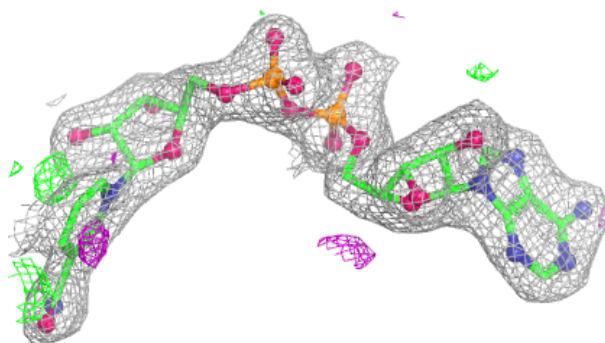


Electron density around NAD C 501:

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

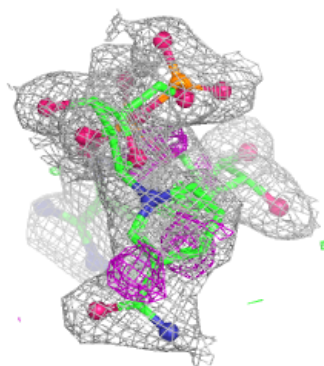
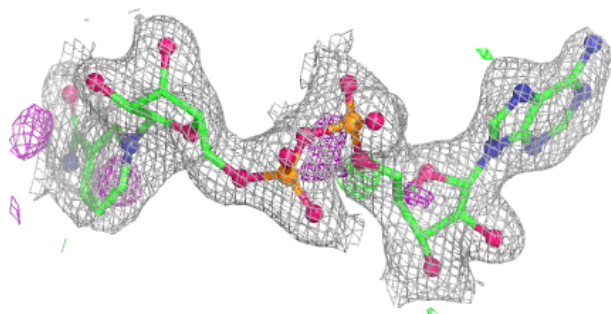
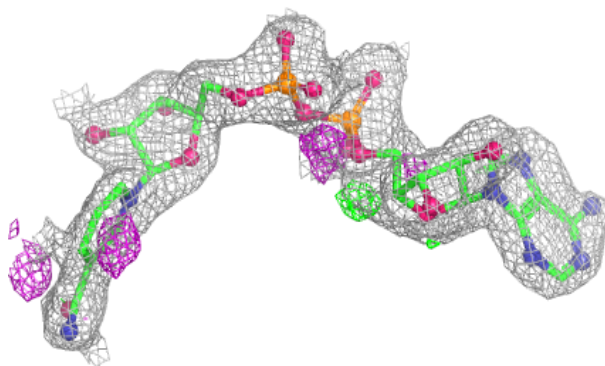
**Electron density around NAD D 501:**

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

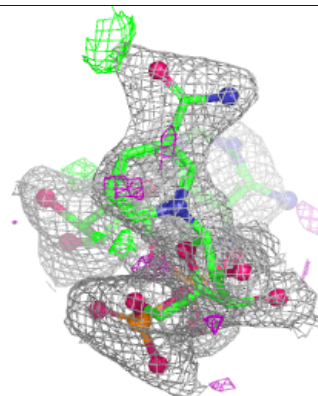
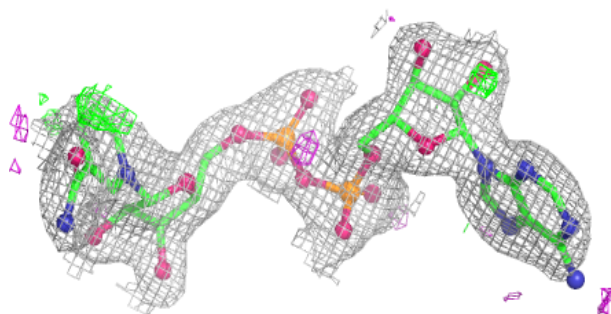
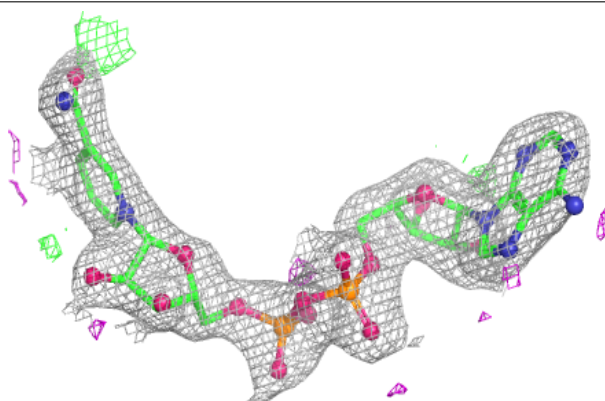


Electron density around NAD E 501:

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

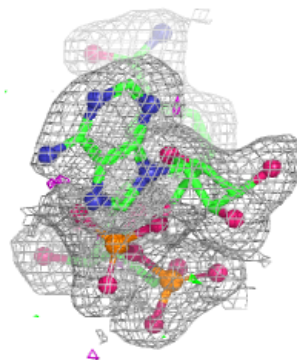
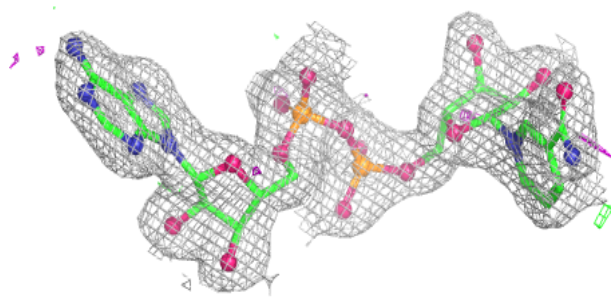
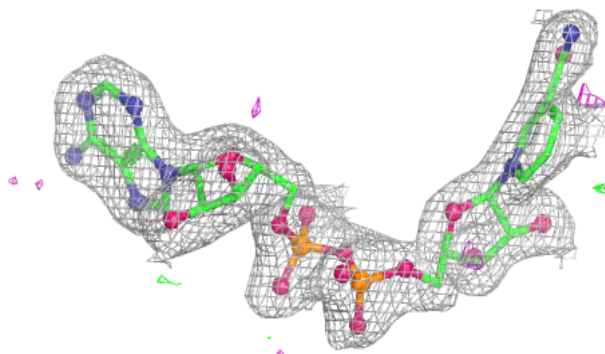
**Electron density around NAD F 501:**

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

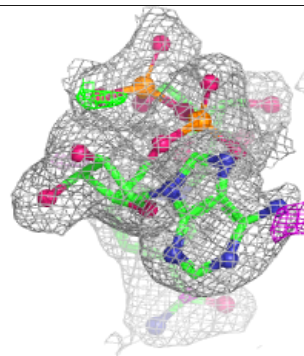
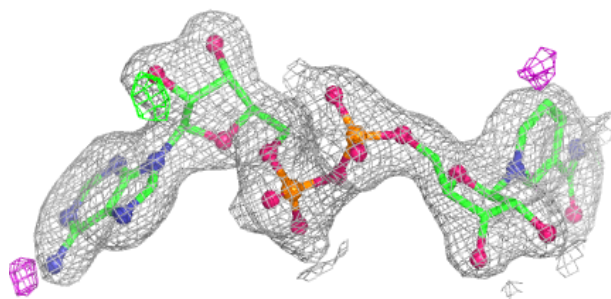
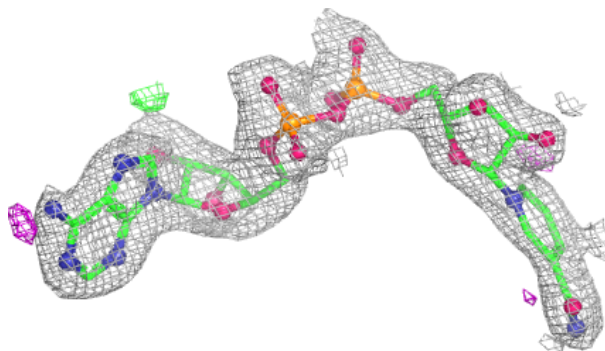


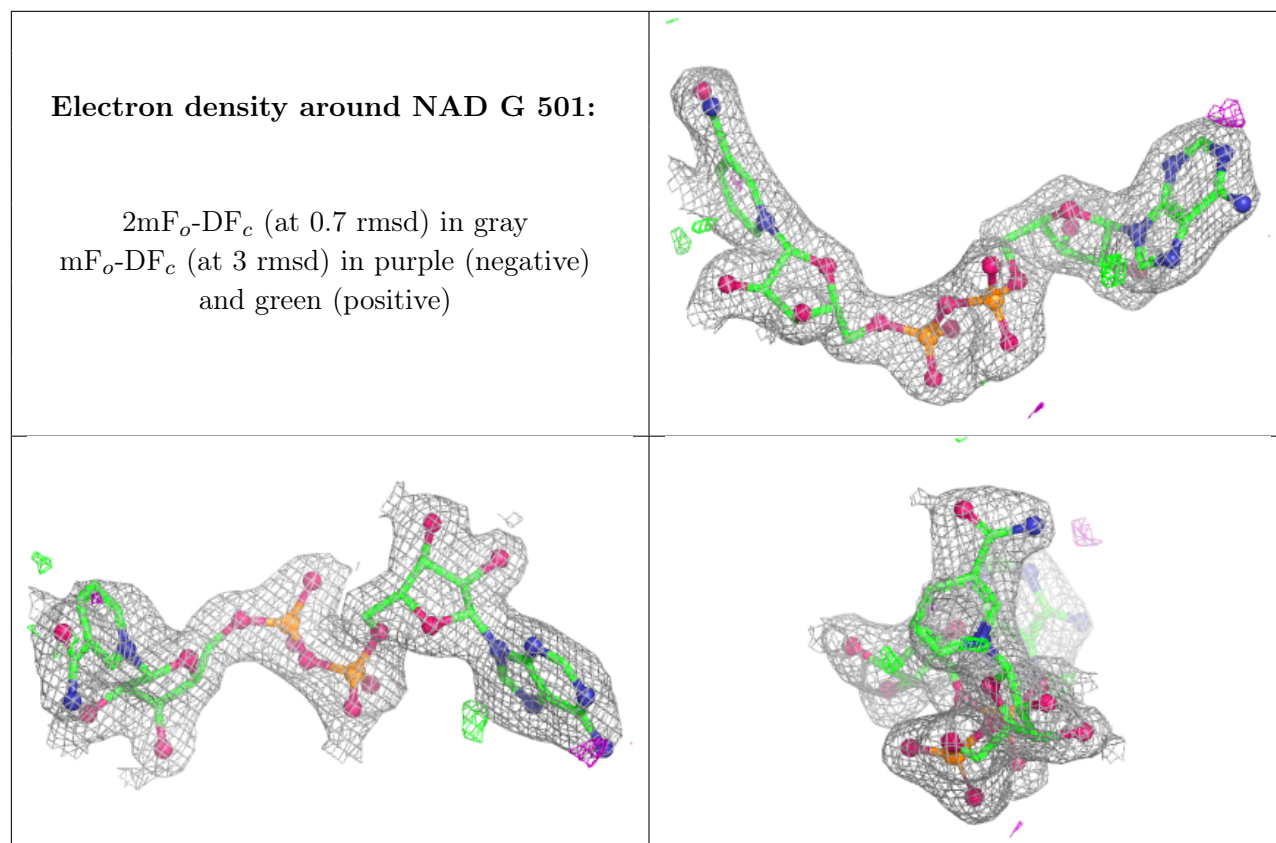
Electron density around NAD A 501:

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

**Electron density around NAD B 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.