



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:01 PM EST

PDB ID : 7UMY
Title : Crystal structure of *Acinetobacter baumannii* FabI in complex with NAD and Fabimycin ((S,E)-3-(7-amino-8-oxo-6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-3-yl)-N-methyl-N-((3-methylbenzofuran-2-yl)methyl)acrylamide)
Authors : Hajian, B.
Deposited on : 2022-04-08
Resolution : 2.74 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:

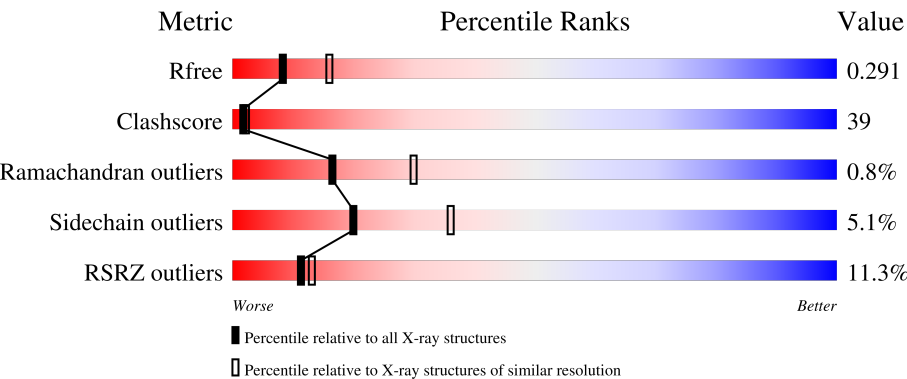
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.74 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}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	271	<div><div>8%</div><div>43%</div><div>47%</div><div>• • •</div></div>
1	B	271	<div><div>13%</div><div>48%</div><div>42%</div><div>• • 6%</div></div>
1	C	271	<div><div>8%</div><div>45%</div><div>48%</div><div>• •</div></div>
1	D	271	<div><div>14%</div><div>42%</div><div>48%</div><div>• • 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	E	271	<div><div></div><div>11%</div><div>48%</div><div>46%</div><div></div><div></div></div>
1	F	271	<div><div></div><div>10%</div><div>52%</div><div>40%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12065 atoms, of which 144 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1917	1219	326	363	9			
1	B	254	Total	C	N	O	S	0	0	0
			1845	1163	316	357	9			
1	C	260	Total	C	N	O	S	0	0	0
			1923	1220	330	364	9			
1	D	258	Total	C	N	O	S	0	0	0
			1899	1208	325	357	9			
1	E	260	Total	C	N	O	S	0	0	0
			1934	1229	332	364	9			
1	F	260	Total	C	N	O	S	0	0	0
			1937	1230	334	364	9			

There are 18 discrepancies between the modelled and reference sequences:

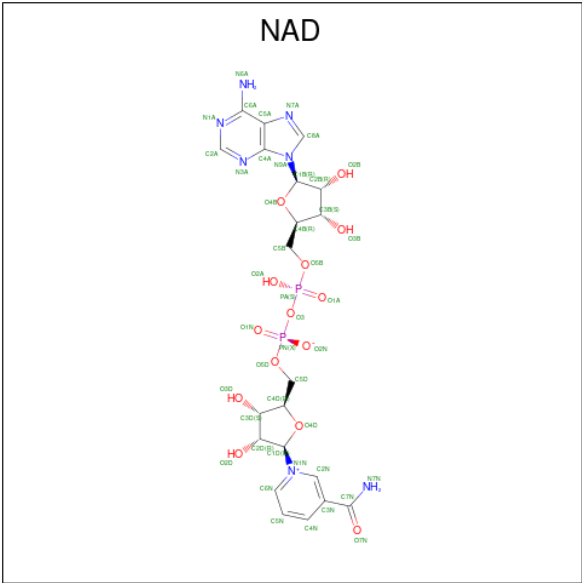
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP D0CAD5
A	-2	ASP	-	expression tag	UNP D0CAD5
A	-1	HIS	-	expression tag	UNP D0CAD5
B	-3	GLY	-	expression tag	UNP D0CAD5
B	-2	ASP	-	expression tag	UNP D0CAD5
B	-1	HIS	-	expression tag	UNP D0CAD5
C	-3	GLY	-	expression tag	UNP D0CAD5
C	-2	ASP	-	expression tag	UNP D0CAD5
C	-1	HIS	-	expression tag	UNP D0CAD5
D	-3	GLY	-	expression tag	UNP D0CAD5
D	-2	ASP	-	expression tag	UNP D0CAD5
D	-1	HIS	-	expression tag	UNP D0CAD5
E	-3	GLY	-	expression tag	UNP D0CAD5
E	-2	ASP	-	expression tag	UNP D0CAD5
E	-1	HIS	-	expression tag	UNP D0CAD5
F	-3	GLY	-	expression tag	UNP D0CAD5
F	-2	ASP	-	expression tag	UNP D0CAD5

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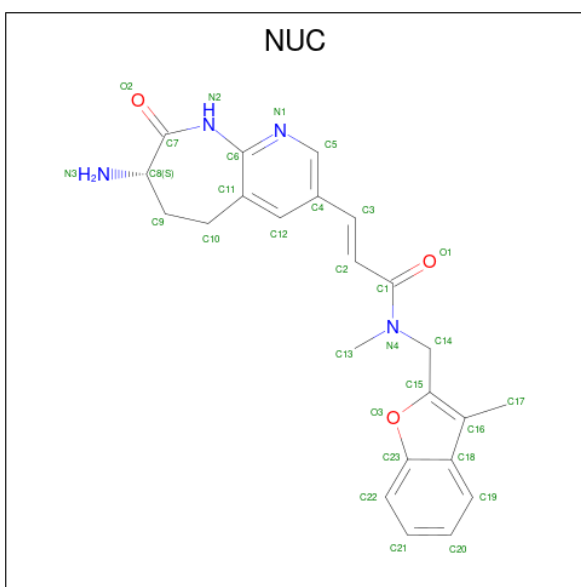
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	expression tag	UNP D0CAD5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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		

- Molecule 3 is (2E)-3-[(7S)-7-amino-8-oxo-6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-3-yl]-N-methyl-N-[(3-methyl-1-benzofuran-2-yl)methyl]prop-2-enamide (three-letter code: NUC) (formula: C₂₃H₂₄N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			54	23	24	4	3		
3	B	1	Total	C	H	N	O	0	0
			54	23	24	4	3		
3	C	1	Total	C	H	N	O	0	0
			54	23	24	4	3		
3	D	1	Total	C	H	N	O	0	0
			54	23	24	4	3		
3	E	1	Total	C	H	N	O	0	0
			54	23	24	4	3		
3	F	1	Total	C	H	N	O	0	0
			54	23	24	4	3		

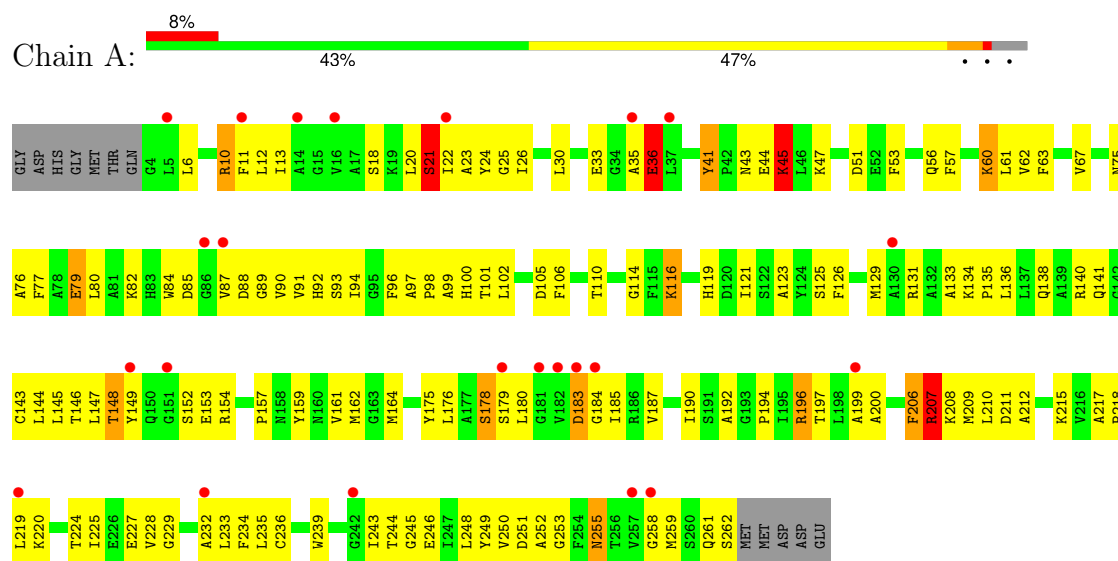
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	2	Total	O	0	0
			2	2		
4	C	9	Total	O	0	0
			9	9		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	4	Total	O	0	0
			4	4		

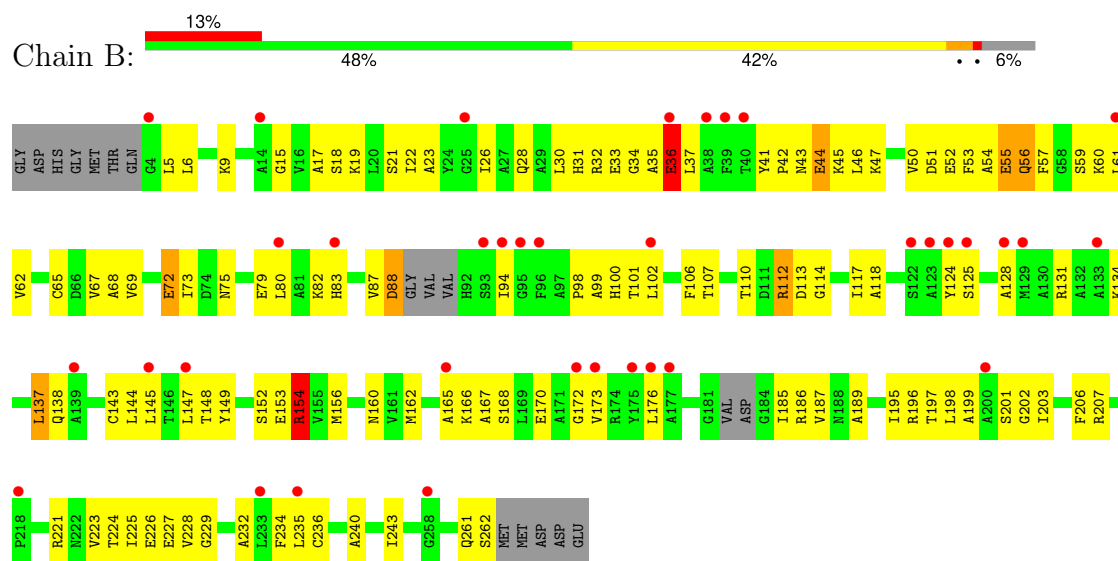
3 Residue-property plots

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

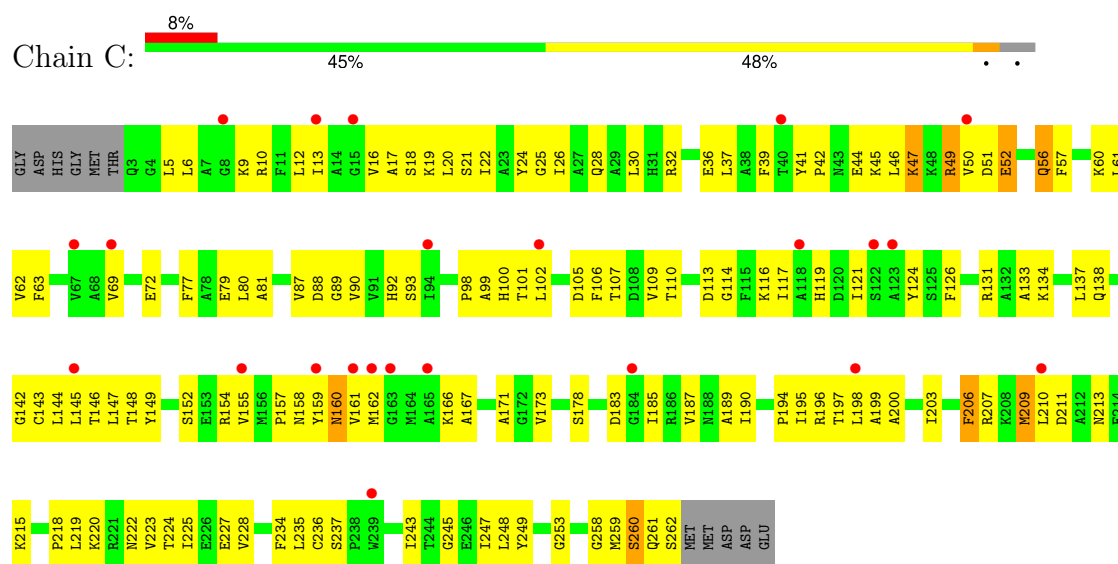
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



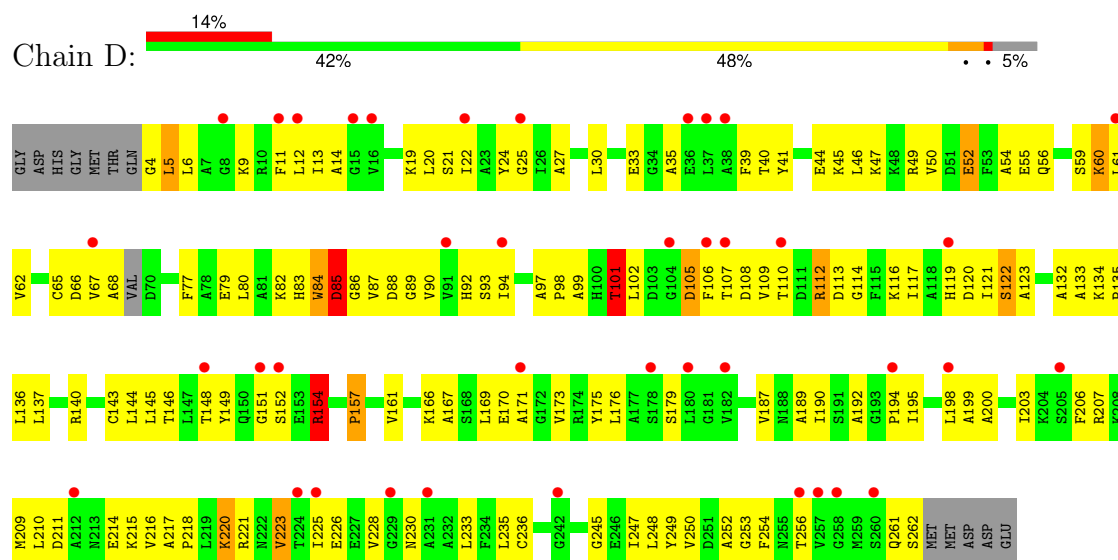
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



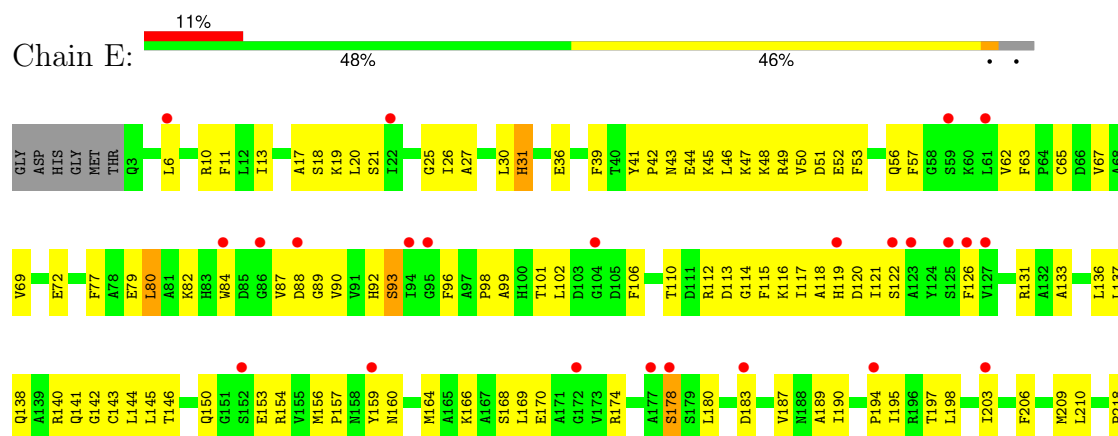
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

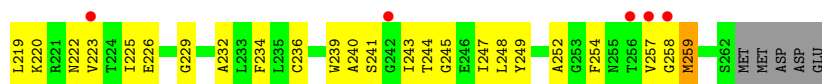


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

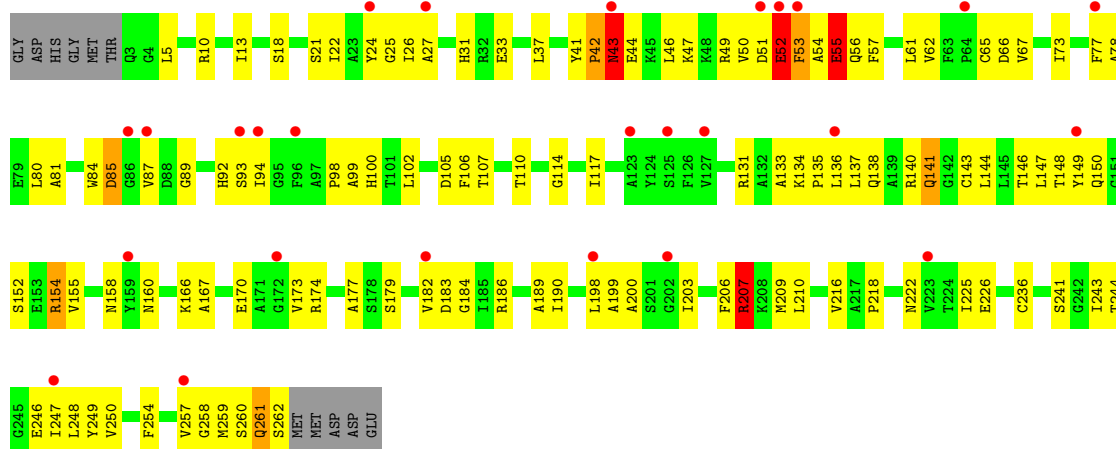


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	256.21Å 79.14Å 89.42Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	28.92 – 2.74 28.92 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (28.92-2.74) 98.1 (28.92-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	59.43 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.256 , 0.296 0.256 , 0.291	Depositor DCC
R_{free} test set	41744 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.177 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12065	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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, NUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/1953	0.75	9/2649 (0.3%)
1	B	0.33	0/1874	0.60	2/2540 (0.1%)
1	C	0.40	1/1958 (0.1%)	0.63	3/2655 (0.1%)
1	D	0.34	0/1933	1.03	13/2618 (0.5%)
1	E	0.35	2/1970 (0.1%)	0.73	5/2669 (0.2%)
1	F	0.40	0/1973	0.74	8/2673 (0.3%)
All	All	0.37	3/11661 (0.0%)	0.76	40/15804 (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	A	0	2
1	B	0	3
1	C	0	2
1	D	1	2
1	F	0	5
All	All	1	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	GLU	CB-CG	7.56	1.66	1.52
1	E	153	GLU	CB-CG	-5.26	1.42	1.52
1	E	153	GLU	CD-OE1	5.09	1.31	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	LEU	CB-CG-CD2	31.59	164.71	111.00
1	E	80	LEU	CB-CG-CD2	-19.90	77.17	111.00
1	D	5	LEU	CB-CG-CD1	-19.46	77.92	111.00
1	F	56	GLN	CA-CB-CG	11.75	139.26	113.40
1	A	207	ARG	CA-CB-CG	-9.80	91.84	113.40
1	A	45	LYS	CA-CB-CG	9.54	134.40	113.40
1	C	52	GLU	OE1-CD-OE2	-9.39	112.03	123.30
1	F	56	GLN	N-CA-CB	8.61	126.09	110.60
1	C	52	GLU	CA-CB-CG	8.59	132.30	113.40
1	E	80	LEU	CB-CG-CD1	7.96	124.53	111.00
1	A	60	LYS	CA-CB-CG	7.77	130.49	113.40
1	D	5	LEU	CA-CB-CG	-7.66	97.67	115.30
1	A	60	LYS	CB-CG-CD	-7.44	92.25	111.60
1	D	60	LYS	CA-CB-CG	7.35	129.57	113.40
1	A	207	ARG	CB-CG-CD	7.13	130.14	111.60
1	D	220	LYS	CA-CB-CG	-6.57	98.95	113.40
1	D	101	THR	OG1-CB-CG2	6.57	125.10	110.00
1	A	207	ARG	CG-CD-NE	6.43	125.31	111.80
1	E	153	GLU	CA-CB-CG	6.39	127.46	113.40
1	F	207	ARG	CA-CB-CG	6.25	127.14	113.40
1	A	21	SER	N-CA-CB	-6.23	101.16	110.50
1	F	56	GLN	CB-CA-C	-6.17	98.05	110.40
1	E	80	LEU	CA-CB-CG	6.10	129.33	115.30
1	B	36	GLU	CA-CB-CG	6.06	126.74	113.40
1	D	5	LEU	CD1-CG-CD2	-6.03	92.41	110.50
1	D	105	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	F	141	GLN	CA-CB-CG	-5.75	100.75	113.40
1	C	52	GLU	CG-CD-OE1	5.57	129.45	118.30
1	F	56	GLN	CB-CG-CD	5.55	126.02	111.60
1	D	220	LYS	CB-CG-CD	5.54	126.01	111.60
1	F	154	ARG	CB-CG-CD	-5.53	97.23	111.60
1	A	36	GLU	CA-CB-CG	-5.51	101.29	113.40
1	D	45	LYS	CA-CB-CG	-5.36	101.61	113.40
1	E	80	LEU	CD1-CG-CD2	-5.34	94.47	110.50
1	A	60	LYS	CB-CA-C	-5.30	99.80	110.40
1	F	55	GLU	C-N-CA	-5.29	108.47	121.70
1	D	154	ARG	CB-CG-CD	-5.21	98.05	111.60
1	D	220	LYS	CG-CD-CE	-5.15	96.45	111.90
1	B	137	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	60	LYS	CB-CG-CD	-5.09	98.38	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	101	THR	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	GLU	Peptide
1	A	60	LYS	Peptide
1	B	154	ARG	Sidechain
1	B	55	GLU	Peptide
1	B	56	GLN	Peptide
1	C	49	ARG	Sidechain
1	C	56	GLN	Sidechain
1	D	154	ARG	Sidechain
1	D	84	TRP	Peptide
1	F	140	ARG	Sidechain
1	F	258	GLY	Peptide
1	F	42	PRO	Peptide
1	F	52	GLU	Peptide
1	F	55	GLU	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	1917	0	1865	197	1
1	B	1845	0	1787	140	3
1	C	1923	0	1885	138	1
1	D	1899	0	1869	180	2
1	E	1934	0	1908	177	0
1	F	1937	0	1912	138	0
2	A	44	0	24	10	0
2	B	44	0	25	10	0
2	C	44	0	24	9	0
2	D	44	0	25	13	0
2	E	44	0	25	4	0
2	F	44	0	25	11	0
3	A	30	24	0	0	0
3	B	30	24	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	30	24	0	2	0
3	D	30	24	0	3	0
3	E	30	24	0	0	0
3	F	30	24	0	1	0
4	A	4	0	0	1	0
4	B	2	0	0	0	0
4	C	9	0	0	2	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	1	0
All	All	11921	144	11374	912	4

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 39.

All (912) 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:B:6:LEU:HD23	1:B:35:ALA:HB2	1.26	1.15
1:B:137:LEU:HD23	1:B:185:ILE:HD13	1.15	1.13
1:D:25:GLY:HA3	1:D:225:ILE:HG22	1.31	1.12
1:A:25:GLY:HA3	1:A:225:ILE:HG22	1.34	1.09
1:A:76:ALA:HA	1:A:79:GLU:OE2	1.55	1.06
1:B:67:VAL:HG21	1:B:125:SER:HB2	1.41	1.03
1:A:197:THR:HG23	1:A:199:ALA:H	1.21	1.02
1:B:6:LEU:HD21	1:B:30:LEU:HD22	1.41	1.00
1:F:49:ARG:O	1:F:53:PHE:HB2	1.60	1.00
1:B:22:ILE:HG12	1:B:225:ILE:HG22	1.43	0.99
1:D:22:ILE:HD12	2:D:301:NAD:PN	2.00	0.99
1:A:41:TYR:CE1	1:A:62:VAL:HG13	1.98	0.99
1:A:207:ARG:HG3	1:A:208:LYS:N	1.39	0.98
1:B:23:ALA:HA	1:B:26:ILE:HD13	1.46	0.98
1:B:113:ASP:O	1:B:117:ILE:HD12	1.66	0.96
1:A:21:SER:HB3	1:A:24:TYR:H	1.27	0.95
1:C:107:THR:HG21	1:E:180:LEU:HD21	1.49	0.95
1:B:195:ILE:HG22	1:B:197:THR:HG23	1.48	0.95
1:F:25:GLY:HA3	1:F:225:ILE:HG22	1.49	0.94
1:C:213:ASN:ND2	1:C:222:ASN:OD1	2.01	0.94
1:B:137:LEU:CD2	1:B:185:ILE:HD13	1.98	0.94
1:A:35:ALA:O	1:A:36:GLU:HG2	1.68	0.93
1:E:10:ARG:HA	1:E:36:GLU:HB2	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD11	1:A:235:LEU:HD11	1.51	0.92
1:E:25:GLY:HA3	1:E:225:ILE:HG22	1.49	0.92
1:B:36:GLU:OE1	1:B:36:GLU:N	2.03	0.92
1:D:214:GLU:O	1:D:220:LYS:HG2	1.70	0.92
1:D:98:PRO:O	1:D:101:THR:OG1	1.89	0.90
1:B:134:LYS:NZ	1:B:138:GLN:OE1	2.05	0.90
1:E:26:ILE:HD11	1:E:232:ALA:HB3	1.52	0.89
1:E:26:ILE:HD13	1:E:229:GLY:HA2	1.52	0.89
1:A:207:ARG:HG3	1:A:208:LYS:H	1.35	0.89
1:E:25:GLY:HA3	1:E:225:ILE:CG2	2.02	0.89
1:B:137:LEU:HD21	1:B:185:ILE:HG21	1.55	0.88
1:E:126:PHE:CE2	1:E:146:THR:HB	2.08	0.87
1:C:28:GLN:O	1:C:32:ARG:HG3	1.73	0.87
1:B:101:THR:HG21	1:B:114:GLY:HA3	1.56	0.87
1:F:141:GLN:OE1	1:F:184:GLY:HA3	1.74	0.86
1:B:56:GLN:HB3	1:B:57:PHE:CD1	2.08	0.86
1:E:26:ILE:CD1	1:E:232:ALA:HB3	2.05	0.85
1:D:106:PHE:O	1:D:110:THR:OG1	1.93	0.85
1:A:41:TYR:HE1	1:A:62:VAL:HG13	1.41	0.85
1:C:113:ASP:O	1:C:117:ILE:HD12	1.75	0.85
1:E:36:GLU:HB3	1:E:84:TRP:CZ2	2.10	0.85
1:E:113:ASP:O	1:E:117:ILE:HD12	1.75	0.85
1:D:207:ARG:HA	1:D:210:LEU:CD1	2.06	0.85
1:F:42:PRO:HG2	1:F:43:ASN:HB3	1.58	0.84
1:A:197:THR:HG21	2:A:301:NAD:O1N	1.76	0.83
1:A:76:ALA:HA	1:A:79:GLU:CD	1.98	0.83
1:A:136:LEU:HD12	1:A:136:LEU:H	1.44	0.83
1:D:136:LEU:HD12	1:D:136:LEU:H	1.44	0.83
1:D:253:GLY:O	1:D:256:THR:HG22	1.80	0.82
1:D:195:ILE:HD11	1:D:223:VAL:O	1.80	0.82
1:F:51:ASP:HA	1:F:62:VAL:HG21	1.62	0.82
1:B:162:MET:HE3	1:B:165:ALA:HB3	1.62	0.82
1:A:53:PHE:HA	1:A:56:GLN:OE1	1.80	0.81
1:F:42:PRO:CG	1:F:43:ASN:HB3	2.10	0.81
1:A:148:THR:OG1	1:A:149:TYR:N	2.12	0.81
1:D:6:LEU:HD13	1:D:30:LEU:HD23	1.61	0.81
1:E:80:LEU:HD12	1:E:84:TRP:HB2	1.62	0.81
1:E:42:PRO:HG2	1:E:46:LEU:HD22	1.62	0.81
1:E:258:GLY:HA2	1:F:154:ARG:CD	2.10	0.81
1:F:42:PRO:CB	1:F:43:ASN:HB3	2.11	0.80
1:A:248:LEU:HD11	1:E:243:ILE:HD13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ILE:O	1:E:30:LEU:HD12	1.82	0.80
1:F:37:LEU:HD12	1:F:57:PHE:HB3	1.64	0.80
1:B:41:TYR:CE2	1:B:47:LYS:HG3	2.17	0.80
1:D:206:PHE:HD1	1:D:210:LEU:HD11	1.46	0.80
1:E:36:GLU:HB3	1:E:84:TRP:HZ2	1.47	0.79
1:B:80:LEU:HD12	1:B:83:HIS:HB2	1.64	0.79
1:A:76:ALA:CA	1:A:79:GLU:OE2	2.30	0.79
1:F:225:ILE:HD12	1:F:225:ILE:H	1.46	0.79
1:D:211:ASP:HA	1:D:214:GLU:OE2	1.83	0.78
1:A:207:ARG:HA	1:A:210:LEU:HB2	1.64	0.78
1:C:41:TYR:CE1	1:C:62:VAL:HG12	2.19	0.78
1:F:207:ARG:HA	1:F:210:LEU:HB2	1.64	0.78
1:E:156:MET:SD	1:F:259:MET:HB2	2.24	0.77
1:A:249:TYR:O	1:E:243:ILE:HG23	1.83	0.77
1:D:80:LEU:HD11	1:D:84:TRP:CE3	2.20	0.77
1:E:26:ILE:CD1	1:E:229:GLY:HA2	2.14	0.77
1:D:133:ALA:O	1:D:137:LEU:HG	1.85	0.77
1:C:87:VAL:HG13	1:C:137:LEU:HD23	1.68	0.76
1:B:113:ASP:CG	1:B:117:ILE:HD11	2.05	0.76
1:D:59:SER:OG	1:D:61:LEU:HD12	1.85	0.76
1:B:224:THR:O	1:B:228:VAL:HG23	1.86	0.76
1:D:50:VAL:HG23	1:D:62:VAL:HG11	1.68	0.76
1:A:97:ALA:HB3	1:A:102:LEU:HD11	1.68	0.75
1:A:192:ALA:HA	1:A:250:VAL:HG23	1.69	0.75
1:C:224:THR:O	1:C:228:VAL:HG23	1.86	0.74
1:D:6:LEU:CD1	1:D:30:LEU:HD23	2.17	0.74
1:F:47:LYS:NZ	1:F:51:ASP:OD1	2.19	0.74
1:A:23:ALA:HA	1:A:26:ILE:CG2	2.18	0.74
1:B:106:PHE:O	1:B:110:THR:HG23	1.87	0.74
1:D:87:VAL:HG23	1:D:136:LEU:HB3	1.70	0.74
1:A:207:ARG:CG	1:A:208:LYS:N	2.35	0.74
1:D:82:LYS:HB2	1:D:83:HIS:HD2	1.53	0.74
1:C:12:LEU:HD12	1:C:80:LEU:HD22	1.68	0.74
1:B:67:VAL:HG21	1:B:125:SER:CB	2.17	0.74
1:D:41:TYR:CZ	1:D:47:LYS:HG2	2.22	0.74
1:E:48:LYS:HB3	1:E:49:ARG:HH11	1.52	0.74
1:E:194:PRO:CG	1:E:209:MET:HE3	2.17	0.74
2:E:302:NAD:H52A	2:E:302:NAD:H52N	1.69	0.74
1:A:10:ARG:HH12	1:A:85:ASP:H	1.33	0.74
1:B:152:SER:HB3	1:B:166:LYS:HB3	1.69	0.74
1:C:173:VAL:HG13	1:C:187:VAL:HG12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LYS:O	1:C:138:GLN:HG3	1.86	0.73
1:D:250:VAL:HG23	1:D:250:VAL:O	1.87	0.73
1:A:141:GLN:NE2	1:A:183:ASP:O	2.19	0.73
1:E:69:VAL:HG12	1:E:72:GLU:H	1.52	0.73
1:A:61:LEU:HD22	1:A:63:PHE:HZ	1.51	0.73
1:B:137:LEU:HD21	1:B:185:ILE:CG2	2.18	0.73
1:E:10:ARG:HB3	1:E:84:TRP:CZ3	2.23	0.73
1:B:6:LEU:HD23	1:B:35:ALA:CB	2.12	0.73
1:E:41:TYR:CE2	1:E:47:LYS:HG2	2.22	0.73
1:B:69:VAL:HB	1:B:72:GLU:OE2	1.89	0.73
1:D:105:ASP:OD1	1:D:107:THR:N	2.22	0.73
1:D:207:ARG:HA	1:D:210:LEU:HD12	1.69	0.73
1:B:195:ILE:CG2	1:B:197:THR:HG23	2.19	0.73
1:E:87:VAL:HG12	1:E:136:LEU:HB3	1.70	0.73
1:E:195:ILE:HD11	1:E:223:VAL:O	1.87	0.73
1:C:32:ARG:NH1	1:C:32:ARG:HB3	2.04	0.72
1:B:6:LEU:CD2	1:B:30:LEU:HD22	2.16	0.72
1:A:10:ARG:HH12	1:A:85:ASP:N	1.88	0.72
1:B:172:GLY:O	1:B:176:LEU:HD12	1.89	0.72
1:D:113:ASP:O	1:D:117:ILE:HD12	1.90	0.72
1:E:45:LYS:HD2	1:E:45:LYS:O	1.90	0.72
1:D:85:ASP:OD1	1:D:140:ARG:HD2	1.89	0.72
1:A:161:VAL:HG23	1:A:164:MET:HE3	1.72	0.71
1:B:172:GLY:C	1:B:176:LEU:HD12	2.10	0.71
1:B:148:THR:HA	1:B:166:LYS:CE	2.21	0.71
1:B:148:THR:HA	1:B:166:LYS:HE3	1.73	0.71
1:D:206:PHE:CD1	1:D:210:LEU:HD11	2.25	0.71
1:F:41:TYR:HE2	1:F:44:GLU:HG2	1.55	0.71
1:B:152:SER:OG	1:B:170:GLU:OE2	2.09	0.71
1:E:87:VAL:HG22	1:E:89:GLY:H	1.54	0.71
1:B:144:LEU:HD12	1:B:187:VAL:HG22	1.71	0.71
1:C:105:ASP:O	1:C:109:VAL:HG22	1.91	0.71
1:C:116:LYS:NZ	1:E:120:ASP:HB2	2.05	0.71
1:D:41:TYR:HB3	1:D:50:VAL:HG11	1.73	0.71
1:E:79:GLU:O	1:E:82:LYS:HB2	1.90	0.71
1:B:41:TYR:CZ	1:B:47:LYS:HG3	2.25	0.70
1:C:189:ALA:HB3	1:C:247:ILE:CD1	2.20	0.70
1:D:93:SER:OG	2:D:301:NAD:H52N	1.90	0.70
1:A:21:SER:HB3	1:A:24:TYR:N	2.05	0.70
1:E:126:PHE:CD2	1:E:146:THR:HB	2.26	0.70
1:B:22:ILE:O	1:B:26:ILE:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:PHE:O	1:D:210:LEU:HD12	1.91	0.70
1:A:206:PHE:O	1:A:209:MET:HB3	1.91	0.70
1:B:137:LEU:HD23	1:B:185:ILE:CD1	2.09	0.70
1:D:195:ILE:HD11	1:D:223:VAL:C	2.11	0.70
1:A:41:TYR:CE1	1:A:62:VAL:CG1	2.75	0.70
1:A:157:PRO:HD3	1:C:259:MET:O	1.92	0.69
1:E:10:ARG:HB3	1:E:84:TRP:CH2	2.27	0.69
1:B:56:GLN:HG2	1:B:57:PHE:CE1	2.27	0.69
1:D:145:LEU:HD12	1:D:146:THR:N	2.07	0.69
1:A:190:ILE:HD13	1:A:248:LEU:HB3	1.74	0.69
1:E:48:LYS:HB3	1:E:49:ARG:NH1	2.07	0.69
1:B:60:LYS:O	1:B:62:VAL:HG23	1.93	0.69
1:D:85:ASP:OD1	1:D:86:GLY:N	2.25	0.69
1:E:80:LEU:CD1	1:E:84:TRP:HB2	2.23	0.69
1:B:41:TYR:HB3	1:B:50:VAL:HG21	1.73	0.68
1:E:52:GLU:O	1:E:56:GLN:HG2	1.93	0.68
1:E:63:PHE:CE1	1:E:79:GLU:HB3	2.28	0.68
1:F:18:SER:OG	1:F:198:LEU:HD21	1.93	0.68
1:A:43:ASN:OD1	1:A:45:LYS:HB2	1.94	0.68
1:F:206:PHE:O	1:F:209:MET:HB2	1.94	0.68
1:E:258:GLY:HA2	1:F:154:ARG:HD2	1.73	0.67
1:A:89:GLY:HA2	1:A:143:CYS:O	1.94	0.67
1:D:101:THR:HG22	1:D:161:VAL:HG12	1.77	0.67
1:A:207:ARG:HA	1:A:210:LEU:HD12	1.75	0.67
1:F:43:ASN:OD1	1:F:46:LEU:HD23	1.94	0.67
1:A:187:VAL:O	1:A:245:GLY:N	2.24	0.67
1:B:195:ILE:HG22	1:B:197:THR:CG2	2.24	0.67
1:F:42:PRO:HG2	1:F:43:ASN:CB	2.25	0.67
1:A:21:SER:HB2	1:A:24:TYR:HB2	1.77	0.67
1:B:221:ARG:NH2	1:B:227:GLU:OE2	2.27	0.66
1:E:195:ILE:HD11	1:E:223:VAL:C	2.14	0.66
1:A:87:VAL:HG22	1:A:89:GLY:H	1.59	0.66
1:C:211:ASP:O	1:C:215:LYS:HG3	1.95	0.66
1:D:25:GLY:HA3	1:D:225:ILE:CG2	2.17	0.66
1:E:67:VAL:HG22	2:E:302:NAD:C6A	2.26	0.66
1:F:189:ALA:HB3	1:F:247:ILE:HD13	1.76	0.66
1:F:106:PHE:O	1:F:110:THR:OG1	2.10	0.66
1:C:106:PHE:HA	1:C:160:ASN:HD22	1.59	0.66
1:E:26:ILE:CG2	1:E:30:LEU:HD11	2.24	0.66
1:C:113:ASP:C	1:C:117:ILE:HD12	2.15	0.66
1:A:91:VAL:HG13	1:A:145:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:CG1	1:C:62:VAL:HG13	2.25	0.66
1:A:194:PRO:HA	2:A:301:NAD:O7N	1.95	0.66
1:E:20:LEU:O	1:E:225:ILE:HD11	1.95	0.66
1:F:198:LEU:HD22	1:F:198:LEU:H	1.61	0.66
1:B:195:ILE:HD11	1:B:223:VAL:O	1.96	0.66
1:D:101:THR:CG2	1:D:161:VAL:HG11	2.26	0.66
1:A:26:ILE:O	1:A:30:LEU:HD12	1.96	0.65
1:C:50:VAL:HG12	1:C:62:VAL:HG13	1.76	0.65
1:D:87:VAL:HB	1:D:137:LEU:HD23	1.78	0.65
1:F:154:ARG:HH12	1:F:254:PHE:HE2	1.41	0.65
1:A:61:LEU:HD22	1:A:63:PHE:CZ	2.29	0.65
1:A:85:ASP:OD2	1:B:202:GLY:N	2.25	0.65
1:E:65:CYS:HA	1:E:72:GLU:HG2	1.79	0.65
1:D:105:ASP:O	1:D:109:VAL:HG22	1.96	0.65
1:A:25:GLY:HA3	1:A:225:ILE:CG2	2.17	0.65
1:D:80:LEU:HD23	1:D:136:LEU:HD22	1.77	0.65
1:F:105:ASP:OD1	1:F:107:THR:N	2.30	0.65
1:A:21:SER:HB2	1:A:24:TYR:CB	2.26	0.65
1:A:141:GLN:OE1	1:A:141:GLN:HA	1.96	0.65
1:F:31:HIS:HB2	1:F:37:LEU:HD11	1.79	0.65
1:A:244:THR:HG21	1:E:219:LEU:CD1	2.27	0.65
1:C:5:LEU:HG	1:C:6:LEU:HD12	1.77	0.65
1:D:215:LYS:C	1:D:220:LYS:HZ2	1.99	0.65
1:C:32:ARG:HB3	1:C:32:ARG:HH11	1.61	0.65
1:A:98:PRO:HG2	1:A:114:GLY:HA2	1.76	0.65
1:D:105:ASP:OD1	1:D:106:PHE:N	2.29	0.65
1:D:60:LYS:O	1:D:62:VAL:HG23	1.96	0.64
1:D:20:LEU:O	1:D:225:ILE:HD11	1.97	0.64
1:D:190:ILE:HD11	1:D:235:LEU:HD12	1.79	0.64
1:E:145:LEU:HD11	1:E:190:ILE:HG13	1.78	0.64
1:A:41:TYR:HE1	1:A:62:VAL:CG1	2.11	0.64
1:D:101:THR:HG21	1:D:161:VAL:HG11	1.78	0.64
1:B:65:CYS:SG	1:B:73:ILE:HD13	2.37	0.64
1:A:76:ALA:O	1:A:79:GLU:OE2	2.16	0.64
1:C:18:SER:HB3	1:C:198:LEU:HD11	1.79	0.64
1:E:17:ALA:HB1	1:E:198:LEU:HD12	1.80	0.64
1:E:67:VAL:HG22	2:E:302:NAD:N1A	2.13	0.64
1:C:18:SER:HB3	1:C:198:LEU:CD1	2.28	0.64
1:D:22:ILE:HG21	1:D:228:VAL:HG11	1.79	0.64
1:D:67:VAL:HG22	2:D:301:NAD:N1A	2.13	0.64
1:E:170:GLU:HG2	1:E:247:ILE:HD12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLY:HA2	1:D:143:CYS:O	1.97	0.64
1:A:82:LYS:O	1:B:207:ARG:HD3	1.96	0.64
1:C:106:PHE:O	1:C:110:THR:OG1	2.13	0.64
1:D:122:SER:O	1:D:169:LEU:HD13	1.98	0.63
1:C:106:PHE:HD1	1:C:160:ASN:HB3	1.64	0.63
1:F:207:ARG:HG2	1:F:207:ARG:HH11	1.61	0.63
1:D:19:LYS:HA	1:D:24:TYR:CD2	2.34	0.63
1:A:35:ALA:C	1:A:36:GLU:HG2	2.17	0.63
1:A:97:ALA:CB	1:A:102:LEU:HD11	2.28	0.63
1:E:17:ALA:CB	1:E:198:LEU:HD12	2.28	0.63
1:B:61:LEU:HD13	1:B:80:LEU:CD1	2.28	0.63
1:D:190:ILE:HD11	1:D:235:LEU:CD1	2.28	0.63
1:A:26:ILE:HD12	1:A:232:ALA:CB	2.29	0.63
1:B:56:GLN:HG2	1:B:57:PHE:CZ	2.33	0.63
1:E:90:VAL:HB	1:E:144:LEU:HD23	1.79	0.63
1:D:80:LEU:HD11	1:D:84:TRP:HE3	1.61	0.63
1:F:61:LEU:HD22	1:F:61:LEU:H	1.64	0.63
1:D:166:LYS:O	1:D:170:GLU:HG3	1.98	0.62
1:E:157:PRO:HD3	1:F:259:MET:O	1.98	0.62
1:C:219:LEU:O	1:C:220:LYS:HB2	1.99	0.62
1:A:43:ASN:OD1	1:A:45:LYS:HG2	1.99	0.62
1:F:102:LEU:HD23	1:F:158:ASN:O	1.99	0.62
1:F:43:ASN:OD1	1:F:46:LEU:HB2	2.00	0.62
1:C:39:PHE:HB3	1:C:50:VAL:HG13	1.80	0.62
1:A:192:ALA:HA	1:A:250:VAL:CG2	2.30	0.62
1:B:145:LEU:CD2	1:B:232:ALA:HB1	2.29	0.62
1:C:41:TYR:HE1	1:C:62:VAL:HG12	1.65	0.62
1:E:258:GLY:CA	1:F:154:ARG:HD2	2.29	0.62
1:A:33:GLU:HG3	1:A:233:LEU:HD21	1.82	0.61
1:B:42:PRO:HD2	1:B:43:ASN:H	1.64	0.61
1:A:91:VAL:HG13	1:A:145:LEU:CD2	2.31	0.61
1:C:105:ASP:OD1	1:C:107:THR:OG1	2.17	0.61
1:E:98:PRO:HG2	1:E:114:GLY:HA2	1.82	0.61
1:F:248:LEU:HD22	1:F:250:VAL:HG22	1.81	0.61
1:C:253:GLY:HA3	1:F:244:THR:HG22	1.83	0.61
1:A:106:PHE:O	1:A:110:THR:OG1	2.15	0.61
1:D:14:ALA:HA	1:D:40:THR:HG22	1.83	0.61
1:B:162:MET:HE3	1:B:162:MET:HA	1.83	0.61
1:C:87:VAL:CG1	1:C:137:LEU:HD23	2.31	0.61
1:E:21:SER:O	1:E:225:ILE:HD13	2.01	0.61
1:E:42:PRO:CG	1:E:46:LEU:HD22	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:O	1:A:26:ILE:HG23	2.01	0.60
1:B:69:VAL:HB	1:B:72:GLU:CD	2.21	0.60
1:B:131:ARG:HB3	1:B:131:ARG:CZ	2.30	0.60
1:D:214:GLU:O	1:D:220:LYS:HA	2.01	0.60
1:F:51:ASP:O	1:F:54:ALA:HB3	2.01	0.60
1:B:31:HIS:O	1:B:34:GLY:N	2.25	0.60
1:E:150:GLN:HE22	1:E:254:PHE:HD2	1.50	0.60
1:F:5:LEU:H	1:F:33:GLU:HG3	1.66	0.60
1:F:13:ILE:HD12	1:F:27:ALA:HB2	1.83	0.60
1:B:144:LEU:HD12	1:B:187:VAL:CG2	2.32	0.60
1:D:11:PHE:CE1	1:D:89:GLY:HA3	2.36	0.60
1:D:56:GLN:O	1:D:56:GLN:HG2	2.00	0.60
1:E:187:VAL:O	1:E:245:GLY:N	2.28	0.60
1:E:47:LYS:HD2	1:E:51:ASP:OD2	2.02	0.60
1:F:67:VAL:HG22	2:F:302:NAD:N1A	2.16	0.60
1:B:195:ILE:CG2	1:B:197:THR:CG2	2.79	0.60
1:C:224:THR:HB	4:C:405:HOH:O	2.02	0.60
1:A:26:ILE:HD13	1:A:91:VAL:HG11	1.83	0.59
1:A:51:ASP:OD2	1:A:62:VAL:HG11	2.02	0.59
1:D:210:LEU:O	1:D:214:GLU:OE1	2.20	0.59
1:C:117:ILE:O	1:C:121:ILE:HG12	2.02	0.59
1:D:187:VAL:O	1:D:245:GLY:N	2.32	0.59
1:F:42:PRO:CA	1:F:43:ASN:HB3	2.30	0.59
1:B:28:GLN:HA	1:B:57:PHE:HE2	1.68	0.59
1:B:138:GLN:HA	1:B:185:ILE:HD11	1.85	0.59
1:D:49:ARG:HA	1:D:52:GLU:CD	2.22	0.59
1:F:80:LEU:HD13	1:F:80:LEU:O	2.03	0.59
1:D:207:ARG:HA	1:D:210:LEU:HD13	1.83	0.59
1:F:98:PRO:HG2	1:F:114:GLY:HA2	1.84	0.59
1:F:94:ILE:HG23	2:F:302:NAD:C1B	2.32	0.59
1:D:101:THR:HG22	1:D:161:VAL:CG1	2.32	0.58
1:D:228:VAL:HG22	1:D:250:VAL:HG21	1.84	0.58
1:F:89:GLY:HA2	1:F:143:CYS:O	2.03	0.58
1:F:137:LEU:O	1:F:141:GLN:N	2.36	0.58
1:B:75:ASN:O	1:B:79:GLU:HG3	2.02	0.58
1:C:44:GLU:O	1:C:45:LYS:C	2.40	0.58
1:C:243:ILE:HD13	1:F:248:LEU:HD21	1.85	0.58
1:A:141:GLN:HE22	1:A:183:ASP:C	2.06	0.58
1:B:113:ASP:C	1:B:117:ILE:HD12	2.23	0.58
1:D:49:ARG:HA	1:D:52:GLU:OE1	2.04	0.58
1:C:206:PHE:O	1:C:209:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD11	1:A:235:LEU:CD1	2.30	0.58
1:C:42:PRO:HD2	1:C:46:LEU:CB	2.34	0.58
1:C:195:ILE:HG22	1:C:197:THR:HG23	1.84	0.58
1:D:192:ALA:HA	1:D:250:VAL:HG22	1.86	0.58
1:E:41:TYR:HB3	1:E:50:VAL:HG21	1.86	0.58
1:E:195:ILE:CD1	1:E:223:VAL:HG23	2.33	0.58
1:A:6:LEU:HB3	1:A:35:ALA:HB2	1.85	0.58
1:B:42:PRO:CG	1:B:46:LEU:HD22	2.34	0.58
1:E:39:PHE:O	1:E:62:VAL:HA	2.02	0.58
1:F:248:LEU:HD23	1:F:249:TYR:N	2.19	0.58
1:A:250:VAL:HG23	1:A:250:VAL:O	2.04	0.58
1:B:17:ALA:HB2	2:B:302:NAD:O3B	2.04	0.58
1:F:41:TYR:CE2	1:F:44:GLU:HG2	2.36	0.58
1:A:105:ASP:OD1	1:F:179:SER:OG	2.21	0.58
1:B:173:VAL:HG13	1:B:187:VAL:HG12	1.86	0.58
1:C:113:ASP:O	1:C:116:LYS:N	2.37	0.58
1:D:12:LEU:CD2	1:D:90:VAL:HG13	2.34	0.58
1:C:89:GLY:HA2	1:C:143:CYS:O	2.04	0.57
1:E:26:ILE:HG23	1:E:30:LEU:HD11	1.86	0.57
1:C:203:ILE:HD12	3:C:301:NUC:C21	2.35	0.57
1:E:101:THR:C	1:E:102:LEU:HD23	2.24	0.57
1:A:131:ARG:NH2	1:F:110:THR:O	2.37	0.57
1:B:37:LEU:HD12	1:B:57:PHE:CG	2.39	0.57
1:C:189:ALA:HB3	1:C:247:ILE:HD13	1.85	0.57
1:B:173:VAL:HG21	1:B:189:ALA:HB2	1.86	0.57
1:D:44:GLU:O	1:D:47:LYS:HB2	2.05	0.57
1:A:80:LEU:HD11	1:A:84:TRP:HE3	1.70	0.57
1:D:151:GLY:HA2	1:D:154:ARG:O	2.04	0.57
1:E:17:ALA:HB2	2:E:302:NAD:O3B	2.04	0.57
1:C:69:VAL:HB	1:C:72:GLU:HG3	1.86	0.57
1:D:98:PRO:HG2	1:D:114:GLY:HA2	1.87	0.57
1:B:145:LEU:HD21	1:B:232:ALA:HB1	1.86	0.57
1:C:152:SER:O	1:E:174:ARG:NH2	2.23	0.57
1:C:194:PRO:HA	2:C:302:NAD:O7N	2.05	0.57
1:D:101:THR:CG2	1:D:161:VAL:CG1	2.82	0.57
1:A:207:ARG:O	1:A:211:ASP:N	2.35	0.57
1:E:89:GLY:HA2	1:E:143:CYS:O	2.04	0.57
1:E:143:CYS:SG	1:E:236:CYS:HA	2.44	0.57
1:C:26:ILE:O	1:C:30:LEU:HD13	2.04	0.56
1:B:98:PRO:HG2	1:B:114:GLY:HA2	1.86	0.56
1:D:189:ALA:HB3	1:D:247:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:ILE:CD1	1:E:232:ALA:HB2	2.35	0.56
1:D:46:LEU:O	1:D:50:VAL:HG13	2.05	0.56
1:D:192:ALA:HA	1:D:250:VAL:CG2	2.36	0.56
1:F:22:ILE:HB	2:F:302:NAD:H51N	1.86	0.56
1:A:80:LEU:HD13	1:A:80:LEU:O	2.05	0.56
1:C:210:LEU:HD22	1:C:222:ASN:ND2	2.20	0.56
1:D:194:PRO:HA	2:D:301:NAD:O7N	2.06	0.56
1:D:152:SER:HB3	1:D:166:LYS:HB2	1.86	0.56
1:E:159:TYR:OH	1:E:166:LYS:HD2	2.06	0.56
1:F:85:ASP:O	1:F:136:LEU:HD22	2.05	0.56
1:C:39:PHE:HB3	1:C:50:VAL:CG1	2.35	0.56
1:D:12:LEU:HD22	1:D:90:VAL:HG13	1.88	0.56
1:B:18:SER:N	1:B:21:SER:OG	2.36	0.56
1:D:200:ALA:HA	1:D:203:ILE:HD13	1.88	0.56
1:D:121:ILE:N	1:D:121:ILE:HD12	2.21	0.56
1:D:152:SER:OG	1:D:170:GLU:OE2	2.21	0.56
1:F:37:LEU:HD12	1:F:57:PHE:CB	2.34	0.56
1:C:206:PHE:O	1:C:210:LEU:N	2.33	0.56
1:C:234:PHE:O	1:C:237:SER:OG	2.24	0.56
1:E:194:PRO:HG2	1:E:209:MET:HE3	1.88	0.56
1:A:251:ASP:OD2	1:A:255:ASN:HB3	2.06	0.55
1:D:13:ILE:HD12	1:D:27:ALA:HB2	1.88	0.55
1:E:145:LEU:CD2	1:E:232:ALA:HB1	2.37	0.55
1:E:210:LEU:HD12	1:E:222:ASN:HD22	1.70	0.55
1:A:94:ILE:HG23	2:A:301:NAD:C1B	2.36	0.55
1:C:227:GLU:HG2	1:F:241:SER:OG	2.06	0.55
1:D:77:PHE:CE1	1:D:133:ALA:HB2	2.41	0.55
1:D:90:VAL:HG23	1:D:137:LEU:HD21	1.88	0.55
1:F:152:SER:HB3	1:F:166:LYS:HB2	1.87	0.55
1:A:77:PHE:CE1	1:A:133:ALA:HB2	2.41	0.55
1:B:26:ILE:HG13	1:B:229:GLY:HA2	1.89	0.55
1:B:44:GLU:OE2	1:B:45:LYS:HE3	2.06	0.55
1:B:67:VAL:HG12	2:B:302:NAD:C6A	2.36	0.55
1:D:157:PRO:O	1:D:209:MET:HE1	2.06	0.55
1:D:206:PHE:HD1	1:D:210:LEU:CD1	2.16	0.55
1:E:146:THR:HG21	1:E:169:LEU:HD11	1.87	0.55
1:B:203:ILE:N	1:B:203:ILE:HD12	2.21	0.55
1:C:149:TYR:CD1	2:C:302:NAD:H5N	2.41	0.55
1:D:145:LEU:HD12	1:D:146:THR:H	1.70	0.55
1:D:123:ALA:HA	1:D:169:LEU:CD1	2.36	0.55
1:D:217:ALA:O	1:D:220:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HG3	1:F:107:THR:HG22	1.88	0.55
1:B:221:ARG:HH11	1:B:221:ARG:HG3	1.72	0.55
1:D:6:LEU:HD11	1:D:233:LEU:CD1	2.37	0.55
1:D:9:LYS:HD2	1:D:88:ASP:CG	2.27	0.55
1:B:6:LEU:CD2	1:B:35:ALA:HB2	2.18	0.55
1:C:145:LEU:HD11	1:C:190:ILE:HG13	1.88	0.55
1:C:249:TYR:HB2	1:F:246:GLU:OE1	2.07	0.55
1:A:227:GLU:OE1	1:E:241:SER:OG	2.24	0.55
1:D:120:ASP:HB3	1:D:121:ILE:HD12	1.88	0.55
1:F:131:ARG:HB3	1:F:131:ARG:NH1	2.21	0.55
1:A:76:ALA:C	1:A:79:GLU:OE2	2.46	0.54
1:B:152:SER:HB2	1:B:167:ALA:CA	2.38	0.54
1:E:258:GLY:CA	1:F:154:ARG:CD	2.83	0.54
1:F:210:LEU:HG	1:F:222:ASN:ND2	2.22	0.54
1:A:22:ILE:O	1:A:26:ILE:HG22	2.07	0.54
1:C:235:LEU:HD21	1:C:248:LEU:HD12	1.89	0.54
1:D:22:ILE:HD12	2:D:301:NAD:O2N	2.06	0.54
1:D:152:SER:HB3	1:D:166:LYS:CB	2.37	0.54
1:F:203:ILE:N	1:F:203:ILE:HD12	2.22	0.54
1:A:43:ASN:OD1	1:A:45:LYS:CG	2.55	0.54
1:E:117:ILE:HD12	1:E:117:ILE:H	1.72	0.54
1:A:134:LYS:O	1:A:138:GLN:HG3	2.07	0.54
1:D:22:ILE:HA	1:D:225:ILE:HG23	1.89	0.54
1:E:189:ALA:HB3	1:E:247:ILE:HD13	1.88	0.54
1:E:195:ILE:HD11	1:E:223:VAL:HG23	1.88	0.54
1:A:11:PHE:CE1	1:A:89:GLY:HA3	2.42	0.54
1:A:259:MET:O	1:C:157:PRO:HD3	2.08	0.54
1:D:25:GLY:CA	1:D:225:ILE:HG22	2.21	0.54
1:C:44:GLU:O	1:C:46:LEU:N	2.40	0.54
1:A:92:HIS:ND1	1:A:146:THR:HG23	2.22	0.54
1:B:61:LEU:HD13	1:B:80:LEU:HD11	1.90	0.54
1:E:88:ASP:C	1:E:142:GLY:HA3	2.28	0.54
1:E:93:SER:O	1:E:93:SER:OG	2.25	0.54
1:A:143:CYS:SG	1:A:236:CYS:HA	2.48	0.53
1:D:22:ILE:HD12	2:D:301:NAD:O1N	2.08	0.53
1:D:22:ILE:HD13	2:D:301:NAD:O4D	2.08	0.53
1:D:171:ALA:O	1:D:175:TYR:HD2	1.91	0.53
1:A:102:LEU:HD12	1:A:102:LEU:N	2.23	0.53
1:B:101:THR:HG21	1:B:114:GLY:CA	2.31	0.53
1:B:148:THR:HA	1:B:166:LYS:HE2	1.90	0.53
1:C:5:LEU:HG	1:C:6:LEU:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:GLU:OE1	1:F:226:GLU:N	2.39	0.53
1:B:152:SER:HB2	1:B:167:ALA:HA	1.91	0.53
1:E:96:PHE:HB3	1:E:121:ILE:HG21	1.89	0.53
1:F:52:GLU:HA	1:F:55:GLU:H	1.72	0.53
1:A:10:ARG:HD3	1:A:84:TRP:CE2	2.44	0.53
1:C:148:THR:OG1	1:C:149:TYR:N	2.42	0.53
1:D:207:ARG:CA	1:D:210:LEU:HD12	2.39	0.53
1:E:106:PHE:HD1	1:E:160:ASN:HB3	1.73	0.53
1:E:257:VAL:HG12	1:E:259:MET:N	2.24	0.53
1:B:67:VAL:HG22	1:B:67:VAL:O	2.08	0.53
1:E:138:GLN:NE2	1:E:183:ASP:OD2	2.41	0.53
1:E:210:LEU:HD12	1:E:222:ASN:ND2	2.24	0.53
1:E:25:GLY:HA3	1:E:225:ILE:HG21	1.86	0.53
1:A:224:THR:O	1:A:228:VAL:HG23	2.08	0.53
1:B:234:PHE:CD2	1:B:235:LEU:HD22	2.44	0.53
1:A:100:HIS:CE1	1:A:101:THR:HG23	2.44	0.52
1:B:46:LEU:O	1:B:50:VAL:HG23	2.08	0.52
1:B:106:PHE:HB2	1:B:160:ASN:OD1	2.09	0.52
1:C:225:ILE:HG12	4:C:405:HOH:O	2.09	0.52
1:F:44:GLU:HA	1:F:47:LYS:HB2	1.91	0.52
1:F:135:PRO:HA	1:F:138:GLN:OE1	2.10	0.52
1:A:98:PRO:HG2	1:A:114:GLY:CA	2.39	0.52
1:B:94:ILE:HG12	2:B:302:NAD:O4B	2.10	0.52
1:C:19:LYS:HA	1:C:24:TYR:CD1	2.44	0.52
1:C:98:PRO:HG2	1:C:114:GLY:HA2	1.91	0.52
1:C:253:GLY:HA3	1:F:244:THR:CG2	2.39	0.52
1:F:42:PRO:HG2	1:F:43:ASN:CG	2.29	0.52
1:A:22:ILE:HB	2:A:301:NAD:H51N	1.91	0.52
1:B:137:LEU:CD2	1:B:185:ILE:HG21	2.34	0.52
1:C:116:LYS:HZ1	1:E:120:ASP:HB2	1.72	0.52
1:D:105:ASP:HB3	1:D:108:ASP:HB2	1.91	0.52
1:D:116:LYS:HZ2	1:D:117:ILE:N	2.07	0.52
1:E:26:ILE:HG22	1:E:30:LEU:HD11	1.90	0.52
1:F:207:ARG:HG2	1:F:207:ARG:NH1	2.24	0.52
1:B:18:SER:HB3	1:B:198:LEU:HD13	1.92	0.52
1:D:80:LEU:HD23	1:D:136:LEU:CD2	2.40	0.52
1:C:87:VAL:HG13	1:C:137:LEU:CD2	2.39	0.52
1:C:101:THR:HG21	1:C:161:VAL:HG11	1.92	0.52
1:D:40:THR:OG1	1:D:65:CYS:HB3	2.10	0.52
1:D:41:TYR:HB3	1:D:50:VAL:HG21	1.92	0.52
1:E:234:PHE:CE1	1:E:240:ALA:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:PHE:HB2	1:D:132:ALA:HB1	1.93	0.51
1:D:87:VAL:HG23	1:D:136:LEU:CB	2.39	0.51
1:D:117:ILE:HG23	1:D:121:ILE:HD13	1.91	0.51
1:B:162:MET:HA	1:B:162:MET:CE	2.40	0.51
1:C:17:ALA:HB2	2:C:302:NAD:O3B	2.10	0.51
1:D:170:GLU:OE1	1:D:247:ILE:HD12	2.10	0.51
1:D:195:ILE:CD1	1:D:223:VAL:HG23	2.40	0.51
1:A:136:LEU:H	1:A:136:LEU:CD1	2.19	0.51
1:A:234:PHE:CD2	1:E:234:PHE:CD2	2.98	0.51
1:B:65:CYS:O	2:B:302:NAD:H2A	2.11	0.51
1:D:11:PHE:CZ	1:D:236:CYS:HB3	2.44	0.51
1:E:43:ASN:N	1:E:43:ASN:OD1	2.43	0.51
1:F:198:LEU:HD22	1:F:198:LEU:N	2.25	0.51
1:B:221:ARG:HG3	1:B:221:ARG:NH1	2.24	0.51
1:C:107:THR:O	1:E:131:ARG:NH1	2.43	0.51
1:D:79:GLU:HA	1:D:82:LYS:HE3	1.92	0.51
1:A:234:PHE:HE1	1:A:239:TRP:C	2.13	0.51
1:C:90:VAL:HB	1:C:144:LEU:HD23	1.92	0.51
1:A:13:ILE:HD13	1:A:91:VAL:HG21	1.92	0.51
1:A:85:ASP:OD1	1:B:201:SER:HA	2.11	0.51
1:C:93:SER:OG	2:C:302:NAD:H51N	2.11	0.51
1:A:44:GLU:HA	1:A:44:GLU:OE1	2.10	0.51
1:B:28:GLN:HA	1:B:57:PHE:CE2	2.46	0.51
2:D:301:NAD:O3B	2:D:301:NAD:O1A	2.28	0.51
1:B:26:ILE:HD12	1:B:26:ILE:H	1.76	0.51
1:F:149:TYR:HB2	2:F:302:NAD:C5N	2.40	0.51
1:B:148:THR:OG1	1:B:149:TYR:N	2.43	0.51
1:D:50:VAL:HG23	1:D:62:VAL:CG1	2.39	0.51
1:E:19:LYS:HG3	1:E:53:PHE:CZ	2.45	0.51
1:E:26:ILE:HD11	1:E:232:ALA:CB	2.32	0.51
1:C:61:LEU:HB3	1:C:63:PHE:HE1	1.76	0.50
1:C:124:TYR:CZ	1:E:112:ARG:HA	2.47	0.50
1:C:187:VAL:O	1:C:245:GLY:N	2.37	0.50
1:D:22:ILE:HD11	2:D:301:NAD:H71N	1.76	0.50
1:A:88:ASP:OD1	1:A:140:ARG:HB3	2.11	0.50
1:D:22:ILE:CG2	1:D:228:VAL:HG11	2.42	0.50
1:D:195:ILE:CD1	1:D:223:VAL:O	2.56	0.50
1:F:199:ALA:HB1	3:F:301:NUC:C13	2.42	0.50
1:A:26:ILE:HA	1:A:229:GLY:HA2	1.93	0.50
1:A:98:PRO:O	1:A:99:ALA:HB3	2.10	0.50
1:A:233:LEU:O	1:A:233:LEU:HD12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:HD2	1:C:88:ASP:CG	2.32	0.50
1:D:113:ASP:C	1:D:117:ILE:HD12	2.32	0.50
1:F:170:GLU:HG2	1:F:247:ILE:HD12	1.92	0.50
1:A:11:PHE:CZ	1:A:236:CYS:HB3	2.46	0.50
1:A:141:GLN:NE2	1:A:184:GLY:HA3	2.27	0.50
1:B:131:ARG:HB3	1:B:131:ARG:NH1	2.27	0.50
1:E:98:PRO:O	1:E:101:THR:OG1	2.26	0.50
1:E:219:LEU:HB2	1:E:252:ALA:HB1	1.93	0.50
1:F:22:ILE:HA	1:F:225:ILE:HG23	1.94	0.50
1:A:10:ARG:HB3	1:A:84:TRP:CZ2	2.46	0.50
1:A:98:PRO:CG	1:A:114:GLY:HA2	2.41	0.50
1:A:207:ARG:CA	1:A:210:LEU:HB2	2.38	0.50
1:D:6:LEU:HD22	1:D:11:PHE:HE2	1.76	0.50
1:D:82:LYS:HB2	1:D:83:HIS:CD2	2.40	0.50
1:D:113:ASP:OD2	1:D:117:ILE:HD11	2.12	0.50
1:E:11:PHE:CZ	1:E:236:CYS:HB3	2.46	0.50
1:A:93:SER:OG	2:A:301:NAD:H51N	2.11	0.50
1:A:146:THR:HG22	1:A:147:LEU:N	2.27	0.50
1:A:206:PHE:HE1	1:A:210:LEU:HD11	1.76	0.50
1:A:225:ILE:H	1:A:225:ILE:HD12	1.77	0.50
1:F:61:LEU:HD22	1:F:61:LEU:N	2.27	0.50
1:A:146:THR:HG22	1:A:147:LEU:H	1.77	0.49
1:D:136:LEU:H	1:D:136:LEU:CD1	2.20	0.49
1:B:186:ARG:HD2	1:B:243:ILE:O	2.12	0.49
1:C:116:LYS:HE2	1:E:120:ASP:OD1	2.12	0.49
1:D:6:LEU:HD13	1:D:30:LEU:CD2	2.38	0.49
1:D:215:LYS:O	1:D:220:LYS:NZ	2.42	0.49
1:E:258:GLY:O	1:E:259:MET:HB2	2.12	0.49
1:A:77:PHE:CZ	1:A:133:ALA:HB2	2.47	0.49
1:A:196:ARG:NH2	1:A:207:ARG:HB3	2.27	0.49
1:A:10:ARG:HD3	1:A:84:TRP:NE1	2.26	0.49
1:A:116:LYS:HA	4:A:403:HOH:O	2.11	0.49
1:B:106:PHE:HD1	1:B:160:ASN:HB3	1.77	0.49
1:C:51:ASP:HA	1:C:62:VAL:HG21	1.95	0.49
1:D:199:ALA:HB1	3:D:302:NUC:C3	2.41	0.49
1:F:51:ASP:HA	1:F:62:VAL:HG11	1.95	0.49
1:A:25:GLY:CA	1:A:225:ILE:HG22	2.24	0.49
1:A:253:GLY:HA3	1:E:244:THR:CG2	2.43	0.49
1:C:13:ILE:HG12	1:C:37:LEU:HD22	1.94	0.49
1:C:41:TYR:HB3	1:C:50:VAL:HG21	1.94	0.49
1:D:226:GLU:O	1:D:230:ASN:OD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LEU:HD23	1:F:248:LEU:C	2.32	0.49
1:A:13:ILE:HD13	1:A:91:VAL:CG2	2.43	0.49
1:A:22:ILE:HG21	1:A:147:LEU:HG	1.93	0.49
1:A:75:ASN:O	1:A:79:GLU:HG3	2.13	0.49
1:A:243:ILE:HG23	1:E:249:TYR:O	2.12	0.49
1:C:22:ILE:HA	1:C:225:ILE:HG22	1.94	0.49
1:A:11:PHE:CE1	1:A:236:CYS:HB3	2.48	0.49
1:A:26:ILE:HD12	1:A:232:ALA:HB1	1.94	0.49
1:A:149:TYR:HB2	2:A:301:NAD:C5N	2.43	0.49
1:B:196:ARG:NH1	1:B:196:ARG:HG3	2.28	0.49
1:D:134:LYS:HB3	1:D:135:PRO:HD3	1.94	0.49
1:B:106:PHE:HD1	1:B:160:ASN:CB	2.26	0.49
1:D:123:ALA:HA	1:D:169:LEU:HD12	1.95	0.49
1:B:54:ALA:HB1	1:B:59:SER:O	2.13	0.49
1:D:211:ASP:HA	1:D:214:GLU:CD	2.34	0.49
1:F:149:TYR:HB2	2:F:302:NAD:H5N	1.95	0.49
1:A:148:THR:O	2:A:301:NAD:H6N	2.13	0.48
1:A:251:ASP:OD2	1:A:255:ASN:N	2.44	0.48
1:B:5:LEU:HD12	1:B:5:LEU:O	2.12	0.48
1:D:20:LEU:O	1:D:225:ILE:CD1	2.60	0.48
1:E:156:MET:SD	1:F:259:MET:CB	2.99	0.48
1:E:234:PHE:HE1	1:E:239:TRP:C	2.16	0.48
1:F:248:LEU:HD22	1:F:250:VAL:CG2	2.42	0.48
1:A:67:VAL:HG22	2:A:301:NAD:N1A	2.28	0.48
1:A:94:ILE:HG23	2:A:301:NAD:N9A	2.28	0.48
1:C:5:LEU:HD12	1:C:5:LEU:O	2.13	0.48
1:F:46:LEU:O	1:F:50:VAL:HG23	2.14	0.48
1:C:243:ILE:HG23	1:F:249:TYR:O	2.13	0.48
1:F:42:PRO:HA	1:F:65:CYS:O	2.13	0.48
1:A:207:ARG:O	1:A:210:LEU:HB2	2.12	0.48
1:C:149:TYR:HB2	2:C:302:NAD:H5N	1.95	0.48
1:C:195:ILE:N	2:C:302:NAD:O7N	2.42	0.48
1:E:11:PHE:CE1	1:E:89:GLY:HA3	2.49	0.48
1:E:92:HIS:O	1:E:146:THR:HA	2.13	0.48
1:E:190:ILE:HD12	1:E:232:ALA:HB2	1.95	0.48
1:B:113:ASP:OD2	1:B:117:ILE:HD11	2.14	0.48
1:F:67:VAL:HA	1:F:73:ILE:HD11	1.96	0.48
1:B:22:ILE:O	1:B:26:ILE:CD1	2.61	0.48
1:B:101:THR:OG1	1:B:102:LEU:HD13	2.14	0.48
1:A:85:ASP:OD2	1:B:201:SER:HA	2.14	0.48
1:E:41:TYR:HD2	1:E:43:ASN:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:O	1:F:174:ARG:NH2	2.33	0.48
1:A:21:SER:HB2	1:A:24:TYR:HB3	1.96	0.47
1:B:143:CYS:SG	1:B:236:CYS:HA	2.54	0.47
1:C:260:SER:O	1:C:262:SER:N	2.46	0.47
1:D:94:ILE:HG12	2:D:301:NAD:C1B	2.43	0.47
1:E:154:ARG:NH1	1:F:154:ARG:HE	2.12	0.47
1:C:20:LEU:O	1:C:197:THR:HG22	2.15	0.47
1:F:24:TYR:CE1	1:F:53:PHE:HE1	2.31	0.47
1:F:152:SER:HB2	1:F:167:ALA:CA	2.44	0.47
1:E:115:PHE:HE2	1:E:164:MET:HE2	1.79	0.47
1:E:258:GLY:HA2	1:F:154:ARG:HD3	1.95	0.47
1:C:21:SER:HA	2:C:302:NAD:O3	2.15	0.47
1:D:4:GLY:HA3	1:D:33:GLU:OE1	2.14	0.47
1:D:49:ARG:HA	1:D:52:GLU:CG	2.45	0.47
1:E:26:ILE:C	1:E:30:LEU:HD12	2.33	0.47
1:F:42:PRO:HB2	1:F:43:ASN:HB3	1.94	0.47
1:F:65:CYS:O	2:F:302:NAD:H2A	2.14	0.47
1:F:98:PRO:CG	1:F:117:ILE:HD12	2.44	0.47
1:B:224:THR:OG1	1:B:226:GLU:OE1	2.30	0.47
1:D:90:VAL:HB	1:D:144:LEU:HD23	1.96	0.47
1:E:137:LEU:O	1:E:141:GLN:N	2.48	0.47
1:A:218:PRO:HB3	1:E:178:SER:HA	1.97	0.47
1:B:145:LEU:HD21	1:B:232:ALA:CB	2.43	0.47
1:E:6:LEU:HD13	1:E:11:PHE:HE2	1.79	0.47
1:E:140:ARG:O	1:E:141:GLN:HG2	2.13	0.47
1:F:225:ILE:H	1:F:225:ILE:CD1	2.21	0.47
1:C:39:PHE:HZ	1:C:57:PHE:HD2	1.63	0.47
1:D:85:ASP:CG	1:D:86:GLY:N	2.68	0.47
1:A:96:PHE:HB3	1:A:121:ILE:HG21	1.97	0.47
1:B:186:ARG:NH2	1:B:235:LEU:O	2.47	0.47
1:D:189:ALA:O	1:D:190:ILE:HD13	2.14	0.47
1:A:135:PRO:HD2	1:A:136:LEU:HD12	1.97	0.47
1:C:249:TYR:O	1:F:243:ILE:HG23	2.15	0.47
1:F:77:PHE:CE1	1:F:133:ALA:HB2	2.50	0.47
1:E:26:ILE:HD13	1:E:229:GLY:CA	2.37	0.46
1:E:77:PHE:CZ	1:E:133:ALA:HB2	2.49	0.46
1:C:152:SER:HB2	1:C:167:ALA:HB2	1.98	0.46
1:D:250:VAL:O	1:D:250:VAL:CG2	2.59	0.46
1:E:13:ILE:CD1	1:E:27:ALA:HB2	2.45	0.46
1:A:250:VAL:HG12	1:E:243:ILE:HG12	1.96	0.46
1:B:9:LYS:HD2	1:B:88:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:HE2	1:E:168:SER:HG	1.55	0.46
1:A:43:ASN:OD1	1:A:45:LYS:CB	2.61	0.46
1:A:106:PHE:HE1	1:A:164:MET:HE2	1.81	0.46
1:A:175:TYR:CD1	1:F:155:VAL:HG13	2.50	0.46
1:D:94:ILE:HG12	2:D:301:NAD:H1B	1.97	0.46
1:C:60:LYS:HE3	1:C:60:LYS:HB2	1.68	0.46
1:C:143:CYS:SG	1:C:236:CYS:HA	2.56	0.46
1:E:31:HIS:HD2	1:E:57:PHE:CD1	2.34	0.46
1:E:206:PHE:CE2	1:E:210:LEU:HD21	2.50	0.46
1:F:77:PHE:CZ	1:F:133:ALA:HB2	2.51	0.46
1:A:23:ALA:HA	1:A:26:ILE:HG22	1.97	0.46
1:A:47:LYS:O	1:A:51:ASP:OD1	2.33	0.46
1:B:186:ARG:NE	1:B:240:ALA:O	2.48	0.46
1:F:190:ILE:HG23	1:F:250:VAL:HG23	1.97	0.46
1:A:190:ILE:CD1	1:A:235:LEU:HD11	2.33	0.46
1:C:92:HIS:CE1	1:C:126:PHE:HB2	2.51	0.46
1:D:145:LEU:HD11	1:D:190:ILE:HG12	1.97	0.46
1:E:113:ASP:O	1:E:116:LYS:N	2.49	0.46
1:F:150:GLN:HB3	1:F:249:TYR:HE2	1.81	0.46
1:A:178:SER:HA	1:E:218:PRO:HB3	1.97	0.46
1:B:61:LEU:HD13	1:B:80:LEU:HD13	1.96	0.46
1:D:13:ILE:O	1:D:39:PHE:HA	2.16	0.46
1:E:52:GLU:HG2	1:E:56:GLN:HE21	1.81	0.46
1:B:106:PHE:CD1	1:B:160:ASN:HA	2.51	0.46
1:B:153:GLU:C	1:B:154:ARG:HG2	2.36	0.46
1:C:92:HIS:O	1:C:146:THR:HA	2.16	0.46
1:C:107:THR:CG2	1:E:180:LEU:HD21	2.32	0.46
1:D:21:SER:HA	2:D:301:NAD:PN	2.56	0.46
1:D:49:ARG:HA	1:D:52:GLU:HG3	1.96	0.46
1:E:90:VAL:HB	1:E:144:LEU:CD2	2.46	0.46
1:F:10:ARG:HB3	1:F:84:TRP:CH2	2.51	0.46
1:A:176:LEU:O	1:A:180:LEU:HD23	2.16	0.46
1:C:199:ALA:HB1	3:C:301:NUC:C13	2.46	0.46
1:F:85:ASP:C	1:F:85:ASP:OD2	2.55	0.46
1:F:143:CYS:SG	1:F:236:CYS:HA	2.56	0.46
1:A:126:PHE:CE1	1:A:144:LEU:HD22	2.51	0.45
1:C:142:GLY:O	1:C:185:ILE:HA	2.16	0.45
1:C:158:ASN:C	1:C:160:ASN:OD1	2.54	0.45
1:A:11:PHE:CD1	1:A:89:GLY:HA3	2.52	0.45
1:E:27:ALA:HA	1:E:30:LEU:CD1	2.46	0.45
1:E:87:VAL:O	1:E:137:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ILE:HG22	1:E:197:THR:CG2	2.46	0.45
1:F:94:ILE:HG23	2:F:302:NAD:N9A	2.31	0.45
1:A:63:PHE:CE2	1:A:80:LEU:HD23	2.51	0.45
1:C:159:TYR:OH	1:C:166:LYS:HE3	2.16	0.45
1:C:18:SER:CB	1:C:198:LEU:HD11	2.46	0.45
1:D:214:GLU:O	1:D:220:LYS:CA	2.62	0.45
1:F:51:ASP:O	1:F:62:VAL:HG21	2.17	0.45
1:F:134:LYS:O	1:F:138:GLN:HG3	2.17	0.45
1:A:252:ALA:C	1:E:244:THR:HG22	2.37	0.45
1:B:15:GLY:O	2:B:302:NAD:H4B	2.16	0.45
1:C:44:GLU:O	1:C:47:LYS:N	2.31	0.45
1:C:131:ARG:NH2	1:E:110:THR:O	2.50	0.45
1:C:259:MET:HE2	1:C:259:MET:HB2	1.69	0.45
1:E:13:ILE:HD11	1:E:30:LEU:HD13	1.98	0.45
1:E:19:LYS:HG3	1:E:53:PHE:HZ	1.80	0.45
1:F:25:GLY:CA	1:F:225:ILE:HG22	2.35	0.45
1:A:180:LEU:N	1:A:180:LEU:HD22	2.30	0.45
1:A:212:ALA:CB	1:C:259:MET:HE1	2.47	0.45
1:B:112:ARG:HA	1:B:112:ARG:HD2	1.42	0.45
1:E:26:ILE:HD12	1:E:232:ALA:HB3	1.91	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.88	0.45
1:A:179:SER:HB3	1:A:180:LEU:HD22	1.99	0.45
1:B:32:ARG:HB3	1:B:33:GLU:OE1	2.17	0.45
1:B:144:LEU:HB2	1:B:187:VAL:HG22	1.98	0.45
1:D:217:ALA:O	1:D:220:LYS:N	2.47	0.45
1:E:226:GLU:OE2	1:E:226:GLU:N	2.49	0.45
1:A:119:HIS:O	1:A:123:ALA:HB3	2.17	0.45
1:C:200:ALA:HB2	1:C:206:PHE:CZ	2.51	0.45
1:F:106:PHE:HD1	1:F:160:ASN:HB3	1.82	0.45
1:A:26:ILE:HA	1:A:229:GLY:CA	2.47	0.45
1:A:159:TYR:CZ	1:A:162:MET:HB3	2.51	0.45
1:D:190:ILE:HD12	1:D:248:LEU:HB3	1.98	0.45
1:E:44:GLU:O	1:E:47:LYS:HB2	2.16	0.45
1:A:21:SER:O	1:A:225:ILE:HG21	2.17	0.44
1:A:92:HIS:CD2	1:A:94:ILE:HD12	2.52	0.44
1:B:22:ILE:HG22	1:B:26:ILE:HD11	1.98	0.44
1:C:149:TYR:HB2	2:C:302:NAD:C5N	2.47	0.44
1:B:134:LYS:O	1:B:138:GLN:N	2.43	0.44
1:C:98:PRO:O	1:C:100:HIS:N	2.50	0.44
1:E:31:HIS:CD2	1:E:57:PHE:HB3	2.52	0.44
1:F:105:ASP:OD1	1:F:105:ASP:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:VAL:HG13	1:F:183:ASP:OD1	2.17	0.44
1:A:53:PHE:O	1:A:57:PHE:CD1	2.71	0.44
1:D:83:HIS:CD2	1:D:83:HIS:N	2.83	0.44
1:E:194:PRO:HB2	1:E:209:MET:HE1	1.99	0.44
1:E:195:ILE:O	1:E:197:THR:HG23	2.18	0.44
1:A:26:ILE:HG12	1:A:30:LEU:CD1	2.47	0.44
1:D:216:VAL:HB	1:D:254:PHE:CE2	2.52	0.44
1:F:200:ALA:C	1:F:203:ILE:HD13	2.38	0.44
1:C:77:PHE:CE2	1:C:133:ALA:HB2	2.53	0.44
1:C:79:GLU:OE2	1:C:79:GLU:HA	2.17	0.44
1:D:77:PHE:CZ	1:D:133:ALA:HB2	2.52	0.44
1:D:211:ASP:O	1:D:214:GLU:HG2	2.17	0.44
1:E:10:ARG:HG2	1:E:84:TRP:CZ2	2.53	0.44
1:E:218:PRO:HD2	1:E:252:ALA:O	2.17	0.44
1:F:22:ILE:O	1:F:26:ILE:HG13	2.18	0.44
1:A:21:SER:CB	1:A:24:TYR:CB	2.95	0.44
1:A:206:PHE:CE1	1:A:210:LEU:HD11	2.52	0.44
1:A:244:THR:HG21	1:E:219:LEU:HD13	1.98	0.44
1:D:11:PHE:HE1	1:D:89:GLY:HA3	1.80	0.44
1:D:93:SER:OG	1:D:93:SER:O	2.29	0.44
1:F:94:ILE:HG23	2:F:302:NAD:O4B	2.17	0.44
1:B:98:PRO:O	1:B:101:THR:HG23	2.18	0.44
1:B:114:GLY:O	1:B:118:ALA:HB2	2.17	0.44
1:D:220:LYS:HG3	1:D:220:LYS:HZ3	1.57	0.44
1:B:134:LYS:O	1:B:138:GLN:HG3	2.17	0.44
1:D:22:ILE:HD12	2:D:301:NAD:O5D	2.18	0.44
1:D:105:ASP:CG	1:D:108:ASP:H	2.20	0.44
1:D:123:ALA:HA	1:D:169:LEU:HD13	2.00	0.44
1:E:77:PHE:CE1	1:E:133:ALA:HB2	2.52	0.44
1:F:134:LYS:HB3	1:F:135:PRO:HD3	1.99	0.44
1:A:243:ILE:HD13	1:E:248:LEU:HD11	1.99	0.44
1:C:16:VAL:O	1:C:16:VAL:HG13	2.18	0.44
1:D:98:PRO:O	1:D:101:THR:N	2.51	0.44
1:D:105:ASP:HB3	1:D:108:ASP:H	1.83	0.44
1:F:186:ARG:HD2	1:F:243:ILE:O	2.17	0.44
1:A:44:GLU:O	1:A:45:LYS:C	2.56	0.43
1:A:200:ALA:HB2	1:A:206:PHE:CE2	2.53	0.43
1:B:124:TYR:CZ	1:B:128:ALA:HB2	2.53	0.43
1:C:234:PHE:CD2	1:C:235:LEU:HD22	2.52	0.43
1:D:143:CYS:SG	1:D:236:CYS:HA	2.58	0.43
1:F:80:LEU:HD13	1:F:80:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:VAL:HG21	1:F:189:ALA:HB2	2.00	0.43
1:A:33:GLU:CG	1:A:233:LEU:HD21	2.48	0.43
2:A:301:NAD:O1A	2:A:301:NAD:O3B	2.33	0.43
1:D:6:LEU:HB3	1:D:35:ALA:HB2	2.01	0.43
1:F:87:VAL:HG22	1:F:89:GLY:H	1.84	0.43
1:F:105:ASP:OD1	1:F:106:PHE:N	2.51	0.43
1:B:69:VAL:O	1:B:72:GLU:OE2	2.36	0.43
1:D:148:THR:OG1	1:D:149:TYR:N	2.50	0.43
1:E:42:PRO:CD	1:E:46:LEU:HD22	2.48	0.43
1:E:137:LEU:HD23	1:E:137:LEU:HA	1.82	0.43
1:B:224:THR:HG23	1:B:227:GLU:H	1.83	0.43
1:E:46:LEU:N	1:E:46:LEU:HD12	2.33	0.43
1:F:42:PRO:O	1:F:66:ASP:HB2	2.18	0.43
1:A:133:ALA:HA	1:A:136:LEU:HD13	2.01	0.43
1:C:63:PHE:CD1	1:C:63:PHE:N	2.86	0.43
1:E:87:VAL:CG1	1:E:136:LEU:HB3	2.44	0.43
1:A:99:ALA:CA	1:A:102:LEU:HD13	2.49	0.43
1:F:210:LEU:HD12	1:F:210:LEU:HA	1.86	0.43
1:A:154:ARG:HE	1:C:258:GLY:HA2	1.83	0.43
1:C:10:ARG:HA	1:C:36:GLU:O	2.18	0.43
1:A:21:SER:CB	1:A:24:TYR:HB2	2.45	0.43
1:C:253:GLY:CA	1:F:244:THR:HG22	2.47	0.43
1:D:39:PHE:CE2	1:D:54:ALA:HA	2.53	0.43
1:D:40:THR:OG1	1:D:65:CYS:CB	2.67	0.43
1:D:152:SER:HB3	1:D:167:ALA:N	2.33	0.43
1:D:198:LEU:HD12	1:D:198:LEU:HA	1.90	0.43
1:E:47:LYS:NZ	1:E:51:ASP:OD1	2.52	0.43
1:A:36:GLU:OE1	1:A:57:PHE:O	2.37	0.43
1:C:41:TYR:CD1	1:C:62:VAL:HG12	2.52	0.43
1:D:194:PRO:O	1:D:195:ILE:HG13	2.19	0.43
1:E:10:ARG:HG2	1:E:84:TRP:CE2	2.54	0.43
1:E:194:PRO:CB	1:E:209:MET:HE3	2.48	0.43
1:F:78:ALA:O	1:F:81:ALA:HB3	2.19	0.43
1:F:147:LEU:O	1:F:166:LYS:NZ	2.46	0.43
1:A:244:THR:HG21	1:E:219:LEU:HD11	2.00	0.43
1:B:147:LEU:HB3	2:B:302:NAD:O4D	2.19	0.43
1:C:47:LYS:HD2	1:C:51:ASP:OD2	2.19	0.43
1:C:102:LEU:HD12	1:C:102:LEU:N	2.34	0.43
1:C:155:VAL:HG11	1:E:178:SER:CB	2.48	0.43
1:E:63:PHE:CD1	1:E:79:GLU:HB3	2.54	0.43
1:E:190:ILE:HD11	1:E:232:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:HG2	1:B:53:PHE:CZ	2.54	0.42
1:B:131:ARG:NH1	1:B:131:ARG:CB	2.82	0.42
1:B:162:MET:CE	1:B:162:MET:CA	2.97	0.42
1:E:113:ASP:C	1:E:117:ILE:HD12	2.38	0.42
1:F:18:SER:OG	1:F:198:LEU:CD2	2.64	0.42
1:F:131:ARG:HB3	1:F:131:ARG:HH11	1.83	0.42
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.81	0.42
1:A:99:ALA:HA	1:A:102:LEU:HD13	2.01	0.42
1:A:258:GLY:N	1:C:155:VAL:O	2.49	0.42
1:D:176:LEU:HB2	1:D:187:VAL:HG11	2.02	0.42
1:E:17:ALA:HB3	1:E:198:LEU:HD12	1.99	0.42
1:E:203:ILE:HD13	1:E:203:ILE:HA	1.90	0.42
1:A:87:VAL:HG12	1:A:136:LEU:O	2.19	0.42
1:A:211:ASP:O	1:A:215:LYS:HG3	2.19	0.42
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.73	0.42
1:A:261:GLN:O	1:A:262:SER:C	2.57	0.42
1:F:261:GLN:O	1:F:262:SER:C	2.58	0.42
1:C:121:ILE:N	1:C:121:ILE:HD13	2.35	0.42
1:D:261:GLN:O	1:D:262:SER:C	2.57	0.42
1:F:80:LEU:HD12	1:F:136:LEU:CD1	2.50	0.42
1:F:52:GLU:CB	1:F:55:GLU:HB2	2.50	0.42
1:A:253:GLY:HA3	1:E:244:THR:HG23	2.02	0.42
1:B:261:GLN:O	1:B:262:SER:C	2.58	0.42
1:D:200:ALA:HA	1:D:206:PHE:CE2	2.55	0.42
1:D:200:ALA:C	1:D:203:ILE:HD12	2.40	0.42
1:A:138:GLN:HE21	1:A:138:GLN:HB3	1.60	0.42
1:C:13:ILE:CG1	1:C:37:LEU:HD22	2.49	0.42
1:B:94:ILE:HG23	2:B:302:NAD:C8A	2.49	0.42
1:C:47:LYS:CD	1:C:51:ASP:OD2	2.68	0.42
1:E:18:SER:HB3	1:E:198:LEU:HD11	2.01	0.42
1:E:80:LEU:HD11	1:E:84:TRP:HE3	1.84	0.42
1:C:235:LEU:HD21	1:C:248:LEU:CD1	2.50	0.41
1:E:13:ILE:O	1:E:39:PHE:HA	2.20	0.41
1:E:118:ALA:O	1:E:122:SER:OG	2.18	0.41
1:E:150:GLN:NE2	1:E:254:PHE:HD2	2.14	0.41
1:F:207:ARG:HA	1:F:210:LEU:CB	2.43	0.41
1:C:218:PRO:HB3	1:F:177:ALA:O	2.19	0.41
1:C:234:PHE:HD2	1:C:235:LEU:HD22	1.85	0.41
1:F:148:THR:HA	1:F:166:LYS:NZ	2.36	0.41
1:A:23:ALA:HA	1:A:26:ILE:HG21	2.01	0.41
1:A:57:PHE:CD1	1:A:57:PHE:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:CG	1:B:201:SER:HA	2.41	0.41
1:C:17:ALA:HB3	2:C:302:NAD:O1A	2.19	0.41
1:D:136:LEU:HD12	1:D:136:LEU:N	2.24	0.41
1:D:173:VAL:HG13	1:D:187:VAL:HG12	2.02	0.41
1:D:218:PRO:HD2	1:D:252:ALA:O	2.21	0.41
1:E:46:LEU:N	1:E:46:LEU:CD1	2.84	0.41
1:F:92:HIS:O	1:F:146:THR:HA	2.19	0.41
1:A:246:GLU:OE1	1:E:249:TYR:HB2	2.20	0.41
1:D:121:ILE:HD12	1:D:121:ILE:H	1.84	0.41
1:D:225:ILE:HD13	1:D:225:ILE:HG21	1.84	0.41
1:E:46:LEU:O	1:E:50:VAL:HG23	2.20	0.41
1:F:98:PRO:HG3	1:F:117:ILE:HD12	2.01	0.41
1:A:18:SER:O	1:A:21:SER:HB2	2.19	0.41
1:A:220:LYS:HA	1:A:220:LYS:HD2	1.83	0.41
1:B:98:PRO:HB2	1:B:101:THR:HG23	2.01	0.41
1:C:159:TYR:CZ	1:C:162:MET:HB3	2.55	0.41
1:D:203:ILE:HG21	3:D:302:NUC:C20	2.50	0.41
1:B:94:ILE:HG12	2:B:302:NAD:C1B	2.50	0.41
1:C:159:TYR:CE2	1:C:162:MET:HB3	2.55	0.41
1:E:102:LEU:HD23	1:E:102:LEU:N	2.34	0.41
1:A:125:SER:O	1:A:129:MET:HG3	2.20	0.41
1:A:141:GLN:OE1	1:A:141:GLN:CA	2.65	0.41
1:B:17:ALA:N	1:B:21:SER:OG	2.51	0.41
1:B:98:PRO:O	1:B:100:HIS:N	2.54	0.41
1:E:194:PRO:CB	1:E:209:MET:CE	2.98	0.41
1:A:217:ALA:O	1:A:220:LYS:HD3	2.21	0.41
1:B:67:VAL:HG12	2:B:302:NAD:N1A	2.36	0.41
1:B:199:ALA:HB1	3:B:301:NUC:C13	2.51	0.41
1:C:206:PHE:HA	1:C:209:MET:HB2	2.03	0.41
1:D:46:LEU:N	1:D:46:LEU:HD22	2.36	0.41
1:D:92:HIS:O	1:D:146:THR:HA	2.19	0.41
1:E:31:HIS:HD2	1:E:57:PHE:HD1	1.69	0.41
1:F:216:VAL:HG13	1:F:257:VAL:HG11	2.02	0.41
1:A:149:TYR:HD1	1:A:159:TYR:CZ	2.39	0.41
1:A:207:ARG:HH11	1:A:207:ARG:HD2	1.65	0.41
1:C:171:ALA:HB3	1:E:164:MET:HA	2.02	0.41
1:D:97:ALA:HB3	1:D:102:LEU:HD11	2.02	0.41
1:D:195:ILE:HD12	1:D:223:VAL:HG23	2.01	0.41
1:E:11:PHE:HE1	1:E:89:GLY:HA3	1.86	0.41
1:F:5:LEU:N	1:F:33:GLU:HG3	2.33	0.41
1:A:97:ALA:O	1:A:99:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HB2	1:A:252:ALA:HB1	2.03	0.41
1:B:117:ILE:HD12	1:B:117:ILE:H	1.86	0.41
1:E:170:GLU:HG2	1:E:247:ILE:CD1	2.47	0.41
2:B:302:NAD:H2D	2:B:302:NAD:H2N	1.65	0.40
1:D:41:TYR:CE2	1:D:47:LYS:HG2	2.56	0.40
1:D:102:LEU:HD21	3:D:302:NUC:C5	2.51	0.40
1:E:13:ILE:HD12	1:E:27:ALA:HB2	2.03	0.40
1:F:21:SER:HA	2:F:302:NAD:O3	2.21	0.40
1:A:180:LEU:HB3	1:A:185:ILE:HB	2.03	0.40
1:C:98:PRO:HB2	1:C:100:HIS:CE1	2.56	0.40
1:D:44:GLU:O	1:D:47:LYS:N	2.51	0.40
1:D:66:ASP:OD1	1:D:68:ALA:HB3	2.21	0.40
1:D:248:LEU:HD23	1:D:249:TYR:N	2.36	0.40
1:F:98:PRO:O	1:F:100:HIS:N	2.54	0.40
1:F:135:PRO:HD2	4:F:402:HOH:O	2.20	0.40
1:A:10:ARG:HB3	1:A:84:TRP:CH2	2.56	0.40
1:B:51:ASP:O	1:B:55:GLU:OE1	2.38	0.40
1:C:80:LEU:O	1:C:80:LEU:HG	2.20	0.40
1:C:178:SER:HA	1:F:218:PRO:HB3	2.03	0.40
1:C:195:ILE:HD11	1:C:223:VAL:HG23	2.03	0.40
1:E:48:LYS:C	1:E:48:LYS:HD3	2.41	0.40
1:A:12:LEU:HD23	1:A:90:VAL:HG13	2.04	0.40
1:F:67:VAL:HG22	2:F:302:NAD:C2A	2.50	0.40
1:B:87:VAL:HG12	1:B:137:LEU:HA	2.02	0.40
1:C:25:GLY:HA3	1:C:225:ILE:HB	2.03	0.40
1:C:131:ARG:NH1	1:C:131:ARG:HB3	2.36	0.40
1:E:137:LEU:HD22	1:E:142:GLY:CA	2.52	0.40
1:F:42:PRO:HB3	2:F:302:NAD:C2A	2.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:O	1:C:207:ARG:NH2[4_555]	1.97	0.23
1:B:107:THR:OG1	1:D:179:SER:OG[1_556]	2.01	0.19
1:A:207:ARG:NH2	1:B:82:LYS:O[1_545]	2.06	0.14
1:B:68:ALA:O	1:D:112:ARG:NH1[1_556]	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	257/271 (95%)	244 (95%)	10 (4%)	3 (1%)	11	19
1	B	248/271 (92%)	236 (95%)	11 (4%)	1 (0%)	30	48
1	C	258/271 (95%)	244 (95%)	12 (5%)	2 (1%)	16	30
1	D	254/271 (94%)	242 (95%)	10 (4%)	2 (1%)	16	30
1	E	258/271 (95%)	244 (95%)	12 (5%)	2 (1%)	16	30
1	F	258/271 (95%)	241 (93%)	14 (5%)	3 (1%)	11	19
All	All	1533/1626 (94%)	1451 (95%)	69 (4%)	13 (1%)	16	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	45	LYS
1	B	99	ALA
1	C	99	ALA
1	C	261	GLN
1	D	85	ASP
1	D	99	ALA
1	E	99	ALA
1	F	43	ASN
1	F	99	ALA
1	F	261	GLN
1	E	259	MET
1	A	206	PHE

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	188/208 (90%)	176 (94%)	12 (6%)	14	26
1	B	181/208 (87%)	171 (94%)	10 (6%)	18	32
1	C	191/208 (92%)	179 (94%)	12 (6%)	15	27
1	D	188/208 (90%)	177 (94%)	11 (6%)	16	29
1	E	193/208 (93%)	188 (97%)	5 (3%)	41	62
1	F	194/208 (93%)	186 (96%)	8 (4%)	26	45
All	All	1135/1248 (91%)	1077 (95%)	58 (5%)	20	36

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	21	SER
1	A	41	TYR
1	A	79	GLU
1	A	116	LYS
1	A	148	THR
1	A	153	GLU
1	A	178	SER
1	A	183	ASP
1	A	196	ARG
1	A	207	ARG
1	A	255	ASN
1	B	36	GLU
1	B	44	GLU
1	B	52	GLU
1	B	72	GLU
1	B	88	ASP
1	B	112	ARG
1	B	154	ARG
1	B	156	MET
1	B	168	SER
1	B	206	PHE
1	C	47	LYS
1	C	49	ARG
1	C	52	GLU
1	C	56	GLN
1	C	147	LEU

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Mol	Chain	Res	Type
1	C	154	ARG
1	C	160	ASN
1	C	183	ASP
1	C	196	ARG
1	C	206	PHE
1	C	209	MET
1	C	260	SER
1	D	5	LEU
1	D	52	GLU
1	D	55	GLU
1	D	85	ASP
1	D	101	THR
1	D	112	ARG
1	D	119	HIS
1	D	122	SER
1	D	157	PRO
1	D	221	ARG
1	D	223	VAL
1	E	31	HIS
1	E	93	SER
1	E	119	HIS
1	E	178	SER
1	E	220	LYS
1	F	43	ASN
1	F	52	GLU
1	F	53	PHE
1	F	85	ASP
1	F	93	SER
1	F	144	LEU
1	F	207	ARG
1	F	260	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	GLN
1	C	138	GLN
1	D	83	HIS
1	E	31	HIS
1	E	138	GLN
1	E	150	GLN
1	E	213	ASN

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Mol	Chain	Res	Type
1	F	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	A	301	-	42,48,48	4.45	15 (35%)	50,73,73	1.65	6 (12%)
3	NUC	A	302	-	29,33,33	1.06	2 (6%)	28,47,47	1.40	3 (10%)
3	NUC	C	301	-	29,33,33	1.05	2 (6%)	28,47,47	2.00	6 (21%)
3	NUC	E	301	-	29,33,33	1.07	2 (6%)	28,47,47	1.46	4 (14%)
2	NAD	D	301	-	42,48,48	4.36	15 (35%)	50,73,73	1.65	6 (12%)
2	NAD	B	302	-	42,48,48	4.37	15 (35%)	50,73,73	1.54	6 (12%)
3	NUC	B	301	-	29,33,33	1.06	2 (6%)	28,47,47	1.40	3 (10%)
3	NUC	D	302	-	29,33,33	1.05	2 (6%)	28,47,47	1.40	3 (10%)
2	NAD	C	302	-	42,48,48	4.45	15 (35%)	50,73,73	1.69	6 (12%)
2	NAD	E	302	-	42,48,48	4.39	15 (35%)	50,73,73	2.03	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	F	302	-	42,48,48	4.35	16 (38%)	50,73,73	1.74	7 (14%)
3	NUC	F	301	-	29,33,33	1.10	2 (6%)	28,47,47	1.63	4 (14%)

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	A	301	-	-	10/26/62/62	0/5/5/5
3	NUC	A	302	-	-	7/11/26/26	0/4/4/4
3	NUC	C	301	-	-	8/11/26/26	0/4/4/4
3	NUC	E	301	-	-	7/11/26/26	0/4/4/4
2	NAD	D	301	-	-	9/26/62/62	0/5/5/5
2	NAD	B	302	-	-	13/26/62/62	0/5/5/5
3	NUC	B	301	-	-	6/11/26/26	0/4/4/4
3	NUC	D	302	-	-	7/11/26/26	0/4/4/4
2	NAD	C	302	-	-	7/26/62/62	0/5/5/5
2	NAD	E	302	-	-	8/26/62/62	0/5/5/5
2	NAD	F	302	-	-	13/26/62/62	0/5/5/5
3	NUC	F	301	-	-	6/11/26/26	0/4/4/4

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	O4D-C1D	15.55	1.61	1.40
2	B	302	NAD	O4D-C1D	15.51	1.61	1.40
2	C	302	NAD	O4D-C1D	15.49	1.61	1.40
2	E	302	NAD	O4D-C1D	15.37	1.61	1.40
2	D	301	NAD	O4D-C1D	15.21	1.60	1.40
2	F	302	NAD	O4D-C1D	14.99	1.60	1.40
2	C	302	NAD	O4B-C1B	10.69	1.54	1.40
2	A	301	NAD	O4B-C1B	10.67	1.54	1.40
2	C	302	NAD	C7N-N7N	10.65	1.52	1.33
2	B	302	NAD	C7N-N7N	10.64	1.52	1.33
2	F	302	NAD	C7N-N7N	10.63	1.52	1.33
2	D	301	NAD	C7N-N7N	10.63	1.52	1.33
2	B	302	NAD	O4B-C1B	10.62	1.54	1.40
2	E	302	NAD	O4B-C1B	10.61	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	302	NAD	C7N-N7N	10.60	1.52	1.33
2	D	301	NAD	O4B-C1B	10.59	1.54	1.40
2	A	301	NAD	C7N-N7N	10.57	1.52	1.33
2	D	301	NAD	C3B-C4B	-10.35	1.26	1.53
2	F	302	NAD	C3B-C4B	-10.30	1.26	1.53
2	A	301	NAD	C3B-C4B	-10.28	1.26	1.53
2	F	302	NAD	O4B-C1B	10.28	1.54	1.40
2	E	302	NAD	C3B-C4B	-10.23	1.27	1.53
2	B	302	NAD	C3B-C4B	-10.23	1.27	1.53
2	C	302	NAD	C3B-C4B	-10.22	1.27	1.53
2	A	301	NAD	PN-O3	7.69	1.67	1.59
2	C	302	NAD	PN-O3	7.12	1.67	1.59
2	E	302	NAD	PN-O3	7.05	1.67	1.59
2	D	301	NAD	PN-O3	6.70	1.66	1.59
2	F	302	NAD	PN-O3	6.70	1.66	1.59
2	B	302	NAD	PN-O3	6.51	1.66	1.59
2	F	302	NAD	O4D-C4D	-6.44	1.30	1.45
2	C	302	NAD	O4D-C4D	-6.36	1.30	1.45
2	A	301	NAD	O4D-C4D	-6.31	1.31	1.45
2	D	301	NAD	O4D-C4D	-6.24	1.31	1.45
2	B	302	NAD	O4D-C4D	-6.04	1.31	1.45
2	E	302	NAD	O4D-C4D	-6.03	1.31	1.45
2	E	302	NAD	O4B-C4B	5.67	1.57	1.45
2	B	302	NAD	O4B-C4B	5.66	1.57	1.45
2	F	302	NAD	PA-O3	5.63	1.65	1.59
2	C	302	NAD	O4B-C4B	5.56	1.57	1.45
2	E	302	NAD	PA-O3	5.56	1.65	1.59
2	C	302	NAD	PA-O3	5.55	1.65	1.59
2	A	301	NAD	O4B-C4B	5.47	1.57	1.45
2	D	301	NAD	O4B-C4B	5.40	1.57	1.45
2	F	302	NAD	O4B-C4B	5.31	1.56	1.45
2	C	302	NAD	C2B-C3B	5.31	1.67	1.53
2	A	301	NAD	C2B-C3B	5.28	1.67	1.53
2	F	302	NAD	C2B-C3B	5.27	1.67	1.53
2	E	302	NAD	C2B-C3B	5.26	1.67	1.53
2	B	302	NAD	C2B-C3B	5.21	1.67	1.53
2	D	301	NAD	C2B-C3B	5.12	1.67	1.53
2	B	302	NAD	PA-O3	4.96	1.64	1.59
2	D	301	NAD	PA-O3	4.96	1.64	1.59
2	A	301	NAD	PA-O3	4.91	1.64	1.59
2	A	301	NAD	PN-O5D	3.13	1.71	1.59
2	A	301	NAD	O2D-C2D	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	NUC	C1-N4	2.99	1.39	1.35
2	C	302	NAD	O2D-C2D	2.98	1.50	1.43
2	C	302	NAD	PN-O5D	2.96	1.71	1.59
3	C	301	NUC	C1-N4	2.94	1.39	1.35
2	D	301	NAD	PN-O5D	2.88	1.70	1.59
2	F	302	NAD	O3D-C3D	-2.84	1.35	1.43
2	F	302	NAD	PN-O5D	2.77	1.70	1.59
2	B	302	NAD	O3D-C3D	-2.77	1.36	1.43
2	A	301	NAD	O3D-C3D	-2.76	1.36	1.43
2	D	301	NAD	O3D-C3D	-2.74	1.36	1.43
2	C	302	NAD	O3D-C3D	-2.74	1.36	1.43
2	E	302	NAD	O3D-C3D	-2.73	1.36	1.43
3	D	302	NUC	C1-N4	2.64	1.38	1.35
3	E	301	NUC	C1-N4	2.63	1.38	1.35
3	A	302	NUC	C1-N4	2.61	1.38	1.35
2	B	302	NAD	PN-O5D	2.54	1.69	1.59
2	E	302	NAD	PN-O5D	2.54	1.69	1.59
3	B	301	NUC	C1-N4	2.53	1.38	1.35
2	F	302	NAD	C6A-N6A	2.52	1.43	1.34
2	D	301	NAD	O2D-C2D	2.51	1.49	1.43
2	C	302	NAD	C6A-N6A	2.51	1.43	1.34
2	A	301	NAD	O7N-C7N	-2.51	1.19	1.24
2	A	301	NAD	C6A-N6A	2.50	1.43	1.34
2	E	302	NAD	C6A-N6A	2.49	1.43	1.34
2	D	301	NAD	O7N-C7N	-2.48	1.19	1.24
2	B	302	NAD	C6A-N6A	2.48	1.43	1.34
2	D	301	NAD	C6A-N6A	2.48	1.43	1.34
2	F	302	NAD	O7N-C7N	-2.44	1.19	1.24
2	E	302	NAD	O2D-C2D	2.43	1.49	1.43
2	B	302	NAD	O7N-C7N	-2.42	1.19	1.24
2	F	302	NAD	O2D-C2D	2.41	1.48	1.43
2	E	302	NAD	O7N-C7N	-2.41	1.19	1.24
2	B	302	NAD	O2D-C2D	2.41	1.48	1.43
2	C	302	NAD	O7N-C7N	-2.40	1.19	1.24
2	C	302	NAD	C5B-C4B	2.38	1.58	1.51
2	A	301	NAD	C5B-C4B	2.37	1.58	1.51
2	B	302	NAD	C5B-C4B	2.27	1.58	1.51
3	A	302	NUC	C18-C23	-2.25	1.38	1.43
3	C	301	NUC	C18-C23	-2.24	1.38	1.43
3	B	301	NUC	C18-C23	-2.22	1.38	1.43
2	D	301	NAD	C5B-C4B	2.22	1.58	1.51
2	E	302	NAD	C5B-C4B	2.21	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	NUC	C18-C23	-2.21	1.38	1.43
3	E	301	NUC	C18-C23	-2.21	1.38	1.43
3	D	302	NUC	C18-C23	-2.20	1.38	1.43
2	F	302	NAD	C5B-C4B	2.14	1.58	1.51
2	F	302	NAD	PA-O5B	2.10	1.67	1.59

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302	NAD	C4B-O4B-C1B	-10.53	100.29	109.92
2	B	302	NAD	C4B-O4B-C1B	-6.96	103.56	109.92
2	F	302	NAD	C4B-O4B-C1B	-6.57	103.91	109.92
2	A	301	NAD	C4B-O4B-C1B	-6.36	104.10	109.92
2	C	302	NAD	C4B-O4B-C1B	-6.28	104.17	109.92
2	D	301	NAD	C4B-O4B-C1B	-6.02	104.41	109.92
3	C	301	NUC	C8-C7-N2	5.81	127.14	116.15
2	F	302	NAD	C4D-O4D-C1D	-5.63	104.77	109.92
2	C	302	NAD	C4D-O4D-C1D	-5.38	105.00	109.92
3	C	301	NUC	O2-C7-N2	-5.32	112.85	121.61
2	D	301	NAD	C4D-O4D-C1D	-5.03	105.32	109.92
2	E	302	NAD	N3A-C2A-N1A	-4.89	122.04	128.67
2	B	302	NAD	N3A-C2A-N1A	-4.78	122.18	128.67
2	D	301	NAD	N3A-C2A-N1A	-4.78	122.18	128.67
2	A	301	NAD	N3A-C2A-N1A	-4.75	122.22	128.67
2	F	302	NAD	N3A-C2A-N1A	-4.74	122.24	128.67
2	C	302	NAD	N3A-C2A-N1A	-4.71	122.28	128.67
2	A	301	NAD	C4D-O4D-C1D	-4.55	105.76	109.92
3	E	301	NUC	C2-C1-N4	4.05	120.64	117.91
3	F	301	NUC	O2-C7-N2	-4.05	114.95	121.61
3	F	301	NUC	C8-C7-N2	3.92	123.56	116.15
3	D	302	NUC	C2-C1-N4	3.83	120.49	117.91
2	E	302	NAD	C4D-O4D-C1D	-3.73	106.51	109.92
2	E	302	NAD	O4B-C1B-N9A	3.45	113.32	108.75
3	B	301	NUC	C2-C1-N4	3.42	120.21	117.91
3	A	302	NUC	O2-C7-N2	-3.39	116.02	121.61
3	B	301	NUC	O2-C7-N2	-3.37	116.06	121.61
3	E	301	NUC	O2-C7-N2	-3.34	116.11	121.61
3	D	302	NUC	O2-C7-N2	-3.25	116.27	121.61
2	D	301	NAD	C2B-C3B-C4B	3.14	108.69	102.61
3	C	301	NUC	C2-C1-N4	3.14	120.02	117.91
3	F	301	NUC	C2-C1-N4	3.14	120.02	117.91
3	A	302	NUC	C2-C1-N4	3.11	120.00	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	NUC	C10-C9-C8	-3.11	108.35	112.13
2	A	301	NAD	C2B-C3B-C4B	2.97	108.34	102.61
2	C	302	NAD	C2B-C3B-C4B	2.94	108.29	102.61
2	F	302	NAD	C2B-C3B-C4B	2.65	107.72	102.61
3	A	302	NUC	C8-C7-N2	2.64	121.15	116.15
2	B	302	NAD	C4D-O4D-C1D	-2.53	107.61	109.92
3	F	301	NUC	C9-C10-C11	-2.52	107.98	113.48
2	A	301	NAD	C5N-C4N-C3N	-2.52	117.89	120.36
3	D	302	NUC	C8-C7-N2	2.51	120.90	116.15
3	B	301	NUC	C8-C7-N2	2.51	120.90	116.15
2	B	302	NAD	C2B-C3B-C4B	2.50	107.45	102.61
2	B	302	NAD	C5N-C4N-C3N	-2.47	117.93	120.36
3	E	301	NUC	C8-C7-N2	2.42	120.72	116.15
2	E	302	NAD	C4A-C5A-N7A	-2.38	106.82	109.34
2	D	301	NAD	C5N-C4N-C3N	-2.37	118.03	120.36
2	C	302	NAD	C4A-C5A-N7A	-2.37	106.83	109.34
2	A	301	NAD	C4A-C5A-N7A	-2.35	106.86	109.34
2	F	302	NAD	C4A-C5A-N7A	-2.34	106.87	109.34
2	C	302	NAD	C5N-C4N-C3N	-2.28	118.12	120.36
2	E	302	NAD	C2B-C3B-C4B	2.25	106.95	102.61
2	F	302	NAD	C5N-C4N-C3N	-2.25	118.16	120.36
2	D	301	NAD	C4A-C5A-N7A	-2.23	106.98	109.34
3	C	301	NUC	C9-C10-C11	-2.21	108.66	113.48
2	B	302	NAD	C4A-C5A-N7A	-2.15	107.07	109.34
2	E	302	NAD	C5N-C4N-C3N	-2.13	118.27	120.36
3	C	301	NUC	C4-C5-N1	-2.12	122.39	124.39
2	F	302	NAD	O2N-PN-O5D	2.02	116.71	107.57
3	E	301	NUC	O1-C1-N4	-2.01	116.88	121.57

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O3
2	B	302	NAD	C5D-O5D-PN-O3
2	B	302	NAD	C5D-O5D-PN-O2N
2	B	302	NAD	O4D-C1D-N1N-C2N
2	B	302	NAD	O4D-C1D-N1N-C6N
2	B	302	NAD	C2D-C1D-N1N-C2N
2	B	302	NAD	C2D-C1D-N1N-C6N
2	D	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	D	301	NAD	C5D-O5D-PN-O2N
2	E	302	NAD	C5D-O5D-PN-O3
2	E	302	NAD	C5D-O5D-PN-O1N
2	E	302	NAD	O4D-C1D-N1N-C2N
2	F	302	NAD	C5D-O5D-PN-O3
2	F	302	NAD	C5D-O5D-PN-O1N
2	F	302	NAD	C5D-O5D-PN-O2N
3	A	302	NUC	N4-C1-C2-C3
3	A	302	NUC	O1-C1-C2-C3
3	A	302	NUC	C2-C1-N4-C13
3	A	302	NUC	C2-C1-N4-C14
3	A	302	NUC	O1-C1-N4-C13
3	A	302	NUC	O1-C1-N4-C14
3	B	301	NUC	N4-C1-C2-C3
3	B	301	NUC	O1-C1-C2-C3
3	B	301	NUC	C2-C1-N4-C13
3	B	301	NUC	C2-C1-N4-C14
3	B	301	NUC	O1-C1-N4-C13
3	B	301	NUC	O1-C1-N4-C14
3	C	301	NUC	C2-C1-N4-C13
3	C	301	NUC	C2-C1-N4-C14
3	C	301	NUC	O1-C1-N4-C13
3	C	301	NUC	O1-C1-N4-C14
3	C	301	NUC	C15-C14-N4-C1
3	D	302	NUC	N4-C1-C2-C3
3	D	302	NUC	O1-C1-C2-C3
3	D	302	NUC	C2-C1-N4-C13
3	D	302	NUC	C2-C1-N4-C14
3	D	302	NUC	O1-C1-N4-C13
3	D	302	NUC	O1-C1-N4-C14
3	E	301	NUC	N4-C1-C2-C3
3	E	301	NUC	O1-C1-C2-C3
3	E	301	NUC	C2-C1-N4-C13
3	E	301	NUC	C2-C1-N4-C14
3	E	301	NUC	O1-C1-N4-C13
3	E	301	NUC	O1-C1-N4-C14
3	F	301	NUC	C2-C1-N4-C13
3	F	301	NUC	C2-C1-N4-C14
3	F	301	NUC	O1-C1-N4-C13
3	F	301	NUC	O1-C1-N4-C14
2	A	301	NAD	O4B-C4B-C5B-O5B
2	C	302	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	301	NAD	O4B-C4B-C5B-O5B
2	F	302	NAD	O4B-C4B-C5B-O5B
3	C	301	NUC	O1-C1-C2-C3
3	F	301	NUC	O1-C1-C2-C3
2	A	301	NAD	C3B-C4B-C5B-O5B
2	C	302	NAD	C3B-C4B-C5B-O5B
2	D	301	NAD	C3B-C4B-C5B-O5B
2	F	302	NAD	C3B-C4B-C5B-O5B
3	C	301	NUC	N4-C1-C2-C3
3	F	301	NUC	N4-C1-C2-C3
2	B	302	NAD	O4D-C4D-C5D-O5D
2	B	302	NAD	C3D-C4D-C5D-O5D
2	F	302	NAD	PN-O3-PA-O1A
2	D	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	PA-O3-PN-O5D
2	B	302	NAD	PN-O3-PA-O5B
2	C	302	NAD	PN-O3-PA-O5B
2	C	302	NAD	PA-O3-PN-O5D
2	D	301	NAD	PA-O3-PN-O5D
2	E	302	NAD	PN-O3-PA-O5B
2	F	302	NAD	PN-O3-PA-O5B
2	F	302	NAD	PA-O3-PN-O5D
3	A	302	NUC	C15-C14-N4-C13
3	C	301	NUC	C15-C14-N4-C13
3	D	302	NUC	C15-C14-N4-C13
3	E	301	NUC	C15-C14-N4-C13
2	F	302	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	C5D-O5D-PN-O1N
2	B	302	NAD	C5B-O5B-PA-O1A
2	B	302	NAD	C5D-O5D-PN-O1N
2	C	302	NAD	C5D-O5D-PN-O3
2	C	302	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	E	302	NAD	C5D-O5D-PN-O2N
2	C	302	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	PN-O3-PA-O1A
2	E	302	NAD	O4D-C1D-N1N-C6N
2	F	302	NAD	O4D-C1D-N1N-C2N
2	F	302	NAD	O4D-C1D-N1N-C6N
2	B	302	NAD	PA-O3-PN-O1N

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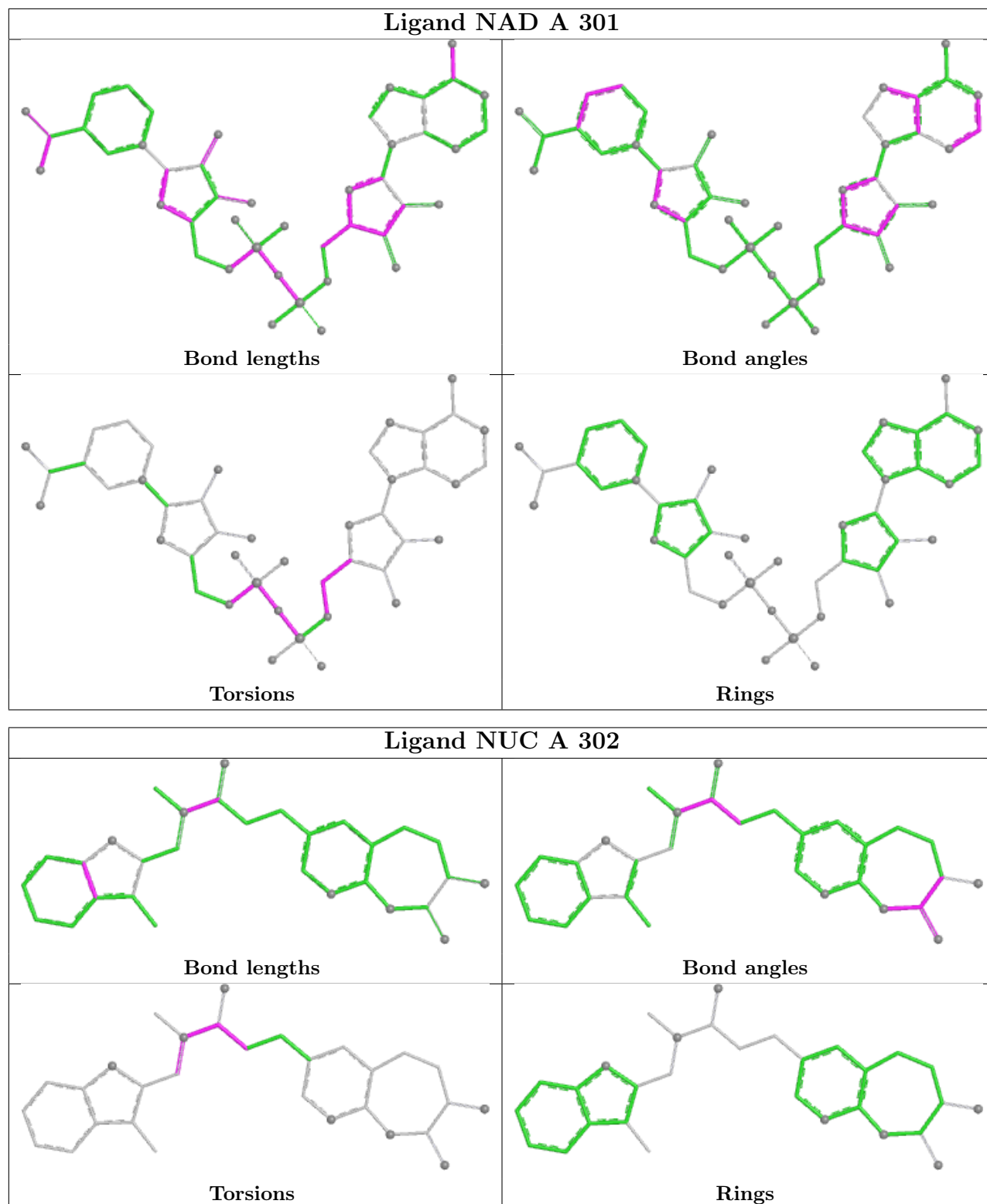
Mol	Chain	Res	Type	Atoms
2	A	301	NAD	PN-O3-PA-O5B
2	B	302	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	PA-O3-PN-O1N
2	A	301	NAD	PA-O3-PN-O2N
2	E	302	NAD	PA-O3-PN-O2N
2	F	302	NAD	PA-O3-PN-O1N
2	F	302	NAD	PA-O3-PN-O2N
2	E	302	NAD	O4B-C4B-C5B-O5B

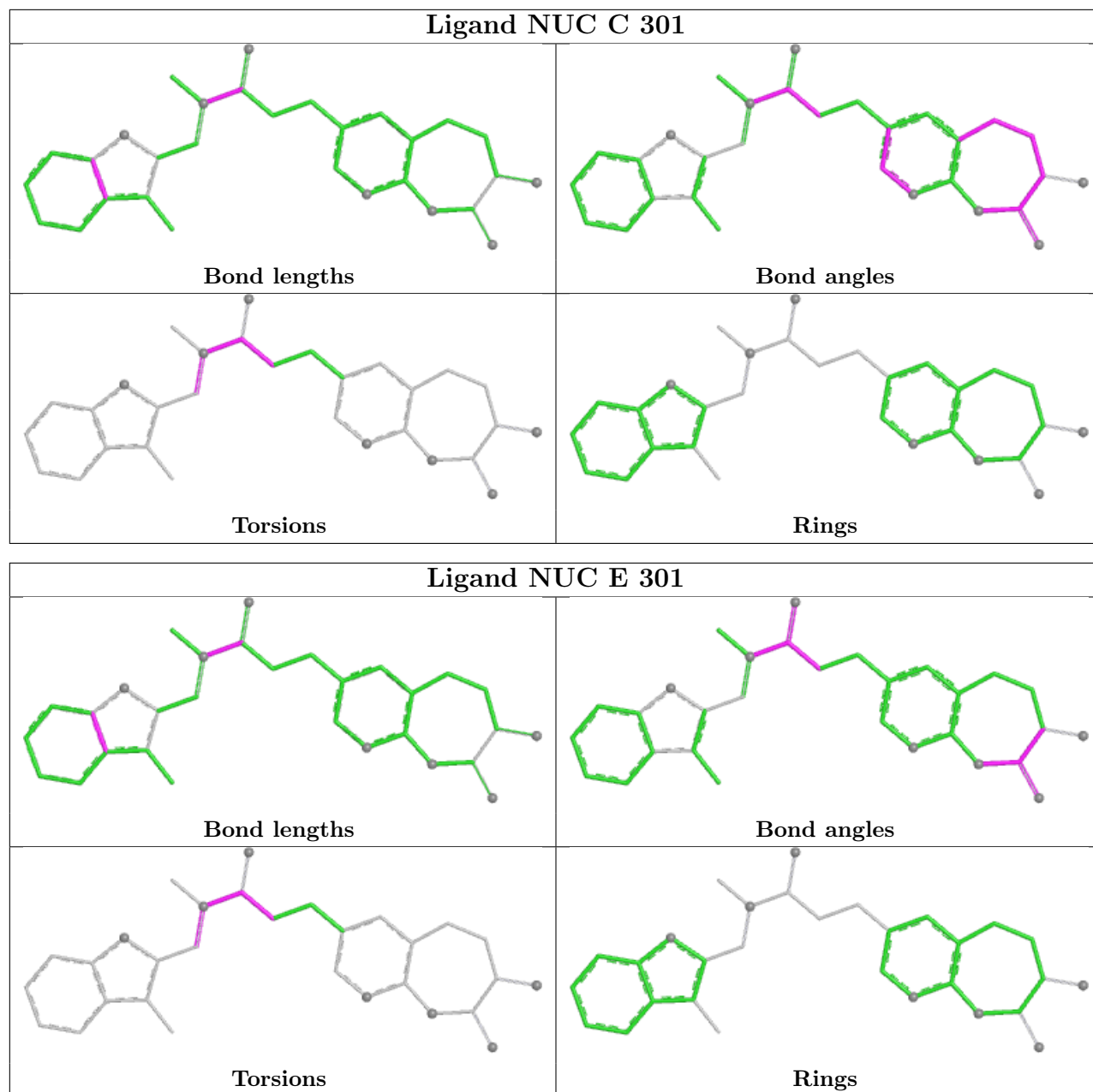
There are no ring outliers.

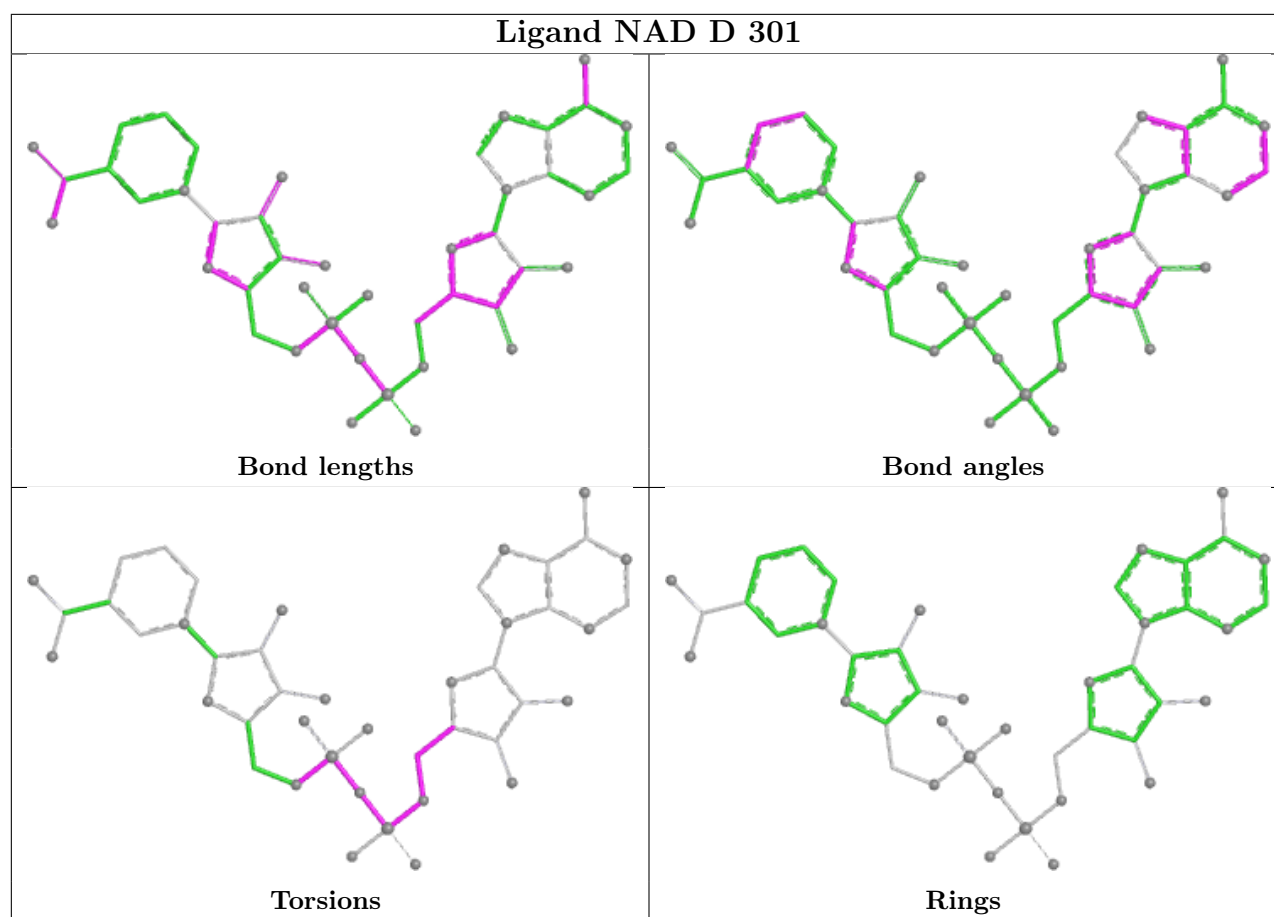
10 monomers are involved in 64 short contacts:

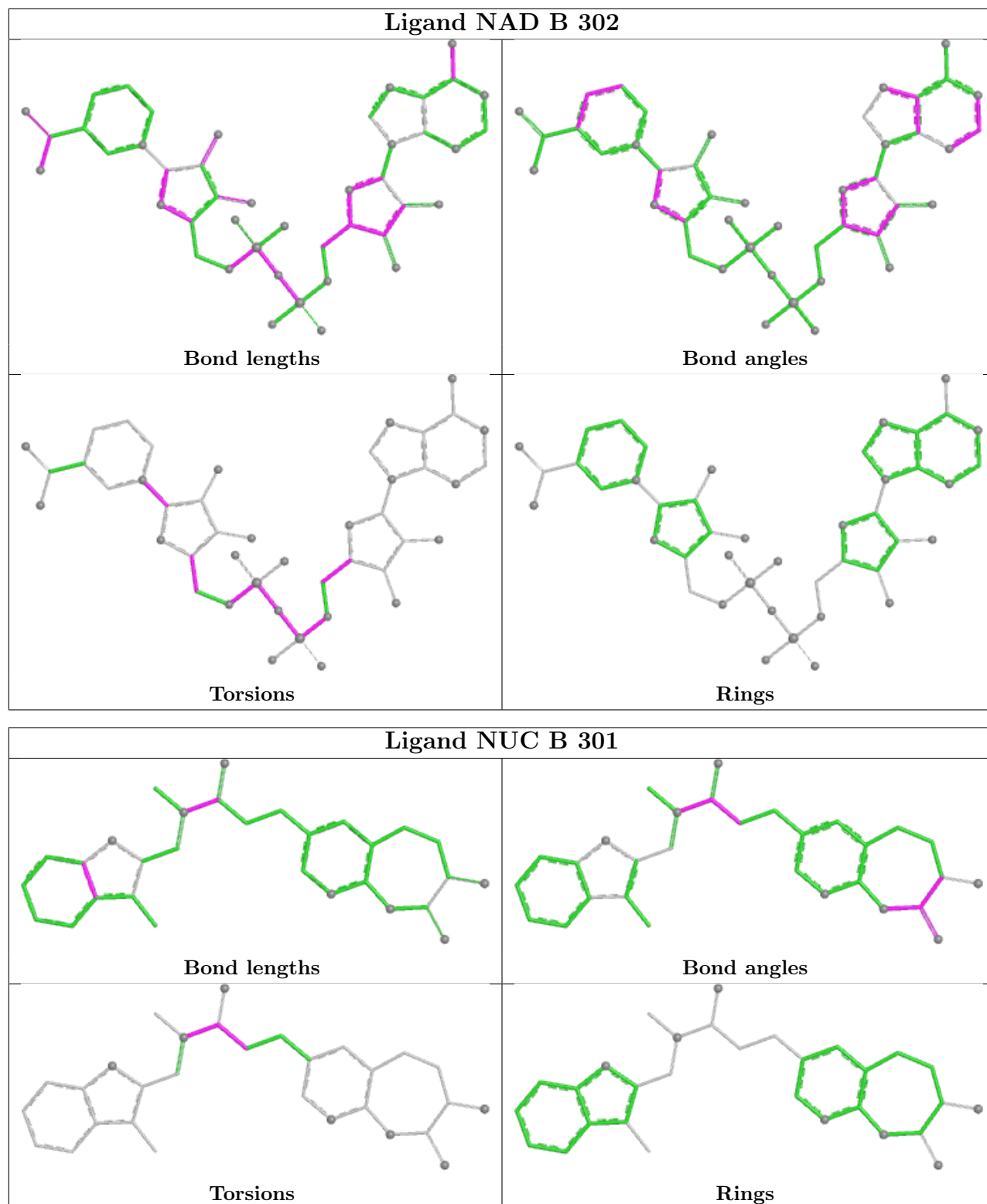
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	10	0
3	C	301	NUC	2	0
2	D	301	NAD	13	0
2	B	302	NAD	10	0
3	B	301	NUC	1	0
3	D	302	NUC	3	0
2	C	302	NAD	9	0
2	E	302	NAD	4	0
2	F	302	NAD	11	0
3	F	301	NUC	1	0

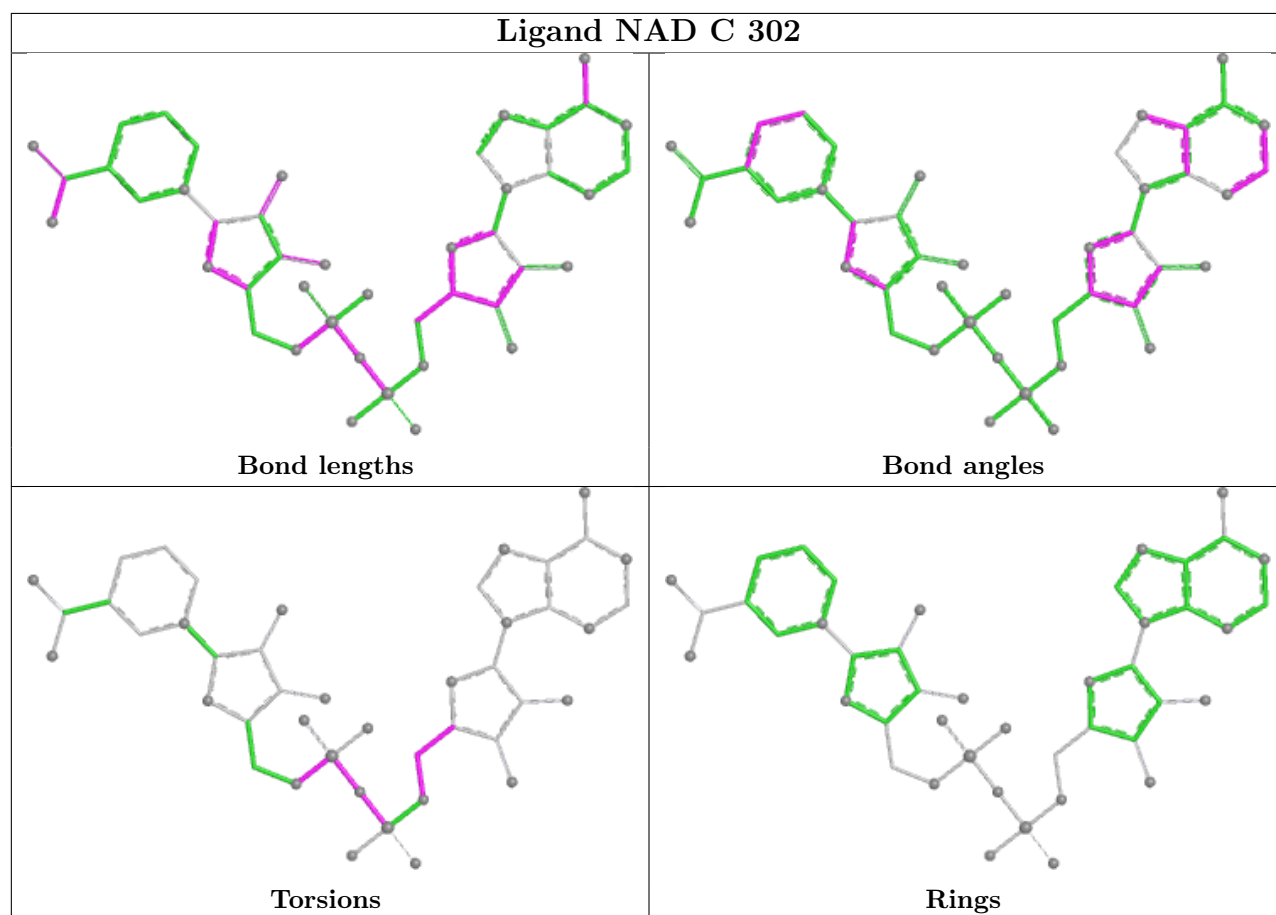
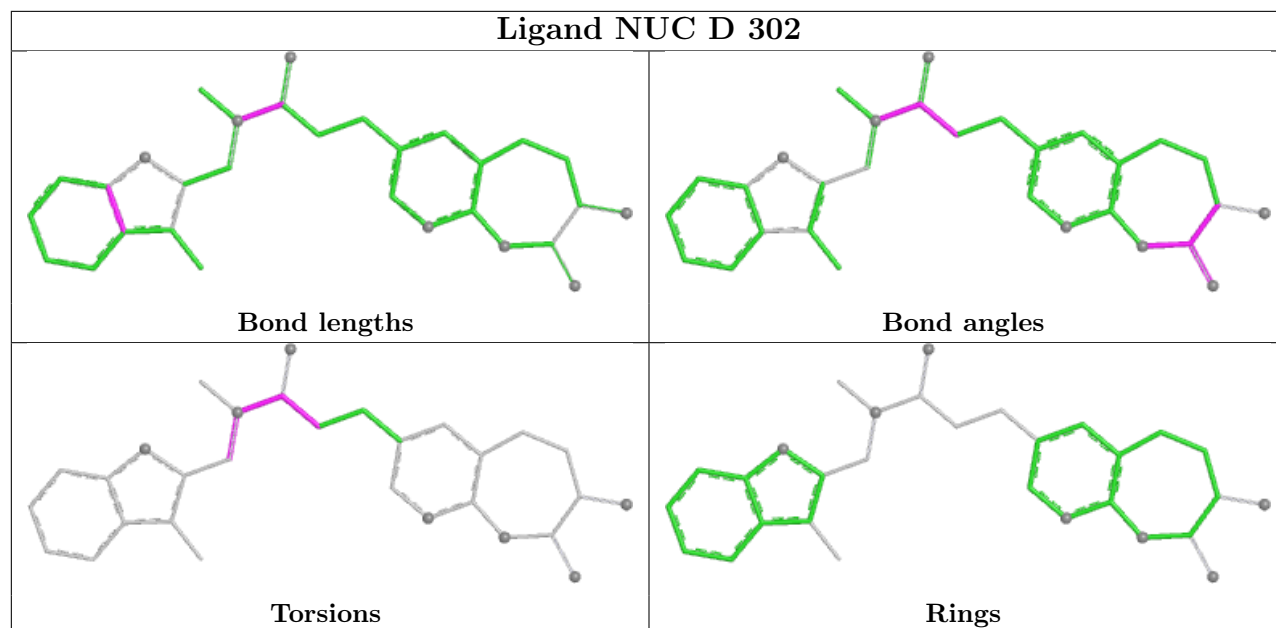
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

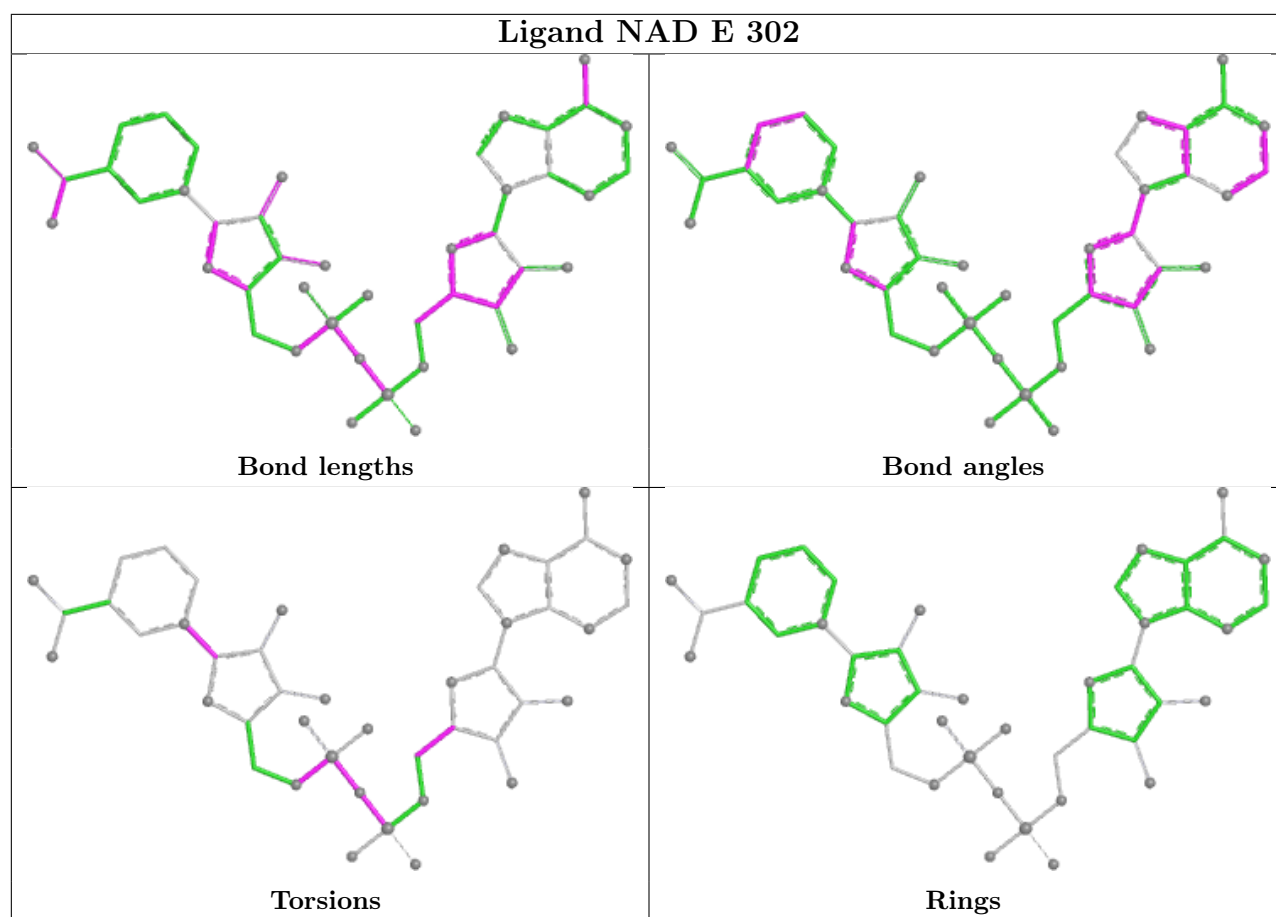


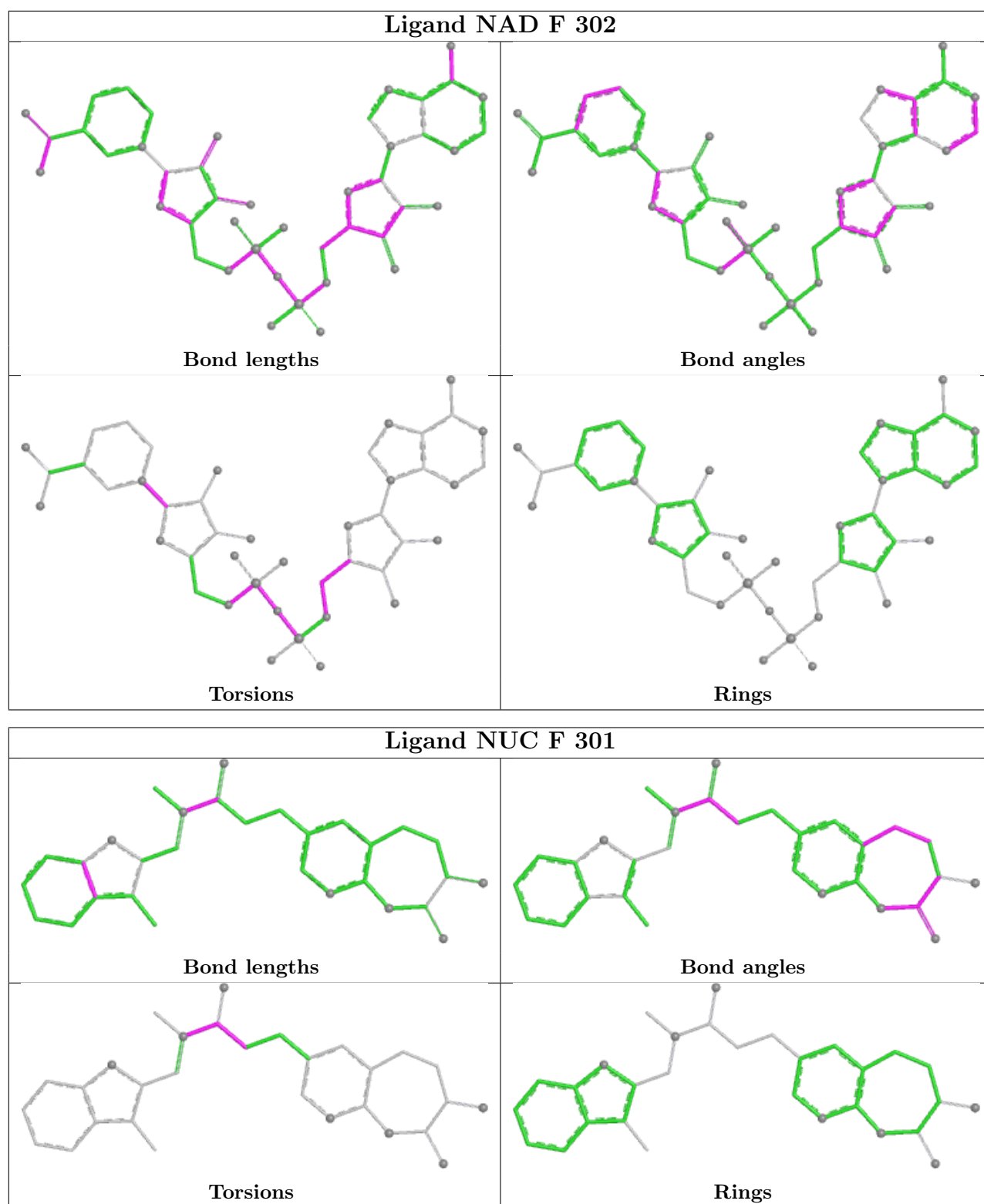












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	259/271 (95%)	0.69	23 (8%)	17 19	50, 86, 135, 232	0
1	B	254/271 (93%)	0.89	36 (14%)	7 9	60, 105, 190, 303	0
1	C	260/271 (95%)	0.73	23 (8%)	17 19	53, 82, 128, 172	0
1	D	258/271 (95%)	1.05	39 (15%)	6 8	63, 96, 143, 276	0
1	E	260/271 (95%)	0.91	29 (11%)	11 13	51, 88, 147, 338	0
1	F	260/271 (95%)	0.84	26 (10%)	14 16	50, 77, 118, 201	0
All	All	1551/1626 (95%)	0.85	176 (11%)	11 13	50, 89, 147, 338	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	SER	4.9
1	E	242	GLY	4.8
1	F	86	GLY	4.7
1	B	93	SER	4.5
1	E	86	GLY	4.4
1	E	22	ILE	4.3
1	E	95	GLY	4.3
1	D	258	GLY	4.1
1	B	123	ALA	4.0
1	F	127	VAL	4.0
1	D	198	LEU	3.7
1	E	61	LEU	3.6
1	A	151	GLY	3.5
1	A	11	PHE	3.5
1	D	22	ILE	3.5
1	D	231	ALA	3.4
1	F	172	GLY	3.4
1	B	139	ALA	3.3
1	B	177	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	94	ILE	3.3
1	A	184	GLY	3.3
1	A	242	GLY	3.3
1	B	258	GLY	3.3
1	A	179	SER	3.2
1	B	40	THR	3.2
1	A	182	VAL	3.2
1	D	242	GLY	3.2
1	C	163	GLY	3.2
1	A	5	LEU	3.2
1	D	94	ILE	3.1
1	F	247	ILE	3.1
1	B	125	SER	3.1
1	D	37	LEU	3.1
1	B	233	LEU	3.1
1	A	232	ALA	3.1
1	D	182	VAL	3.1
1	D	229	GLY	3.1
1	C	165	ALA	3.1
1	D	171	ALA	3.1
1	E	127	VAL	3.1
1	B	95	GLY	3.1
1	D	8	GLY	3.1
1	D	224	THR	3.0
1	E	123	ALA	3.0
1	D	15	GLY	3.0
1	D	151	GLY	3.0
1	C	94	ILE	3.0
1	F	202	GLY	3.0
1	C	145	LEU	3.0
1	E	152	SER	2.9
1	B	102	LEU	2.9
1	B	96	PHE	2.9
1	A	199	ALA	2.9
1	C	8	GLY	2.9
1	F	43	ASN	2.9
1	C	162	MET	2.8
1	F	51	ASP	2.8
1	E	125	SER	2.8
1	D	107	THR	2.8
1	B	172	GLY	2.8
1	C	184	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	36	GLU	2.8
1	D	257	VAL	2.8
1	D	38	ALA	2.8
1	C	159	TYR	2.8
1	D	91	VAL	2.8
1	F	257	VAL	2.8
1	B	80	LEU	2.8
1	F	93	SER	2.7
1	E	6	LEU	2.7
1	A	86	GLY	2.7
1	A	14	ALA	2.7
1	D	11	PHE	2.7
1	D	148	THR	2.7
1	D	194	PRO	2.7
1	E	172	GLY	2.7
1	F	87	VAL	2.6
1	B	218	PRO	2.6
1	F	123	ALA	2.6
1	A	181	GLY	2.6
1	F	136	LEU	2.6
1	F	94	ILE	2.6
1	A	130	ALA	2.6
1	D	178	SER	2.6
1	F	96	PHE	2.5
1	B	83	HIS	2.5
1	A	22	ILE	2.5
1	E	258	GLY	2.5
1	A	183	ASP	2.5
1	C	69	VAL	2.5
1	F	223	VAL	2.5
1	E	256	THR	2.5
1	E	122	SER	2.5
1	B	175	TYR	2.5
1	C	155	VAL	2.5
1	E	183	ASP	2.5
1	E	94	ILE	2.5
1	D	256	THR	2.5
1	B	147	LEU	2.5
1	F	182	VAL	2.5
1	A	258	GLY	2.5
1	C	40	THR	2.5
1	D	36	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	84	TRP	2.4
1	D	16	VAL	2.4
1	B	39	PHE	2.4
1	B	129	MET	2.4
1	D	67	VAL	2.4
1	D	119	HIS	2.4
1	B	38	ALA	2.4
1	B	124	TYR	2.4
1	C	118	ALA	2.4
1	D	110	THR	2.4
1	D	205	SER	2.4
1	E	223	VAL	2.4
1	D	106	PHE	2.4
1	F	125	SER	2.4
1	B	128	ALA	2.4
1	D	212	ALA	2.4
1	A	149	TYR	2.4
1	A	16	VAL	2.3
1	C	161	VAL	2.3
1	C	13	ILE	2.3
1	E	59	SER	2.3
1	C	50	VAL	2.3
1	D	104	GLY	2.3
1	B	145	LEU	2.3
1	B	61	LEU	2.3
1	F	159	TYR	2.3
1	A	87	VAL	2.3
1	F	77	PHE	2.2
1	F	149	TYR	2.2
1	D	225	ILE	2.2
1	F	53	PHE	2.2
1	A	219	LEU	2.2
1	D	260	SER	2.2
1	E	194	PRO	2.2
1	C	67	VAL	2.2
1	B	14	ALA	2.2
1	B	176	LEU	2.2
1	D	61	LEU	2.2
1	C	239	TRP	2.2
1	B	133	ALA	2.2
1	E	119	HIS	2.1
1	F	24	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	165	ALA	2.1
1	E	159	TYR	2.1
1	A	37	LEU	2.1
1	D	12	LEU	2.1
1	D	180	LEU	2.1
1	F	198	LEU	2.1
1	E	178	SER	2.1
1	E	126	PHE	2.1
1	C	102	LEU	2.1
1	C	198	LEU	2.1
1	B	200	ALA	2.1
1	E	177	ALA	2.1
1	B	4	GLY	2.1
1	C	15	GLY	2.1
1	D	25	GLY	2.1
1	F	52	GLU	2.1
1	F	64	PRO	2.1
1	A	257	VAL	2.1
1	E	257	VAL	2.1
1	C	210	LEU	2.1
1	C	123	ALA	2.1
1	E	104	GLY	2.1
1	B	173	VAL	2.0
1	C	122	SER	2.0
1	E	88	ASP	2.0
1	A	35	ALA	2.0
1	B	25	GLY	2.0
1	E	203	ILE	2.0
1	B	235	LEU	2.0
1	B	122	SER	2.0
1	F	27	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 monosaccharides in this entry.

6.4 Ligands

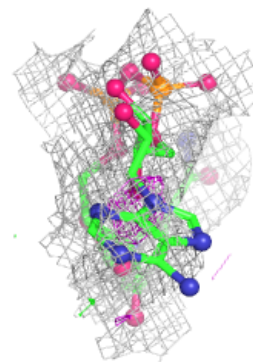
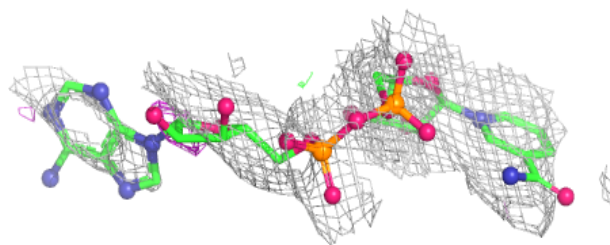
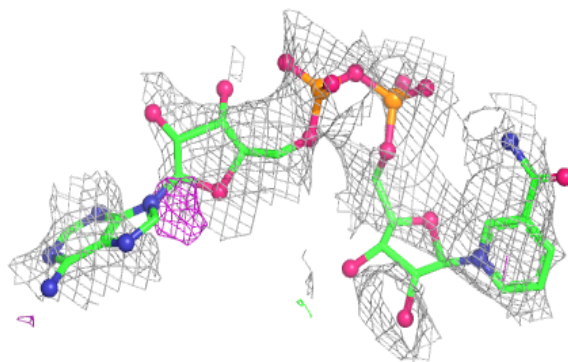
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	302	44/44	0.91	0.16	95,112,121,126	0
2	NAD	F	302	44/44	0.91	0.16	54,62,73,84	0
3	NUC	C	301	30/30	0.92	0.18	81,92,113,120	0
2	NAD	E	302	44/44	0.94	0.16	78,94,108,114	0
3	NUC	F	301	30/30	0.94	0.14	64,85,109,113	0
2	NAD	A	301	44/44	0.95	0.15	84,96,110,119	0
3	NUC	A	302	30/30	0.96	0.18	113,129,157,161	0
2	NAD	B	302	44/44	0.96	0.15	75,106,121,128	0
3	NUC	D	302	30/30	0.96	0.14	114,133,167,171	0
3	NUC	E	301	30/30	0.96	0.16	76,96,126,131	0
2	NAD	D	301	44/44	0.96	0.13	84,97,131,140	0
3	NUC	B	301	30/30	0.97	0.19	144,155,188,190	0

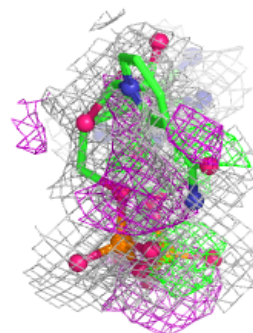
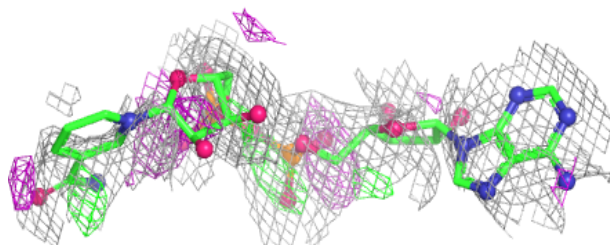
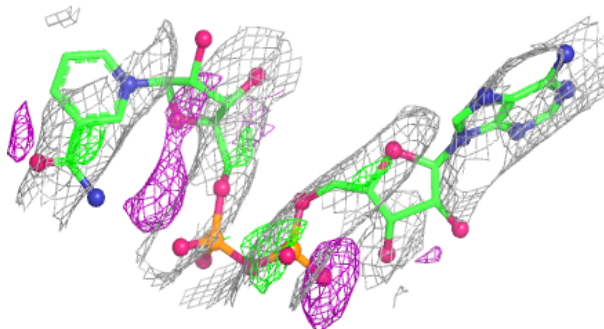
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 302:

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

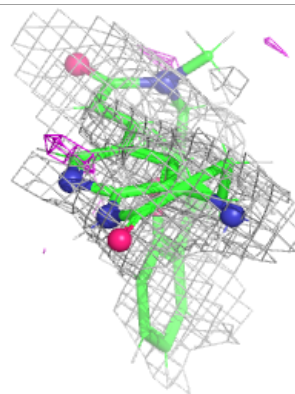
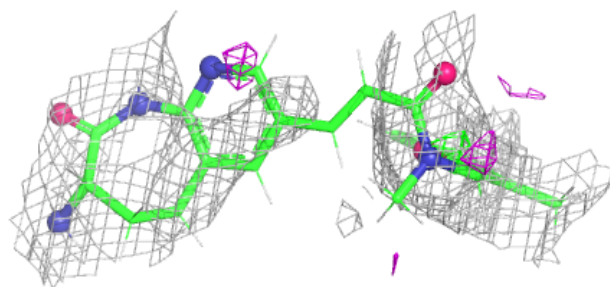
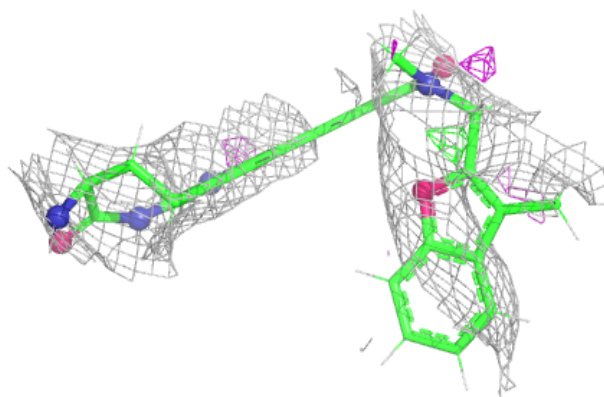
**Electron density around NAD F 302:**

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

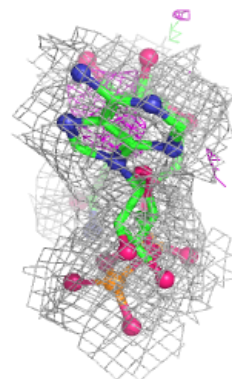
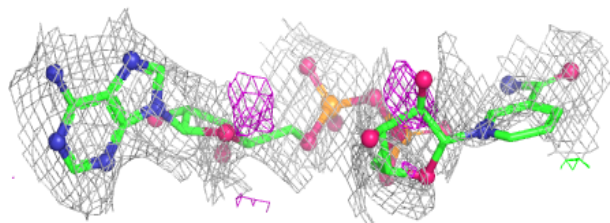
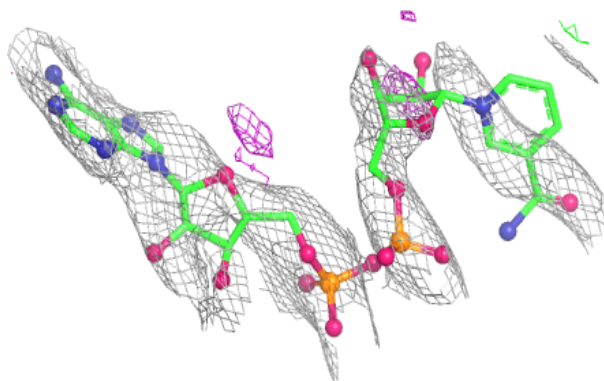


Electron density around NUC C 301:

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

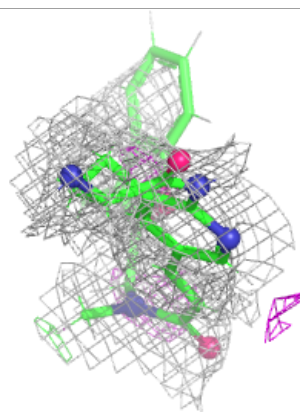
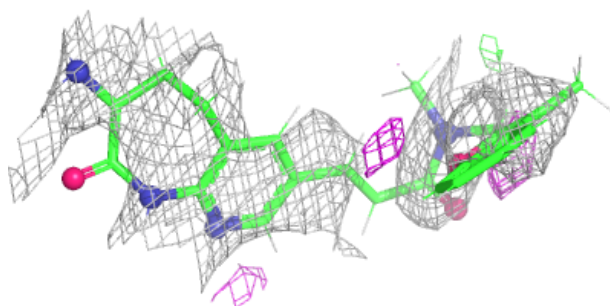
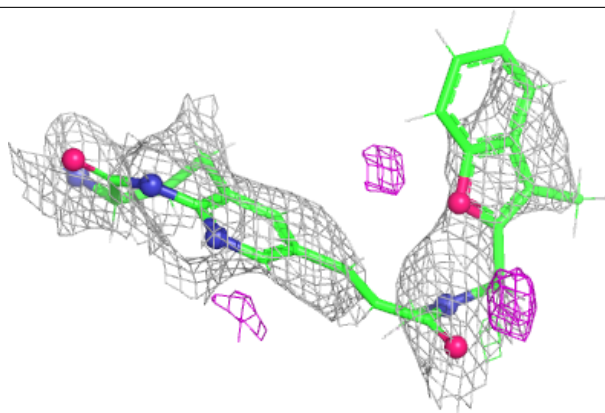
**Electron density around NAD E 302:**

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

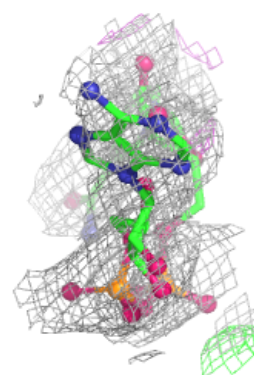
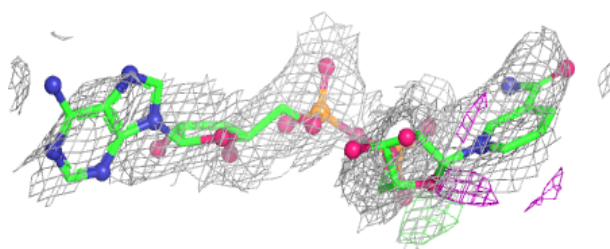
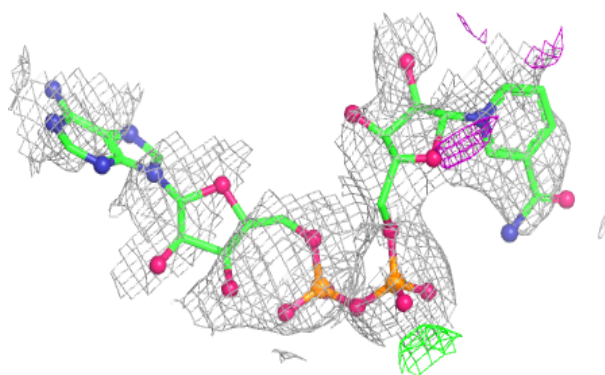


Electron density around NUC F 301:

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

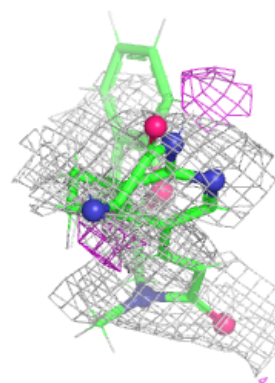
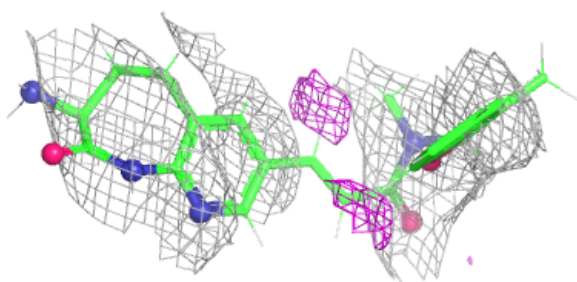
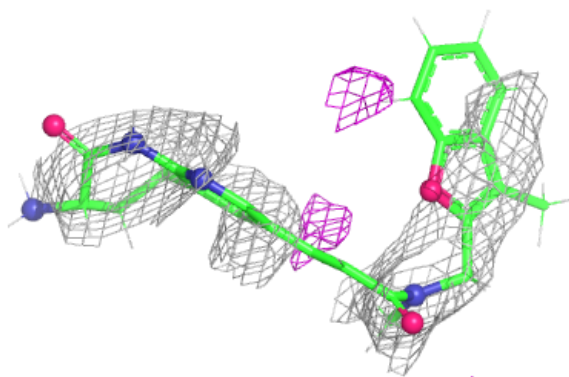
**Electron density around NAD A 301:**

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

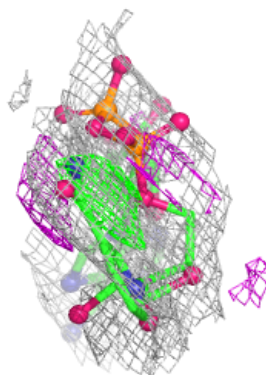
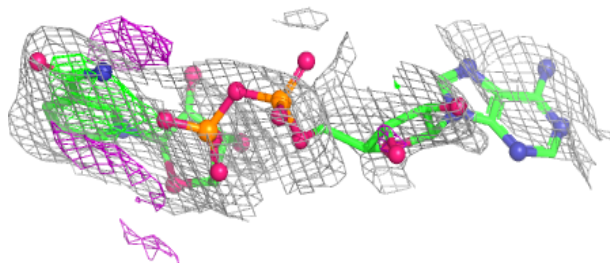
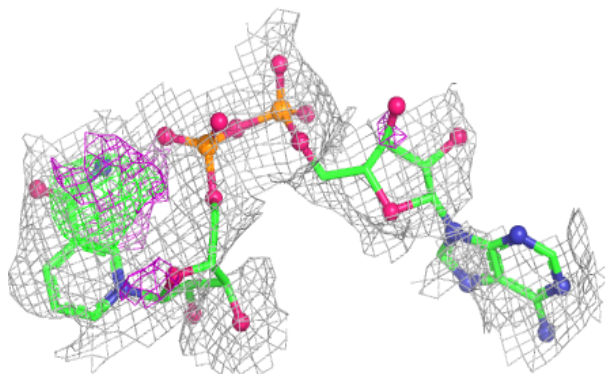


Electron density around NUC A 302:

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

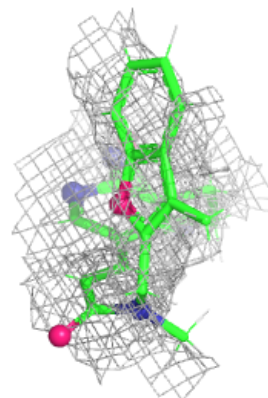
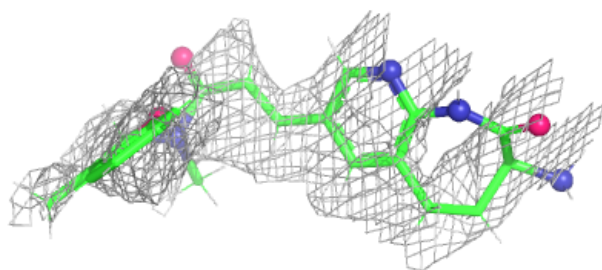
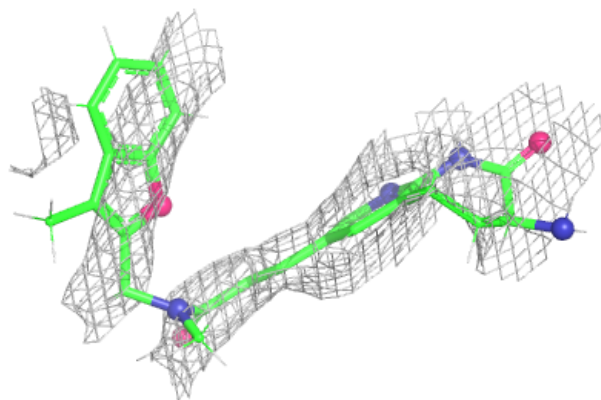
**Electron density around NAD B 302:**

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

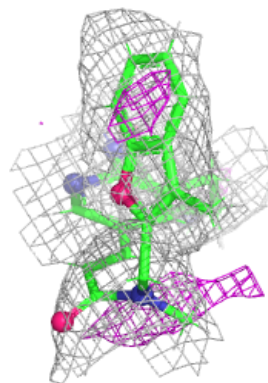
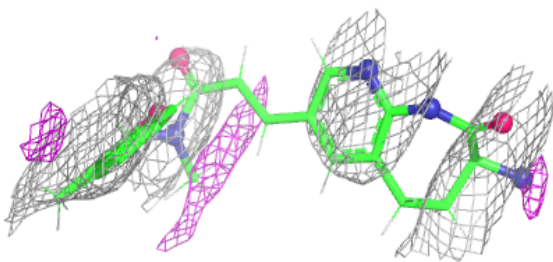
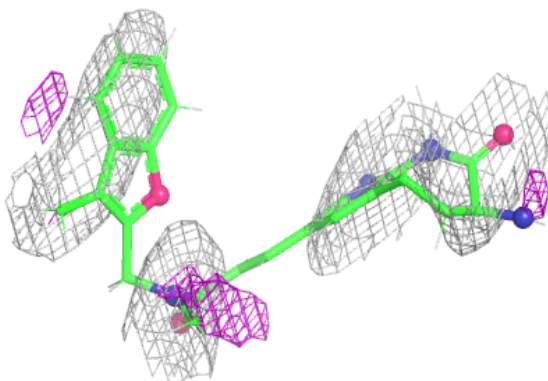


Electron density around NUC D 302:

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

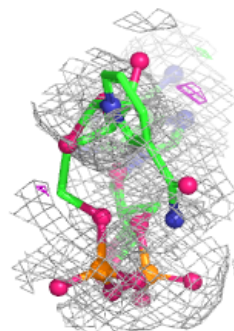
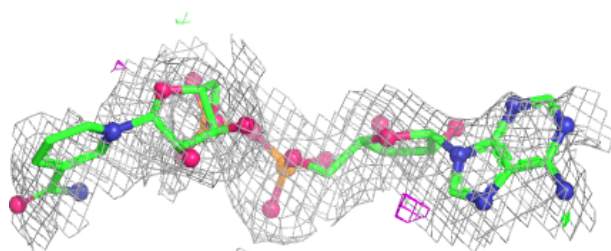
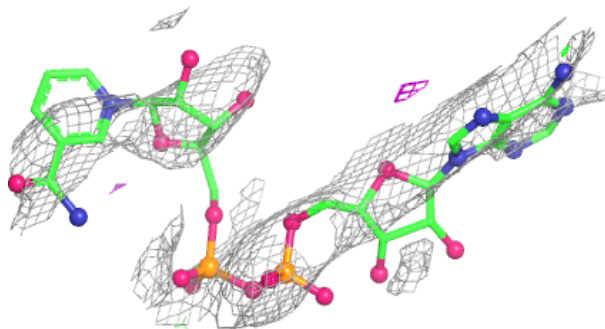
**Electron density around NUC E 301:**

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

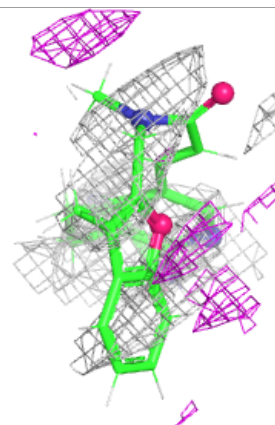
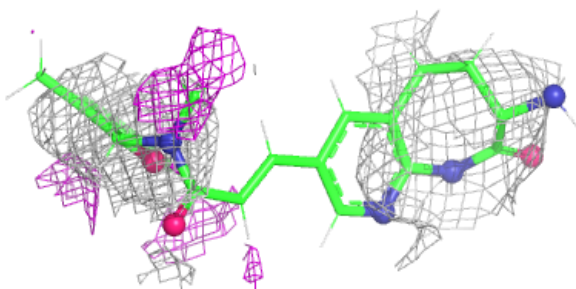
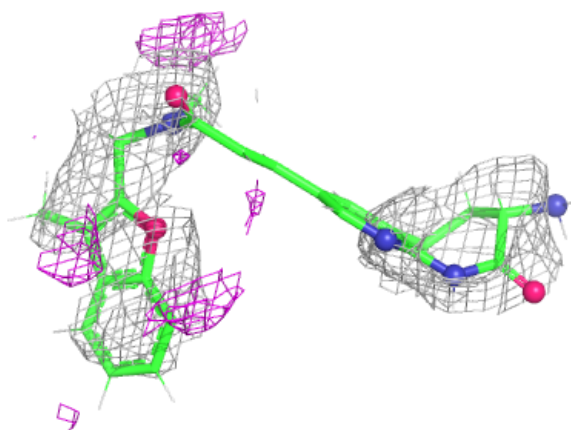


Electron density around NAD D 301:

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

**Electron density around NUC B 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.