



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:42 PM UTC

PDB ID : 1HWY / pdb_00001hwy
Title : BOVINE GLUTAMATE DEHYDROGENASE COMPLEXED WITH NAD
AND 2-OXOGLUTARATE
Authors : Smith, T.J.; Peterson, P.E.; Schmidt, T.; Fang, J.; Stanley, C.A.
Deposited on : 2001-01-10
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

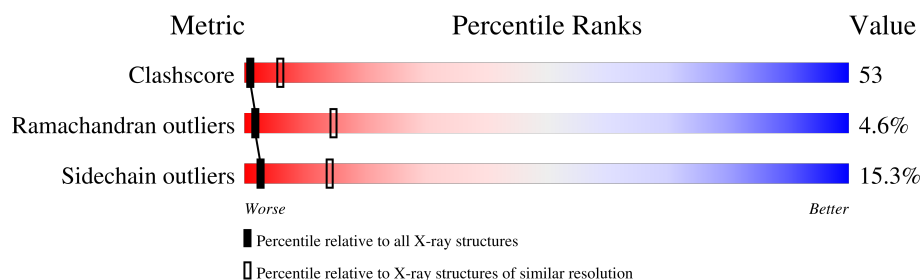
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	501	30% 54% 15% .
1	B	501	28% 55% 15% .
1	C	501	28% 55% 15% .
1	D	501	30% 54% 15% .
1	E	501	28% 55% 15% .
1	F	501	28% 55% 15% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	502	-	-	X	-
2	PO4	A	504	-	-	X	-
2	PO4	B	503	-	-	X	-
2	PO4	B	505	-	-	X	-
2	PO4	C	503	-	-	X	-
2	PO4	C	505	-	-	X	-
2	PO4	D	503	-	-	X	-
2	PO4	D	504	-	-	X	-
2	PO4	E	503	-	-	X	-
2	PO4	E	504	-	-	X	-
2	PO4	F	502	-	-	X	-
2	PO4	F	504	-	-	X	-
3	AKG	A	506	-	-	X	-
3	AKG	B	506	-	-	X	-
3	AKG	C	506	-	-	X	-
3	AKG	D	506	-	-	X	-
3	AKG	E	506	-	-	X	-
3	AKG	F	506	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24468 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 GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	B	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	C	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	D	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	E	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	F	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			

There are 30 discrepancies between the modelled and reference sequences:

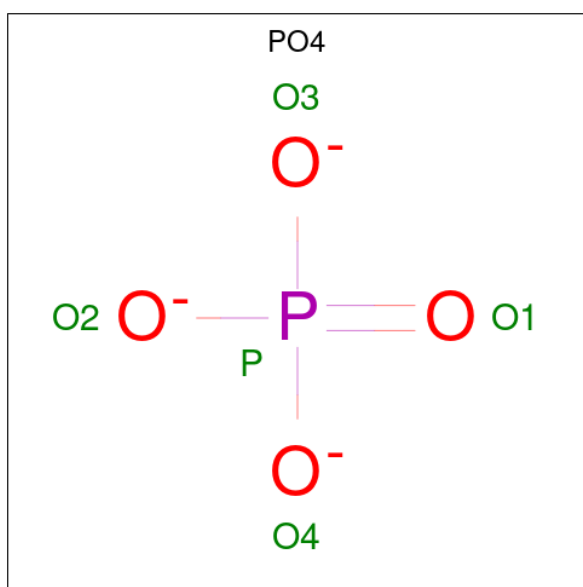
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO	SEE REMARK 999	UNP P00366
B	202	PRO	GLY	SEE REMARK 999	UNP P00366
B	221	HIS	GLY	SEE REMARK 999	UNP P00366
B	222	GLY	HIS	SEE REMARK 999	UNP P00366
C	200	GLY	LYS	SEE REMARK 999	UNP P00366
C	201	LYS	PRO	SEE REMARK 999	UNP P00366
C	202	PRO	GLY	SEE REMARK 999	UNP P00366
C	221	HIS	GLY	SEE REMARK 999	UNP P00366
C	222	GLY	HIS	SEE REMARK 999	UNP P00366
D	200	GLY	LYS	SEE REMARK 999	UNP P00366
D	201	LYS	PRO	SEE REMARK 999	UNP P00366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	PRO	GLY	SEE REMARK 999	UNP P00366
D	221	HIS	GLY	SEE REMARK 999	UNP P00366
D	222	GLY	HIS	SEE REMARK 999	UNP P00366
E	200	GLY	LYS	SEE REMARK 999	UNP P00366
E	201	LYS	PRO	SEE REMARK 999	UNP P00366
E	202	PRO	GLY	SEE REMARK 999	UNP P00366
E	221	HIS	GLY	SEE REMARK 999	UNP P00366
E	222	GLY	HIS	SEE REMARK 999	UNP P00366
F	200	GLY	LYS	SEE REMARK 999	UNP P00366
F	201	LYS	PRO	SEE REMARK 999	UNP P00366
F	202	PRO	GLY	SEE REMARK 999	UNP P00366
F	221	HIS	GLY	SEE REMARK 999	UNP P00366
F	222	GLY	HIS	SEE REMARK 999	UNP P00366

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



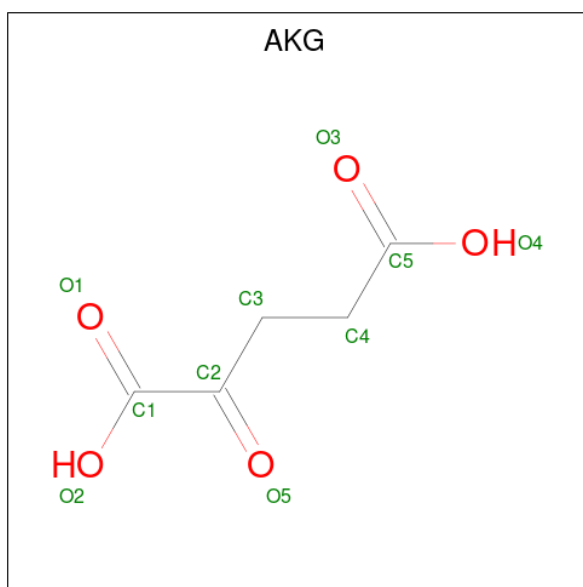
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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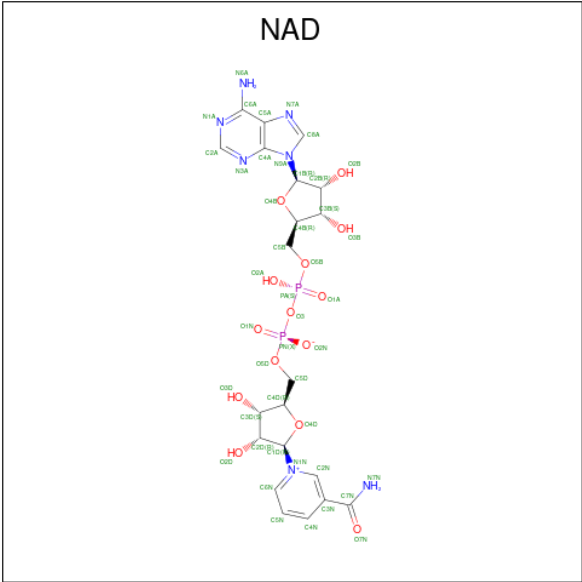
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

- Molecule 5 is water.

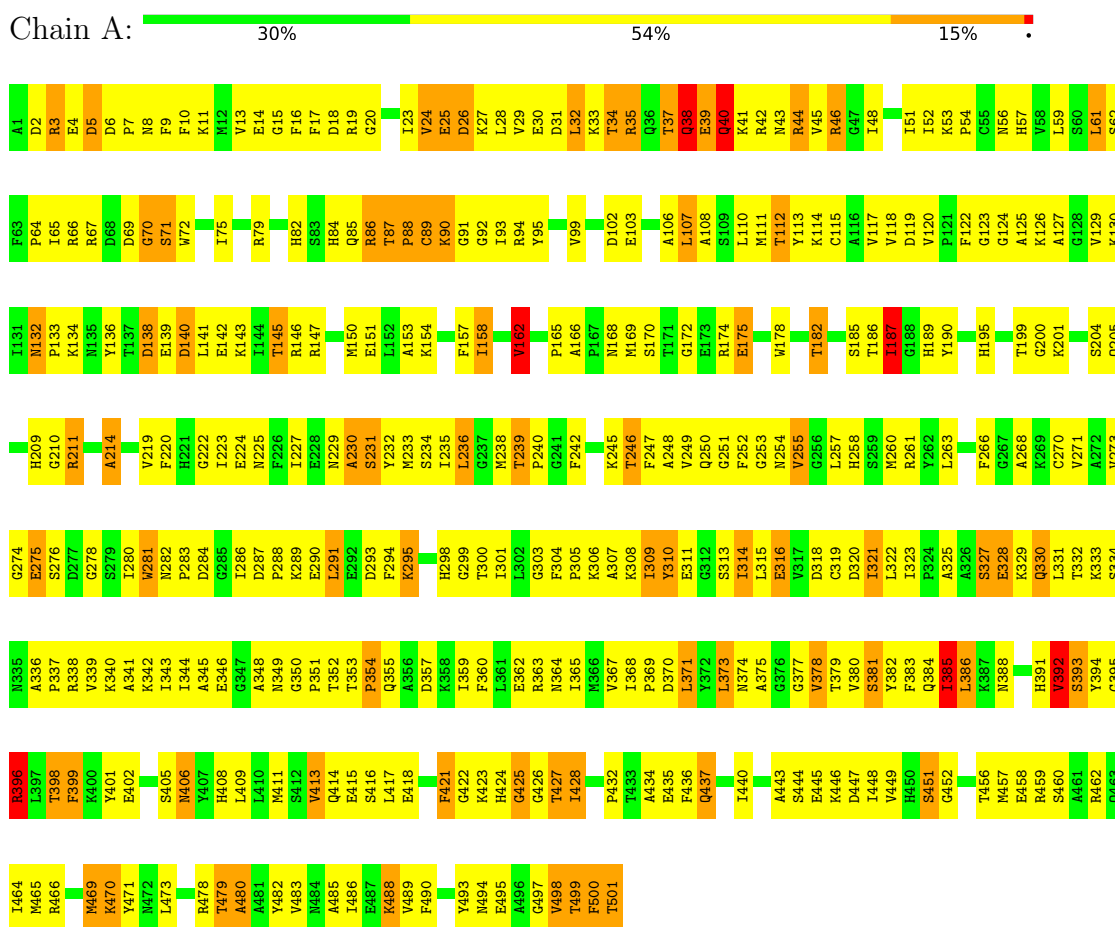
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0
5	C	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0

3 Residue-property plots

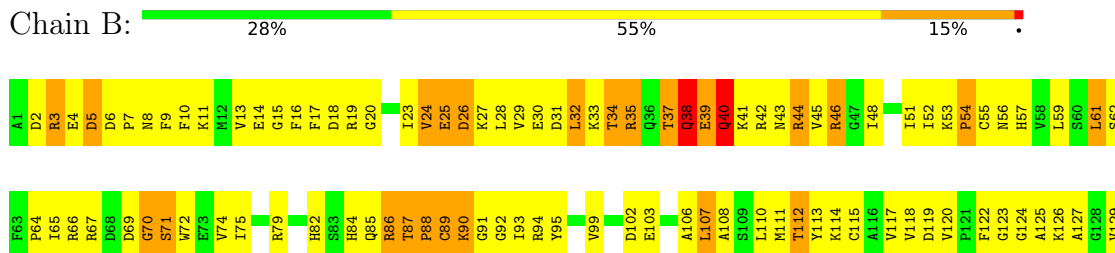
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

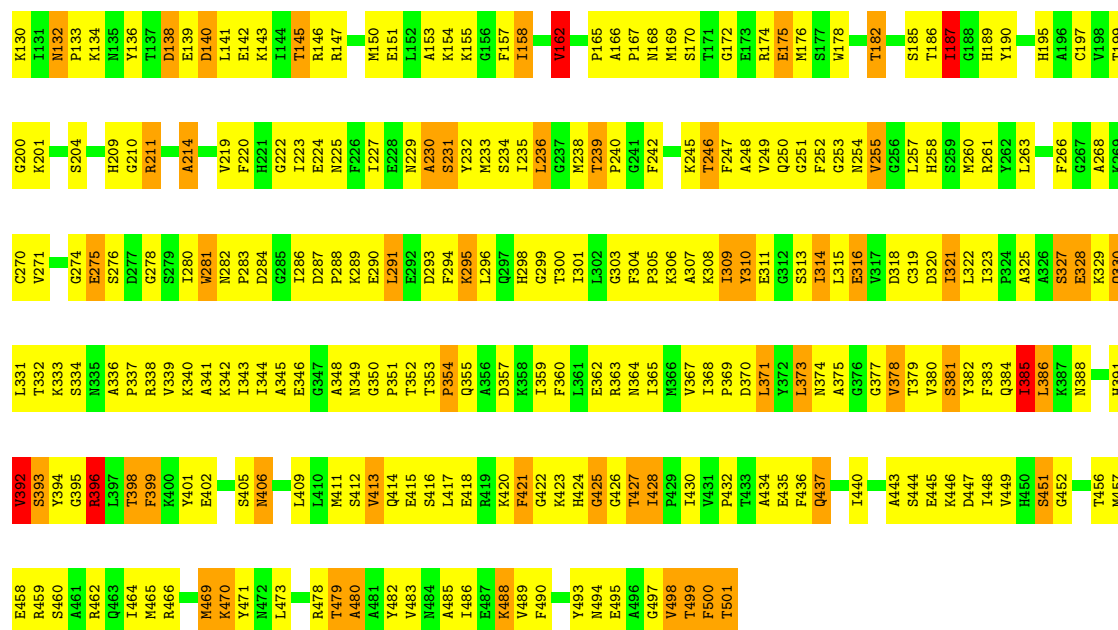
Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE

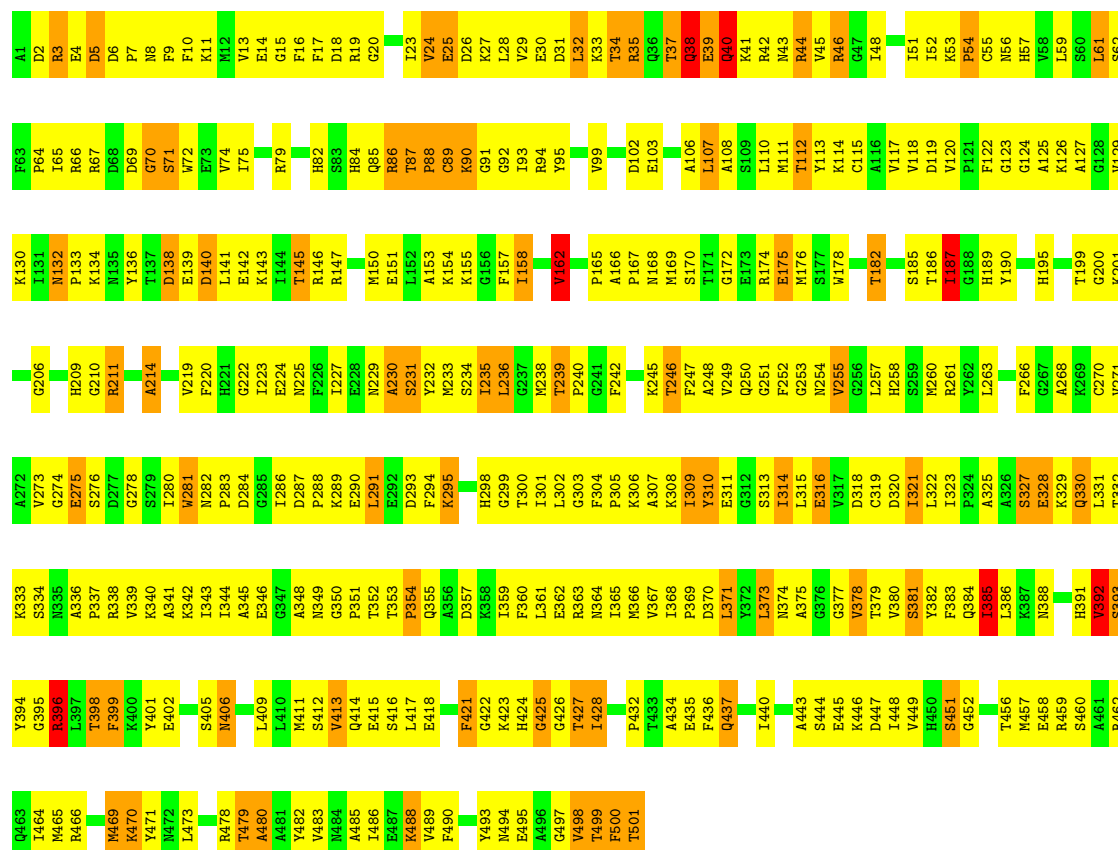


• Molecule 1: GLUTAMATE DEHYDROGENASE

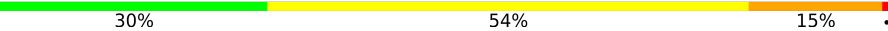


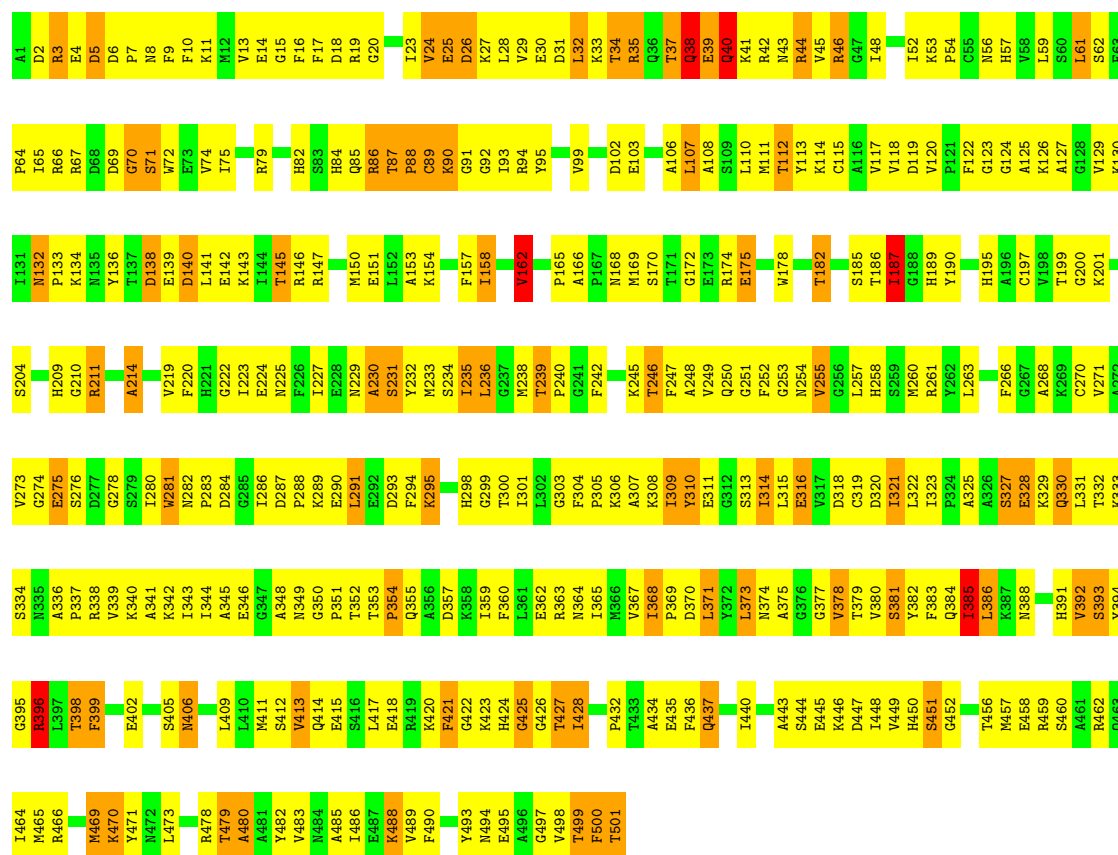


- Molecule 1: GLUTAMATE DEHYDROGENASE



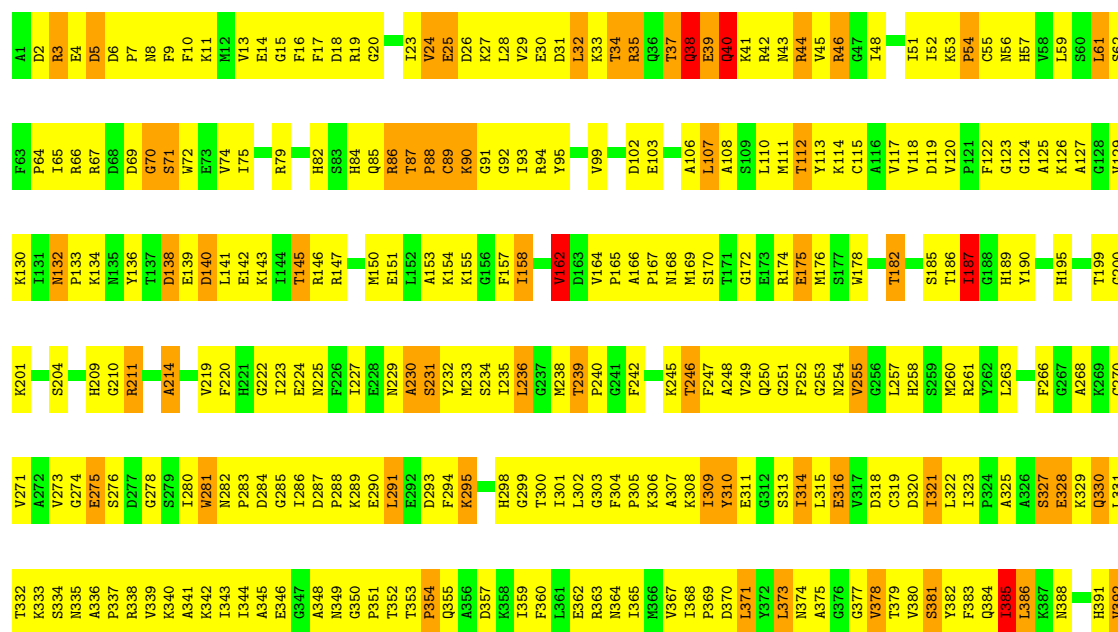
- Molecule 1: GLUTAMATE DEHYDROGENASE

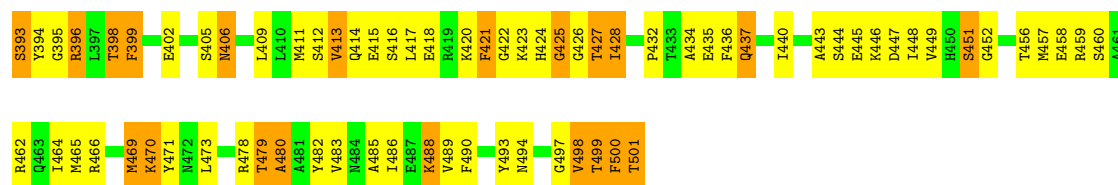
Chain D:  30% 54% 15%



• Molecule 1: GLUTAMATE DEHYDROGENASE

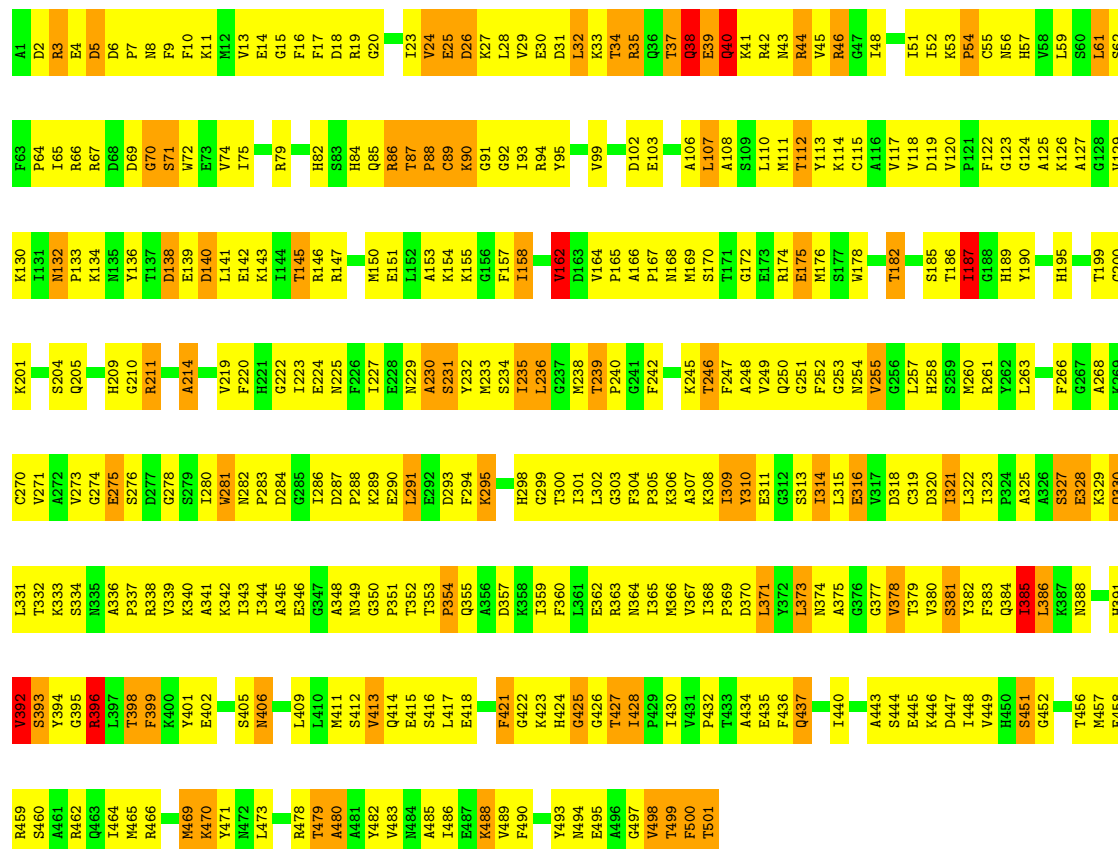
Chain E:  28% 55% 15%





• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 28% 55% 15% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.50Å 101.00Å 164.60Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24468	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAD, AKG

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	0.75	0/3991	1.24	41/5384 (0.8%)
1	B	0.75	0/3991	1.24	41/5384 (0.8%)
1	C	0.75	0/3991	1.24	41/5384 (0.8%)
1	D	0.75	0/3991	1.24	41/5384 (0.8%)
1	E	0.75	0/3991	1.24	41/5384 (0.8%)
1	F	0.75	0/3991	1.24	41/5384 (0.8%)
All	All	0.75	0/23946	1.24	246/32304 (0.8%)

There are no bond length outliers.

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	GLN	N-CA-C	-12.84	97.36	111.36
1	D	40	GLN	N-CA-C	-12.83	97.38	111.36
1	F	40	GLN	N-CA-C	-12.82	97.38	111.36
1	C	40	GLN	N-CA-C	-12.81	97.39	111.36
1	A	40	GLN	N-CA-C	-12.81	97.40	111.36
1	B	40	GLN	N-CA-C	-12.80	97.40	111.36
1	F	162	VAL	CB-CA-C	-9.16	103.92	111.71
1	C	162	VAL	CB-CA-C	-9.14	103.94	111.71
1	E	162	VAL	CB-CA-C	-9.14	103.94	111.71
1	A	162	VAL	CB-CA-C	-9.14	103.94	111.71
1	B	162	VAL	CB-CA-C	-9.12	103.96	111.71
1	D	162	VAL	CB-CA-C	-9.11	103.97	111.71
1	D	425	GLY	N-CA-C	-8.93	102.01	112.73
1	A	425	GLY	N-CA-C	-8.92	102.03	112.73
1	C	6	ASP	CA-C-N	8.91	128.85	120.03
1	C	6	ASP	C-N-CA	8.91	128.85	120.03
1	C	425	GLY	N-CA-C	-8.91	102.04	112.73
1	F	425	GLY	N-CA-C	-8.91	102.04	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	425	GLY	N-CA-C	-8.91	102.04	112.73
1	A	6	ASP	CA-C-N	8.90	128.84	120.03
1	A	6	ASP	C-N-CA	8.90	128.84	120.03
1	F	6	ASP	CA-C-N	8.90	128.84	120.03
1	F	6	ASP	C-N-CA	8.90	128.84	120.03
1	B	425	GLY	N-CA-C	-8.88	102.08	112.73
1	B	6	ASP	CA-C-N	8.87	128.81	120.03
1	B	6	ASP	C-N-CA	8.87	128.81	120.03
1	E	6	ASP	CA-C-N	8.87	128.81	120.03
1	E	6	ASP	C-N-CA	8.87	128.81	120.03
1	D	6	ASP	CA-C-N	8.87	128.81	120.03
1	D	6	ASP	C-N-CA	8.87	128.81	120.03
1	F	140	ASP	N-CA-C	-8.73	101.72	111.07
1	D	140	ASP	N-CA-C	-8.73	101.73	111.07
1	A	140	ASP	N-CA-C	-8.72	101.73	111.07
1	B	140	ASP	N-CA-C	-8.72	101.74	111.07
1	E	140	ASP	N-CA-C	-8.72	101.74	111.07
1	C	140	ASP	N-CA-C	-8.72	101.74	111.07
1	D	86	ARG	N-CA-C	-8.05	94.44	108.69
1	B	86	ARG	N-CA-C	-8.04	94.46	108.69
1	E	86	ARG	N-CA-C	-8.04	94.46	108.69
1	F	86	ARG	N-CA-C	-8.04	94.46	108.69
1	A	86	ARG	N-CA-C	-8.04	94.47	108.69
1	C	86	ARG	N-CA-C	-8.02	94.50	108.69
1	A	39	GLU	N-CA-C	-7.96	102.06	112.41
1	B	39	GLU	N-CA-C	-7.96	102.07	112.41
1	E	39	GLU	N-CA-C	-7.95	102.07	112.41
1	C	39	GLU	N-CA-C	-7.95	102.07	112.41
1	F	39	GLU	N-CA-C	-7.95	102.08	112.41
1	D	39	GLU	N-CA-C	-7.94	102.08	112.41
1	D	24	VAL	N-CA-C	7.94	118.79	112.12
1	E	24	VAL	N-CA-C	7.93	118.78	112.12
1	F	24	VAL	N-CA-C	7.89	118.75	112.12
1	A	24	VAL	N-CA-C	7.88	118.74	112.12
1	B	24	VAL	N-CA-C	7.88	118.74	112.12
1	C	24	VAL	N-CA-C	7.87	118.73	112.12
1	E	281	TRP	N-CA-C	7.67	125.50	114.16
1	F	281	TRP	N-CA-C	7.65	125.49	114.16
1	C	281	TRP	N-CA-C	7.64	125.47	114.16
1	A	281	TRP	N-CA-C	7.64	125.46	114.16
1	B	281	TRP	N-CA-C	7.63	125.45	114.16
1	D	281	TRP	N-CA-C	7.62	125.44	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ILE	CB-CA-C	-7.18	102.78	111.97
1	E	187	ILE	CB-CA-C	-7.18	102.78	111.97
1	A	187	ILE	CB-CA-C	-7.17	102.79	111.97
1	B	187	ILE	CB-CA-C	-7.17	102.79	111.97
1	D	187	ILE	CB-CA-C	-7.16	102.80	111.97
1	C	187	ILE	CB-CA-C	-7.16	102.80	111.97
1	B	235	ILE	N-CA-C	-7.16	103.32	110.62
1	A	235	ILE	N-CA-C	-7.15	103.32	110.62
1	E	235	ILE	N-CA-C	-7.15	103.33	110.62
1	F	235	ILE	N-CA-C	-7.14	103.33	110.62
1	D	235	ILE	N-CA-C	-7.13	103.34	110.62
1	C	65	ILE	N-CA-C	-7.12	98.94	108.35
1	C	235	ILE	N-CA-C	-7.12	103.35	110.62
1	E	65	ILE	N-CA-C	-7.11	98.96	108.35
1	D	65	ILE	N-CA-C	-7.10	98.98	108.35
1	A	65	ILE	N-CA-C	-7.10	98.98	108.35
1	F	65	ILE	N-CA-C	-7.08	99.00	108.35
1	B	65	ILE	N-CA-C	-7.08	99.01	108.35
1	B	278	GLY	N-CA-C	6.90	122.01	110.56
1	A	278	GLY	N-CA-C	6.88	121.98	110.56
1	C	278	GLY	N-CA-C	6.88	121.98	110.56
1	D	278	GLY	N-CA-C	6.88	121.97	110.56
1	F	278	GLY	N-CA-C	6.88	121.97	110.56
1	E	278	GLY	N-CA-C	6.87	121.96	110.56
1	C	87	THR	N-CA-C	6.82	124.88	109.81
1	D	87	THR	N-CA-C	6.82	124.88	109.81
1	B	87	THR	N-CA-C	6.81	124.87	109.81
1	A	87	THR	N-CA-C	6.81	124.86	109.81
1	F	87	THR	N-CA-C	6.81	124.85	109.81
1	E	87	THR	N-CA-C	6.80	124.85	109.81
1	F	123	GLY	N-CA-C	-6.57	102.50	112.89
1	E	123	GLY	N-CA-C	-6.57	102.51	112.89
1	A	123	GLY	N-CA-C	-6.56	102.52	112.89
1	B	123	GLY	N-CA-C	-6.56	102.53	112.89
1	C	123	GLY	N-CA-C	-6.55	102.53	112.89
1	D	123	GLY	N-CA-C	-6.53	102.58	112.89
1	B	480	ALA	N-CA-C	-6.42	103.80	111.69
1	F	480	ALA	N-CA-C	-6.41	103.81	111.69
1	D	480	ALA	N-CA-C	-6.39	103.83	111.69
1	A	480	ALA	N-CA-C	-6.38	103.84	111.69
1	E	480	ALA	N-CA-C	-6.37	103.85	111.69
1	C	480	ALA	N-CA-C	-6.34	103.89	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ILE	CA-C-N	6.30	126.32	119.90
1	D	368	ILE	C-N-CA	6.30	126.32	119.90
1	C	89	CYS	N-CA-C	-6.26	101.67	110.50
1	B	368	ILE	CA-C-N	6.25	126.28	119.90
1	B	368	ILE	C-N-CA	6.25	126.28	119.90
1	A	368	ILE	CA-C-N	6.25	126.28	119.90
1	A	368	ILE	C-N-CA	6.25	126.28	119.90
1	F	368	ILE	CA-C-N	6.25	126.28	119.90
1	F	368	ILE	C-N-CA	6.25	126.28	119.90
1	C	368	ILE	CA-C-N	6.24	126.26	119.90
1	C	368	ILE	C-N-CA	6.24	126.26	119.90
1	E	89	CYS	N-CA-C	-6.24	101.71	110.50
1	E	368	ILE	CA-C-N	6.24	126.26	119.90
1	E	368	ILE	C-N-CA	6.24	126.26	119.90
1	B	89	CYS	N-CA-C	-6.23	101.71	110.50
1	A	89	CYS	N-CA-C	-6.23	101.72	110.50
1	D	89	CYS	N-CA-C	-6.23	101.72	110.50
1	F	89	CYS	N-CA-C	-6.21	101.75	110.50
1	E	385	ILE	N-CA-C	-6.16	104.50	110.42
1	D	385	ILE	N-CA-C	-6.14	104.53	110.42
1	F	385	ILE	N-CA-C	-6.12	104.54	110.42
1	A	385	ILE	N-CA-C	-6.12	104.55	110.42
1	B	385	ILE	N-CA-C	-6.11	104.55	110.42
1	C	385	ILE	N-CA-C	-6.10	104.56	110.42
1	A	38	GLN	N-CA-C	-6.10	97.80	110.80
1	D	38	GLN	N-CA-C	-6.10	97.82	110.80
1	B	38	GLN	N-CA-C	-6.09	97.83	110.80
1	C	38	GLN	N-CA-C	-6.09	97.83	110.80
1	F	38	GLN	N-CA-C	-6.09	97.84	110.80
1	E	38	GLN	N-CA-C	-6.08	97.85	110.80
1	D	488	LYS	N-CA-C	-6.04	103.45	111.24
1	D	214	ALA	N-CA-C	6.03	118.34	111.11
1	B	488	LYS	N-CA-C	-6.02	103.48	111.24
1	A	488	LYS	N-CA-C	-6.01	103.48	111.24
1	C	488	LYS	N-CA-C	-6.01	103.48	111.24
1	F	488	LYS	N-CA-C	-6.01	103.48	111.24
1	E	488	LYS	N-CA-C	-6.01	103.48	111.24
1	C	214	ALA	N-CA-C	5.99	118.30	111.11
1	F	214	ALA	N-CA-C	5.99	118.30	111.11
1	E	214	ALA	N-CA-C	5.99	118.30	111.11
1	B	214	ALA	N-CA-C	5.99	118.33	111.02
1	A	214	ALA	N-CA-C	5.98	118.29	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	497	GLY	N-CA-C	-5.91	107.09	115.30
1	F	497	GLY	N-CA-C	-5.91	107.09	115.30
1	B	497	GLY	N-CA-C	-5.89	107.11	115.30
1	A	497	GLY	N-CA-C	-5.89	107.11	115.30
1	D	497	GLY	N-CA-C	-5.88	107.13	115.30
1	C	497	GLY	N-CA-C	-5.87	107.14	115.30
1	B	424	HIS	N-CA-C	-5.86	104.82	111.14
1	C	424	HIS	N-CA-C	-5.84	104.83	111.14
1	A	424	HIS	N-CA-C	-5.83	104.84	111.14
1	F	6	ASP	N-CA-C	-5.83	98.84	108.75
1	B	6	ASP	N-CA-C	-5.83	98.84	108.75
1	C	6	ASP	N-CA-C	-5.83	98.84	108.75
1	D	6	ASP	N-CA-C	-5.83	98.84	108.75
1	D	424	HIS	N-CA-C	-5.83	104.85	111.14
1	E	6	ASP	N-CA-C	-5.82	98.85	108.75
1	A	6	ASP	N-CA-C	-5.82	98.85	108.75
1	F	424	HIS	N-CA-C	-5.82	104.86	111.14
1	A	44	ARG	N-CA-C	-5.81	104.63	110.97
1	D	44	ARG	N-CA-C	-5.81	104.64	110.97
1	C	44	ARG	N-CA-C	-5.80	104.64	110.97
1	F	44	ARG	N-CA-C	-5.80	104.64	110.97
1	B	44	ARG	N-CA-C	-5.80	104.65	110.97
1	E	424	HIS	N-CA-C	-5.80	104.87	111.14
1	E	44	ARG	N-CA-C	-5.80	104.65	110.97
1	D	87	THR	CA-C-N	-5.76	112.64	119.84
1	D	87	THR	C-N-CA	-5.76	112.64	119.84
1	C	87	THR	CA-C-N	-5.75	112.65	119.84
1	C	87	THR	C-N-CA	-5.75	112.65	119.84
1	A	87	THR	CA-C-N	-5.74	112.66	119.84
1	A	87	THR	C-N-CA	-5.74	112.66	119.84
1	E	87	THR	CA-C-N	-5.72	112.68	119.84
1	E	87	THR	C-N-CA	-5.72	112.68	119.84
1	D	301	ILE	N-CA-C	-5.72	104.98	113.39
1	F	87	THR	CA-C-N	-5.71	112.70	119.84
1	F	87	THR	C-N-CA	-5.71	112.70	119.84
1	F	301	ILE	N-CA-C	-5.71	105.00	113.39
1	C	301	ILE	N-CA-C	-5.71	105.00	113.39
1	B	87	THR	CA-C-N	-5.70	112.71	119.84
1	B	87	THR	C-N-CA	-5.70	112.71	119.84
1	B	301	ILE	N-CA-C	-5.69	105.02	113.39
1	A	301	ILE	N-CA-C	-5.69	105.02	113.39
1	C	132	ASN	CA-C-N	5.68	126.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ASN	C-N-CA	5.68	126.94	119.84
1	E	301	ILE	N-CA-C	-5.67	105.05	113.39
1	F	132	ASN	CA-C-N	5.67	126.92	119.84
1	F	132	ASN	C-N-CA	5.67	126.92	119.84
1	A	132	ASN	CA-C-N	5.64	126.89	119.84
1	A	132	ASN	C-N-CA	5.64	126.89	119.84
1	E	132	ASN	CA-C-N	5.63	126.88	119.84
1	E	132	ASN	C-N-CA	5.63	126.88	119.84
1	B	132	ASN	CA-C-N	5.62	126.86	119.84
1	B	132	ASN	C-N-CA	5.62	126.86	119.84
1	D	132	ASN	CA-C-N	5.62	126.86	119.84
1	D	132	ASN	C-N-CA	5.62	126.86	119.84
1	B	54	PRO	N-CA-C	5.58	119.78	111.41
1	C	54	PRO	N-CA-C	5.58	119.78	111.41
1	E	119	ASP	N-CA-C	5.56	119.11	111.54
1	A	54	PRO	N-CA-C	5.56	119.75	111.41
1	B	119	ASP	N-CA-C	5.56	119.11	111.54
1	D	54	PRO	N-CA-C	5.55	119.74	111.41
1	E	54	PRO	N-CA-C	5.55	119.74	111.41
1	F	119	ASP	N-CA-C	5.55	119.09	111.54
1	D	119	ASP	N-CA-C	5.55	119.08	111.54
1	A	119	ASP	N-CA-C	5.54	119.08	111.54
1	C	119	ASP	N-CA-C	5.54	119.07	111.54
1	F	54	PRO	N-CA-C	5.53	119.70	111.41
1	A	306	LYS	N-CA-C	5.50	119.62	111.87
1	E	306	LYS	N-CA-C	5.50	119.62	111.87
1	B	306	LYS	N-CA-C	5.49	119.61	111.87
1	C	306	LYS	N-CA-C	5.49	119.61	111.87
1	D	306	LYS	N-CA-C	5.49	119.61	111.87
1	F	306	LYS	N-CA-C	5.47	119.58	111.87
1	D	434	ALA	N-CA-C	-5.44	105.25	111.07
1	A	434	ALA	N-CA-C	-5.43	105.26	111.07
1	E	434	ALA	N-CA-C	-5.42	105.27	111.07
1	B	434	ALA	N-CA-C	-5.42	105.27	111.07
1	C	434	ALA	N-CA-C	-5.42	105.27	111.07
1	F	434	ALA	N-CA-C	-5.40	105.29	111.07
1	B	392	VAL	CB-CA-C	-5.27	101.59	110.71
1	A	392	VAL	CB-CA-C	-5.27	101.59	110.71
1	F	392	VAL	CB-CA-C	-5.27	101.59	110.71
1	E	392	VAL	CB-CA-C	-5.27	101.60	110.71
1	C	392	VAL	CB-CA-C	-5.25	101.62	110.71
1	D	392	VAL	CB-CA-C	-5.24	101.64	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	THR	N-CA-C	5.23	120.32	113.88
1	D	398	THR	N-CA-C	5.22	120.30	113.88
1	A	398	THR	N-CA-C	5.20	120.27	113.88
1	E	398	THR	N-CA-C	5.18	120.25	113.88
1	B	398	THR	N-CA-C	5.17	120.24	113.88
1	D	28	LEU	N-CA-C	-5.16	105.55	111.07
1	F	398	THR	N-CA-C	5.16	120.22	113.88
1	C	28	LEU	N-CA-C	-5.14	105.56	111.07
1	A	28	LEU	N-CA-C	-5.14	105.57	111.07
1	E	28	LEU	N-CA-C	-5.14	105.57	111.07
1	B	28	LEU	N-CA-C	-5.13	105.58	111.07
1	F	28	LEU	N-CA-C	-5.09	105.62	111.07
1	C	129	VAL	N-CA-C	-5.07	101.11	109.12
1	E	129	VAL	N-CA-C	-5.05	101.14	109.12
1	D	129	VAL	N-CA-C	-5.05	101.14	109.12
1	A	129	VAL	N-CA-C	-5.05	101.14	109.12
1	B	129	VAL	N-CA-C	-5.04	101.15	109.12
1	F	129	VAL	N-CA-C	-5.04	101.16	109.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3910	0	3888	444	1
1	B	3910	0	3888	469	2
1	C	3910	0	3888	445	2
1	D	3910	0	3888	435	0
1	E	3910	0	3888	451	1
1	F	3910	0	3888	465	0
2	A	20	0	0	6	0
2	B	20	0	0	6	0
2	C	20	0	0	6	0
2	D	20	0	0	6	0
2	E	20	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	20	0	0	6	0
3	A	10	0	4	6	0
3	B	10	0	4	7	0
3	C	10	0	4	7	0
3	D	10	0	4	7	0
3	E	10	0	4	6	0
3	F	10	0	4	7	0
4	A	132	0	78	33	0
4	B	132	0	78	36	0
4	C	132	0	78	39	0
4	D	132	0	77	35	0
4	E	132	0	77	31	0
4	F	132	0	77	34	0
5	A	6	0	0	4	0
5	B	6	0	0	4	0
5	C	6	0	0	4	0
5	D	6	0	0	5	0
5	E	6	0	0	4	0
5	F	6	0	0	4	0
All	All	24468	0	23817	2569	3

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 53.

All (2569) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:CA	4:D:507[A]:NAD:O3D	1.66	1.41
1:F:391:HIS:CA	4:F:508[A]:NAD:O3D	1.66	1.41
1:B:391:HIS:CA	4:B:507[A]:NAD:O3D	1.69	1.40
1:C:391:HIS:CA	4:C:507[A]:NAD:O3D	1.70	1.39
1:A:391:HIS:CA	4:A:507[A]:NAD:O3D	1.69	1.38
1:A:391:HIS:HD2	4:A:507[A]:NAD:O2D	1.28	1.16
1:F:391:HIS:HD2	4:F:508[A]:NAD:O2D	1.29	1.14
1:D:391:HIS:HD2	4:D:507[A]:NAD:O2D	1.30	1.12
1:E:391:HIS:HD2	4:E:507[A]:NAD:O2D	1.30	1.11
1:F:391:HIS:CD2	4:F:508[A]:NAD:O2D	2.04	1.11
1:A:391:HIS:CD2	4:A:507[A]:NAD:O2D	2.06	1.09
1:B:391:HIS:HD2	4:B:507[A]:NAD:O2D	1.36	1.08
1:D:391:HIS:CD2	4:D:507[A]:NAD:O2D	2.06	1.08
1:E:391:HIS:CD2	4:E:507[A]:NAD:O2D	2.07	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:HIS:HA	4:C:507[A]:NAD:O3D	0.87	1.05
1:C:391:HIS:HD2	4:C:507[A]:NAD:O2D	1.39	1.04
1:B:391:HIS:CD2	4:B:507[A]:NAD:O2D	2.11	1.02
1:A:153:ALA:HB1	1:A:187:ILE:HD11	1.41	1.02
1:F:153:ALA:HB1	1:F:187:ILE:HD11	1.41	1.01
1:B:391:HIS:HA	4:B:507[A]:NAD:O3D	0.84	1.00
1:E:153:ALA:HB1	1:E:187:ILE:HD11	1.41	1.00
2:D:504:PO4:O3	5:D:514:HOH:O	1.79	1.00
1:C:153:ALA:HB1	1:C:187:ILE:HD11	1.41	1.00
1:C:391:HIS:CD2	4:C:507[A]:NAD:O2D	2.13	0.99
1:B:153:ALA:HB1	1:B:187:ILE:HD11	1.41	0.99
1:A:391:HIS:HA	4:A:507[A]:NAD:O3D	0.81	0.98
1:D:153:ALA:HB1	1:D:187:ILE:HD11	1.41	0.98
1:F:391:HIS:HA	4:F:508[A]:NAD:O3D	0.80	0.98
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.46	0.97
1:D:378:VAL:HG12	3:D:506:AKG:O4	1.65	0.97
1:D:391:HIS:HA	4:D:507[A]:NAD:O3D	0.80	0.96
2:C:505:PO4:O3	5:C:514:HOH:O	1.82	0.96
1:A:107:LEU:HB3	1:A:126:LYS:HG2	1.46	0.96
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.46	0.96
1:C:378:VAL:HG12	3:C:506:AKG:O4	1.65	0.96
1:B:378:VAL:HG12	3:B:506:AKG:O4	1.65	0.96
1:E:378:VAL:HG12	3:E:506:AKG:O4	1.65	0.96
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.46	0.95
1:A:378:VAL:HG12	3:A:506:AKG:O4	1.65	0.95
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.46	0.95
1:F:378:VAL:HG12	3:F:506:AKG:O4	1.65	0.94
2:E:504:PO4:O4	5:E:513:HOH:O	1.86	0.94
2:D:504:PO4:O4	5:D:511:HOH:O	1.86	0.94
1:B:209:HIS:HD2	2:B:503:PO4:O3	1.51	0.94
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.46	0.93
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.51	0.93
1:A:209:HIS:HD2	2:A:502:PO4:O3	1.51	0.93
1:D:209:HIS:HD2	2:D:503:PO4:O3	1.51	0.93
1:F:209:HIS:HD2	2:F:504:PO4:O3	1.51	0.93
2:F:502:PO4:O4	5:F:513:HOH:O	1.86	0.93
2:A:504:PO4:O4	5:A:511:HOH:O	1.86	0.92
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.51	0.92
1:E:209:HIS:HD2	2:E:503:PO4:O3	1.51	0.92
2:B:505:PO4:O4	5:B:513:HOH:O	1.86	0.92
2:C:505:PO4:O4	5:C:511:HOH:O	1.86	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.51	0.92
1:B:417:LEU:HD21	1:F:417:LEU:CD1	2.00	0.92
1:C:209:HIS:HD2	2:C:503:PO4:O3	1.51	0.92
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.51	0.91
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.51	0.91
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.51	0.91
1:C:391:HIS:CA	4:C:507[A]:NAD:HO3N	1.68	0.91
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.06	0.91
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.06	0.91
1:C:195:HIS:HE1	1:E:87:THR:CG2	1.84	0.91
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.06	0.91
1:F:323:ILE:HG12	1:F:345:ALA:HB3	1.53	0.91
1:C:323:ILE:HG12	1:C:345:ALA:HB3	1.53	0.91
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.06	0.90
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.06	0.90
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.53	0.89
1:A:219:VAL:HG22	1:A:373:LEU:HD13	1.55	0.89
1:D:219:VAL:HG22	1:D:373:LEU:HD13	1.55	0.89
1:D:142:GLU:HG2	1:D:146:ARG:HD2	1.55	0.89
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.06	0.89
1:A:323:ILE:HG12	1:A:345:ALA:HB3	1.53	0.89
1:C:142:GLU:HG2	1:C:146:ARG:HD2	1.55	0.88
1:E:142:GLU:HG2	1:E:146:ARG:HD2	1.55	0.88
1:F:462:ARG:HH21	1:F:466:ARG:HH22	1.21	0.88
2:F:502:PO4:O3	5:F:510:HOH:O	1.89	0.88
1:C:370:ASP:HB2	1:C:374:ASN:HD21	1.39	0.88
1:F:219:VAL:HG22	1:F:373:LEU:HD13	1.55	0.88
1:E:219:VAL:HG22	1:E:373:LEU:HD13	1.55	0.88
1:B:195:HIS:HE1	1:F:87:THR:CG2	1.86	0.88
1:B:391:HIS:CA	4:B:507[A]:NAD:HO3N	1.61	0.88
2:B:505:PO4:O3	5:B:510:HOH:O	1.91	0.88
1:E:370:ASP:HB2	1:E:374:ASN:HD21	1.39	0.88
2:A:505:PO4:O2	5:A:510:HOH:O	1.93	0.87
1:B:142:GLU:HG2	1:B:146:ARG:HD2	1.55	0.87
1:B:370:ASP:HB2	1:B:374:ASN:HD21	1.39	0.87
1:C:169:MET:HE1	1:C:327:SER:HA	1.57	0.87
1:C:462:ARG:HH21	1:C:466:ARG:HH22	1.21	0.87
1:D:323:ILE:HG12	1:D:345:ALA:HB3	1.53	0.87
1:F:370:ASP:HB2	1:F:374:ASN:HD21	1.39	0.87
1:F:142:GLU:HG2	1:F:146:ARG:HD2	1.55	0.87
1:B:219:VAL:HG22	1:B:373:LEU:HD13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HG22	1:C:373:LEU:HD13	1.55	0.87
1:E:323:ILE:HG12	1:E:345:ALA:HB3	1.53	0.87
2:E:505:PO4:O2	5:E:512:HOH:O	1.93	0.87
1:A:142:GLU:HG2	1:A:146:ARG:HD2	1.55	0.87
1:E:281:TRP:HB2	1:E:310:TYR:HD2	1.40	0.86
1:A:370:ASP:HB2	1:A:374:ASN:HD21	1.39	0.86
1:B:169:MET:HE1	1:B:327:SER:HA	1.57	0.86
1:D:281:TRP:HB2	1:D:310:TYR:HD2	1.40	0.86
1:B:462:ARG:HH21	1:B:466:ARG:HH22	1.21	0.86
1:C:209:HIS:CD2	2:C:503:PO4:O3	2.29	0.86
2:D:505:PO4:O2	5:D:510:HOH:O	1.93	0.86
1:A:462:ARG:HH21	1:A:466:ARG:HH22	1.21	0.86
1:F:209:HIS:CD2	2:F:504:PO4:O3	2.29	0.86
1:B:209:HIS:CD2	2:B:503:PO4:O3	2.29	0.86
1:E:169:MET:HE1	1:E:327:SER:HA	1.57	0.85
1:E:209:HIS:CD2	2:E:503:PO4:O3	2.29	0.85
1:F:169:MET:HE1	1:F:327:SER:HA	1.57	0.85
1:D:370:ASP:HB2	1:D:374:ASN:HD21	1.39	0.85
2:F:505:PO4:O2	5:F:512:HOH:O	1.93	0.85
1:B:72:TRP:CZ3	1:E:499:THR:HG22	2.12	0.85
2:C:504:PO4:O2	5:C:510:HOH:O	1.93	0.85
1:D:209:HIS:CD2	2:D:503:PO4:O3	2.29	0.85
1:A:209:HIS:CD2	2:A:502:PO4:O3	2.29	0.85
1:C:281:TRP:HB2	1:C:310:TYR:HD2	1.40	0.85
1:F:281:TRP:HB2	1:F:310:TYR:HD2	1.40	0.85
1:A:169:MET:HE1	1:A:327:SER:HA	1.57	0.85
2:F:503:PO4:O2	5:F:512:HOH:O	1.95	0.85
1:E:141:LEU:O	1:E:145:THR:HG23	1.77	0.85
2:B:504:PO4:O2	5:B:512:HOH:O	1.93	0.85
1:D:462:ARG:HH21	1:D:466:ARG:HH22	1.21	0.85
2:E:504:PO4:O3	5:E:510:HOH:O	1.95	0.84
2:E:502:PO4:O2	5:E:512:HOH:O	1.95	0.84
1:A:281:TRP:HB2	1:A:310:TYR:HD2	1.40	0.84
2:A:503:PO4:O2	5:A:510:HOH:O	1.95	0.84
1:B:281:TRP:HB2	1:B:310:TYR:HD2	1.40	0.84
1:D:169:MET:HE1	1:D:327:SER:HA	1.57	0.84
1:B:118:VAL:HG21	1:B:375:ALA:HB1	1.59	0.84
2:D:502:PO4:O2	5:D:510:HOH:O	1.95	0.84
1:E:462:ARG:HH21	1:E:466:ARG:HH22	1.21	0.84
1:A:141:LEU:O	1:A:145:THR:HG23	1.77	0.84
1:B:9:PHE:HE1	1:B:107:LEU:HD13	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:VAL:HG21	1:F:375:ALA:HB1	1.59	0.84
1:D:141:LEU:O	1:D:145:THR:HG23	1.77	0.84
1:C:9:PHE:HE1	1:C:107:LEU:HD13	1.43	0.83
2:C:502:PO4:O2	5:C:510:HOH:O	1.95	0.83
1:F:141:LEU:O	1:F:145:THR:HG23	1.77	0.83
1:A:46:ARG:HH11	1:A:46:ARG:HG3	1.44	0.83
1:B:46:ARG:HH11	1:B:46:ARG:HG3	1.44	0.83
1:D:46:ARG:HH11	1:D:46:ARG:HG3	1.44	0.83
1:D:118:VAL:HG21	1:D:375:ALA:HB1	1.59	0.83
1:A:9:PHE:HE1	1:A:107:LEU:HD13	1.43	0.83
1:A:118:VAL:HG21	1:A:375:ALA:HB1	1.59	0.83
1:C:118:VAL:HG21	1:C:375:ALA:CB	2.09	0.83
1:C:141:LEU:O	1:C:145:THR:HG23	1.77	0.83
1:D:391:HIS:HD2	4:D:507[A]:NAD:HO2N	1.26	0.83
1:E:118:VAL:HG21	1:E:375:ALA:HB1	1.59	0.83
1:F:9:PHE:HE1	1:F:107:LEU:HD13	1.43	0.83
1:A:118:VAL:HG21	1:A:375:ALA:CB	2.09	0.83
2:B:502:PO4:O2	5:B:512:HOH:O	1.95	0.82
1:B:118:VAL:HG21	1:B:375:ALA:CB	2.09	0.82
1:C:46:ARG:HG3	1:C:46:ARG:HH11	1.44	0.82
1:D:87:THR:H	4:E:507[A]:NAD:H72N	1.27	0.82
1:D:118:VAL:HG21	1:D:375:ALA:CB	2.09	0.82
1:E:118:VAL:HG21	1:E:375:ALA:CB	2.09	0.82
1:E:9:PHE:HE1	1:E:107:LEU:HD13	1.43	0.82
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.44	0.82
2:A:504:PO4:O3	5:A:514:HOH:O	1.97	0.82
1:B:141:LEU:O	1:B:145:THR:HG23	1.77	0.82
1:C:118:VAL:HG21	1:C:375:ALA:HB1	1.59	0.82
1:D:9:PHE:HE1	1:D:107:LEU:HD13	1.43	0.82
1:F:118:VAL:HG21	1:F:375:ALA:CB	2.09	0.82
1:C:242:PHE:HB3	1:C:268:ALA:HB2	1.62	0.82
1:C:87:THR:H	4:D:507[A]:NAD:H72N	1.27	0.81
4:C:507[A]:NAD:H72N	1:E:87:THR:H	1.27	0.81
4:A:507[A]:NAD:H72N	1:B:87:THR:H	1.27	0.81
1:C:87:THR:CG2	1:D:195:HIS:HE1	1.93	0.81
1:A:64:PRO:HG2	1:D:499:THR:HG21	1.61	0.81
3:E:506:AKG:O2	4:E:508:NAD:C5N	2.29	0.81
1:A:242:PHE:HB3	1:A:268:ALA:HB2	1.62	0.81
1:D:391:HIS:HA	4:D:507[A]:NAD:C3D	2.11	0.81
3:B:506:AKG:O2	4:B:508:NAD:C5N	2.29	0.81
3:D:506:AKG:O2	4:D:508:NAD:C5N	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:AKG:O2	4:C:508:NAD:C5N	2.29	0.81
1:F:46:ARG:HG3	1:F:46:ARG:HH11	1.44	0.80
1:F:242:PHE:HB3	1:F:268:ALA:HB2	1.62	0.80
1:F:391:HIS:HA	4:F:508[A]:NAD:C3D	2.11	0.80
3:A:506:AKG:O2	4:A:508:NAD:C5N	2.29	0.80
3:F:506:AKG:O2	4:F:507:NAD:C5N	2.29	0.80
1:B:242:PHE:HB3	1:B:268:ALA:HB2	1.62	0.80
1:E:242:PHE:HB3	1:E:268:ALA:HB2	1.62	0.80
1:A:457:MET:HE2	1:A:457:MET:HA	1.64	0.80
4:B:507[A]:NAD:H72N	1:F:87:THR:H	1.27	0.80
1:C:340:LYS:H	1:C:363:ARG:HH22	1.31	0.79
1:C:457:MET:HE2	1:C:457:MET:HA	1.64	0.79
1:D:242:PHE:HB3	1:D:268:ALA:HB2	1.62	0.79
1:F:340:LYS:H	1:F:363:ARG:HH22	1.31	0.79
1:A:87:THR:CG2	1:F:195:HIS:HE1	1.96	0.79
1:B:457:MET:HA	1:B:457:MET:HE2	1.64	0.79
1:E:275:GLU:OE1	4:E:508:NAD:H1B	1.83	0.79
1:A:87:THR:H	4:F:508[A]:NAD:H72N	1.27	0.79
1:D:275:GLU:OE1	4:D:508:NAD:H1B	1.83	0.79
1:C:275:GLU:OE1	4:C:508:NAD:H1B	1.83	0.79
1:D:457:MET:HE2	1:D:457:MET:HA	1.64	0.78
1:F:457:MET:HE2	1:F:457:MET:HA	1.64	0.78
1:A:275:GLU:OE1	4:A:508:NAD:H1B	1.83	0.78
1:B:275:GLU:OE1	4:B:508:NAD:H1B	1.83	0.78
1:D:340:LYS:H	1:D:363:ARG:HH22	1.31	0.78
1:C:499:THR:HG22	1:F:72:TRP:CZ3	2.19	0.78
1:E:340:LYS:H	1:E:363:ARG:HH22	1.31	0.77
1:B:340:LYS:H	1:B:363:ARG:HH22	1.31	0.77
1:E:457:MET:HE2	1:E:457:MET:HA	1.64	0.77
1:A:340:LYS:H	1:A:363:ARG:HH22	1.31	0.76
1:C:195:HIS:HE1	1:E:87:THR:HG21	1.49	0.76
1:F:275:GLU:OE1	4:F:507:NAD:H1B	1.83	0.76
1:B:72:TRP:HZ3	1:E:499:THR:HG22	1.48	0.76
1:B:282:ASN:ND2	1:B:284:ASP:H	1.84	0.76
1:F:313:SER:HB3	1:F:316:GLU:HB2	1.68	0.76
1:E:282:ASN:ND2	1:E:284:ASP:H	1.84	0.75
1:A:313:SER:HB3	1:A:316:GLU:HB2	1.68	0.75
1:C:282:ASN:ND2	1:C:284:ASP:H	1.84	0.75
1:B:391:HIS:HA	4:B:507[A]:NAD:C3D	2.15	0.75
1:C:298:HIS:O	1:C:300:THR:HG22	1.87	0.75
1:A:298:HIS:O	1:A:300:THR:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:MET:HE1	1:C:378:VAL:HG11	1.69	0.75
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.69	0.75
1:B:298:HIS:O	1:B:300:THR:HG22	1.87	0.75
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.69	0.75
1:D:282:ASN:ND2	1:D:284:ASP:H	1.84	0.75
1:A:282:ASN:ND2	1:A:284:ASP:H	1.84	0.74
1:A:111:MET:HE1	1:A:378:VAL:HG11	1.69	0.74
1:E:298:HIS:O	1:E:300:THR:HG22	1.87	0.74
1:F:298:HIS:O	1:F:300:THR:HG22	1.87	0.74
1:A:2:ASP:HB3	1:A:5:ASP:O	1.88	0.74
1:D:2:ASP:HB3	1:D:5:ASP:O	1.87	0.74
1:B:313:SER:HB3	1:B:316:GLU:HB2	1.68	0.74
1:C:2:ASP:HB3	1:C:5:ASP:O	1.88	0.74
1:C:195:HIS:HE1	1:E:87:THR:HG23	1.52	0.74
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.69	0.74
1:D:313:SER:HB3	1:D:316:GLU:HB2	1.68	0.74
1:A:391:HIS:HA	4:A:507[A]:NAD:C3D	2.15	0.74
1:E:111:MET:HE1	1:E:378:VAL:HG11	1.69	0.74
1:A:24:VAL:HG13	1:A:483:VAL:HG22	1.70	0.73
1:D:298:HIS:O	1:D:300:THR:HG22	1.87	0.73
1:E:2:ASP:HB3	1:E:5:ASP:O	1.87	0.73
1:E:313:SER:HB3	1:E:316:GLU:HB2	1.68	0.73
1:C:313:SER:HB3	1:C:316:GLU:HB2	1.68	0.73
1:A:499:THR:HG21	1:D:64:PRO:HG2	1.70	0.73
1:B:2:ASP:HB3	1:B:5:ASP:O	1.88	0.73
1:F:111:MET:HE1	1:F:378:VAL:HG11	1.69	0.73
1:F:282:ASN:ND2	1:F:284:ASP:H	1.84	0.73
1:B:238:MET:HE2	1:B:245:LYS:HE2	1.70	0.73
1:C:238:MET:HE2	1:C:245:LYS:HE2	1.70	0.73
1:A:195:HIS:HE1	1:B:87:THR:CG2	2.01	0.73
1:B:111:MET:HE1	1:B:378:VAL:HG11	1.69	0.73
1:C:391:HIS:HA	4:C:507[A]:NAD:C3D	2.16	0.73
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.69	0.73
1:E:24:VAL:HG13	1:E:483:VAL:HG22	1.71	0.73
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.69	0.73
1:F:2:ASP:HB3	1:F:5:ASP:O	1.88	0.73
1:F:24:VAL:HG13	1:F:483:VAL:HG22	1.71	0.73
1:F:238:MET:HE2	1:F:245:LYS:HE2	1.70	0.73
1:D:238:MET:HE2	1:D:245:LYS:HE2	1.70	0.73
1:E:20:GLY:O	1:E:24:VAL:HG22	1.89	0.73
1:B:195:HIS:CE1	1:F:87:THR:HG23	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLY:O	1:D:24:VAL:HG22	1.89	0.72
1:B:20:GLY:O	1:B:24:VAL:HG22	1.89	0.72
1:B:195:HIS:HE1	1:F:87:THR:HG23	1.51	0.72
1:C:195:HIS:CE1	1:E:87:THR:HG23	2.24	0.72
1:D:87:THR:CG2	1:E:195:HIS:HE1	2.02	0.72
1:A:20:GLY:O	1:A:24:VAL:HG22	1.89	0.72
1:A:499:THR:HG22	1:D:72:TRP:CZ3	2.23	0.72
1:F:20:GLY:O	1:F:24:VAL:HG22	1.89	0.72
1:A:66:ARG:H	1:D:501:THR:HG22	1.55	0.72
1:B:303:GLY:H	1:B:309:ILE:HD11	1.55	0.72
1:C:72:TRP:CZ3	1:F:499:THR:HG22	2.23	0.72
1:E:238:MET:HE2	1:E:245:LYS:HE2	1.70	0.72
1:C:239:THR:HG22	1:C:245:LYS:HE3	1.72	0.72
1:D:24:VAL:HG13	1:D:483:VAL:HG22	1.70	0.72
1:A:239:THR:HG22	1:A:245:LYS:HE3	1.72	0.72
1:A:391:HIS:HA	4:A:507[A]:NAD:HO3N	0.91	0.72
1:B:136:TYR:HB3	1:B:140:ASP:HB2	1.72	0.72
1:C:20:GLY:O	1:C:24:VAL:HG22	1.89	0.72
1:A:238:MET:HE2	1:A:245:LYS:HE2	1.70	0.72
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.69	0.72
1:B:24:VAL:HG13	1:B:483:VAL:HG22	1.70	0.72
1:D:303:GLY:H	1:D:309:ILE:HD11	1.55	0.72
1:F:303:GLY:H	1:F:309:ILE:HD11	1.55	0.72
1:B:195:HIS:HE1	1:F:87:THR:HG21	1.54	0.71
1:C:303:GLY:H	1:C:309:ILE:HD11	1.55	0.71
1:A:417:LEU:HD21	1:B:417:LEU:CD1	2.20	0.71
1:C:310:TYR:HD1	1:C:311:GLU:N	1.88	0.71
1:D:111:MET:HE1	1:D:378:VAL:HG11	1.69	0.71
1:E:418:GLU:OE2	1:E:427:THR:HA	1.91	0.71
1:F:310:TYR:HD1	1:F:311:GLU:N	1.88	0.71
1:A:136:TYR:HB3	1:A:140:ASP:HB2	1.72	0.71
1:A:418:GLU:OE2	1:A:427:THR:HA	1.91	0.71
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.71	0.71
1:F:136:TYR:HB3	1:F:140:ASP:HB2	1.72	0.71
1:A:391:HIS:CA	4:A:507[A]:NAD:HO3N	1.74	0.71
1:B:418:GLU:OE2	1:B:427:THR:HA	1.91	0.71
1:B:421:PHE:HE1	1:F:421:PHE:HE1	1.38	0.71
1:D:23:ILE:HD13	1:D:473:LEU:HD21	1.73	0.71
1:A:310:TYR:HD1	1:A:311:GLU:N	1.88	0.71
1:B:132:ASN:HD21	1:B:134:LYS:HG3	1.56	0.71
1:C:132:ASN:HD21	1:C:134:LYS:HG3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:H	1:A:309:ILE:HD11	1.55	0.71
1:B:7:PRO:HD2	1:B:329:LYS:HD2	1.73	0.71
1:C:195:HIS:CE1	1:E:87:THR:CG2	2.71	0.71
3:D:506:AKG:C1	4:D:508:NAD:C5N	2.69	0.71
1:E:23:ILE:HD13	1:E:473:LEU:HD21	1.73	0.71
3:E:506:AKG:C1	4:E:508:NAD:C5N	2.69	0.71
1:A:7:PRO:HD2	1:A:329:LYS:HD2	1.73	0.71
1:E:239:THR:HG22	1:E:245:LYS:HE3	1.72	0.71
1:E:310:TYR:HD1	1:E:311:GLU:N	1.88	0.71
1:C:136:TYR:HB3	1:C:140:ASP:HB2	1.72	0.71
1:D:7:PRO:HD2	1:D:329:LYS:HD2	1.73	0.71
1:B:23:ILE:HD13	1:B:473:LEU:HD21	1.73	0.71
1:F:418:GLU:OE2	1:F:427:THR:HA	1.91	0.71
1:E:136:TYR:HB3	1:E:140:ASP:HB2	1.72	0.70
1:B:417:LEU:CD2	1:F:417:LEU:CD1	2.69	0.70
1:C:378:VAL:CG1	3:C:506:AKG:O4	2.39	0.70
1:D:310:TYR:HD1	1:D:311:GLU:N	1.88	0.70
1:B:310:TYR:HD1	1:B:311:GLU:N	1.88	0.70
1:C:417:LEU:HD21	1:E:417:LEU:CD1	2.20	0.70
1:C:418:GLU:OE2	1:C:427:THR:HA	1.91	0.70
1:D:500:PHE:HE2	1:E:185:SER:HB2	1.56	0.70
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.73	0.70
1:F:23:ILE:HD13	1:F:473:LEU:HD21	1.73	0.70
1:F:239:THR:HG22	1:F:245:LYS:HE3	1.72	0.70
3:A:506:AKG:C1	4:A:508:NAD:C5N	2.69	0.70
3:C:506:AKG:C1	4:C:508:NAD:C5N	2.69	0.70
1:D:418:GLU:OE2	1:D:427:THR:HA	1.91	0.70
3:F:506:AKG:C1	4:F:507:NAD:C5N	2.69	0.70
1:B:391:HIS:C	4:B:507[A]:NAD:O3D	2.35	0.70
3:B:506:AKG:C1	4:B:508:NAD:C5N	2.69	0.70
1:D:378:VAL:CG1	3:D:506:AKG:O4	2.39	0.70
1:E:7:PRO:HD2	1:E:329:LYS:HD2	1.73	0.70
1:F:132:ASN:HD21	1:F:134:LYS:HG3	1.56	0.70
1:C:23:ILE:HD13	1:C:473:LEU:HD21	1.73	0.70
4:A:507[B]:NAD:H2D	1:B:459:ARG:NH2	2.07	0.70
1:C:25:GLU:O	1:C:29:VAL:HG23	1.92	0.70
1:E:25:GLU:O	1:E:29:VAL:HG23	1.92	0.70
1:A:459:ARG:NH2	4:F:508[B]:NAD:H2D	2.07	0.70
1:B:87:THR:OG1	1:B:88:PRO:HD3	1.92	0.70
1:C:459:ARG:NH2	4:D:507[B]:NAD:H2D	2.07	0.70
1:D:459:ARG:NH2	4:E:507[B]:NAD:H2D	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:VAL:CG1	3:E:506:AKG:O4	2.39	0.70
1:F:87:THR:OG1	1:F:88:PRO:HD3	1.92	0.70
1:C:7:PRO:HD2	1:C:329:LYS:HD2	1.73	0.69
1:D:132:ASN:HD21	1:D:134:LYS:HG3	1.56	0.69
1:D:239:THR:HG22	1:D:245:LYS:HE3	1.72	0.69
1:A:23:ILE:HD13	1:A:473:LEU:HD21	1.73	0.69
1:A:17:PHE:HA	1:A:482:TYR:CD2	2.28	0.69
1:B:409:LEU:HD11	1:F:409:LEU:HD22	1.73	0.69
1:D:25:GLU:O	1:D:29:VAL:HG23	1.92	0.69
1:E:391:HIS:HD2	4:E:507[A]:NAD:HO2N	1.39	0.69
1:A:25:GLU:O	1:A:29:VAL:HG23	1.92	0.69
1:A:428:ILE:HD13	1:A:428:ILE:N	2.07	0.69
1:E:132:ASN:HD21	1:E:134:LYS:HG3	1.56	0.69
1:D:428:ILE:HD13	1:D:428:ILE:N	2.08	0.69
1:E:87:THR:OG1	1:E:88:PRO:HD3	1.92	0.69
1:F:25:GLU:O	1:F:29:VAL:HG23	1.92	0.69
1:A:444:SER:OG	1:A:446:LYS:HG2	1.93	0.69
1:B:239:THR:HG22	1:B:245:LYS:HE3	1.72	0.69
1:D:87:THR:OG1	1:D:88:PRO:HD3	1.92	0.69
1:E:17:PHE:HA	1:E:482:TYR:CD2	2.28	0.69
1:E:460:SER:O	1:E:464:ILE:HG13	1.92	0.69
1:A:72:TRP:CZ3	1:D:499:THR:HG22	2.28	0.69
1:B:17:PHE:HA	1:B:482:TYR:CD2	2.28	0.69
1:B:25:GLU:O	1:B:29:VAL:HG23	1.92	0.69
1:C:46:ARG:HG3	1:C:46:ARG:NH1	2.07	0.69
1:F:444:SER:OG	1:F:446:LYS:HG2	1.93	0.69
1:F:460:SER:O	1:F:464:ILE:HG13	1.92	0.69
1:A:132:ASN:HD21	1:A:134:LYS:HG3	1.56	0.69
1:B:62:SER:HA	1:B:75:ILE:O	1.93	0.69
1:B:428:ILE:HD13	1:B:428:ILE:N	2.07	0.69
1:D:136:TYR:HB3	1:D:140:ASP:HB2	1.72	0.69
1:E:303:GLY:H	1:E:309:ILE:HD11	1.55	0.69
1:E:428:ILE:HD13	1:E:428:ILE:N	2.07	0.69
1:F:391:HIS:C	4:F:508[A]:NAD:O3D	2.36	0.69
1:F:391:HIS:N	4:F:508[A]:NAD:O3D	2.25	0.69
1:A:87:THR:OG1	1:A:88:PRO:HD3	1.92	0.69
1:B:444:SER:OG	1:B:446:LYS:HG2	1.93	0.69
4:B:507[B]:NAD:H2D	1:F:459:ARG:NH2	2.07	0.69
1:A:31:ASP:O	1:A:33:LYS:HG2	1.93	0.69
1:B:499:THR:HG22	1:E:72:TRP:CZ3	2.26	0.69
1:C:31:ASP:O	1:C:33:LYS:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:PHE:HA	1:F:482:TYR:CD2	2.28	0.69
1:F:378:VAL:CG1	3:F:506:AKG:O4	2.39	0.69
1:F:428:ILE:HD13	1:F:428:ILE:N	2.07	0.69
1:A:62:SER:HA	1:A:75:ILE:O	1.93	0.68
1:B:460:SER:O	1:B:464:ILE:HG13	1.92	0.68
1:C:428:ILE:HD13	1:C:428:ILE:N	2.07	0.68
1:D:460:SER:O	1:D:464:ILE:HG13	1.92	0.68
1:F:31:ASP:O	1:F:33:LYS:HG2	1.93	0.68
1:D:391:HIS:N	4:D:507[A]:NAD:O3D	2.27	0.68
1:C:87:THR:HG23	1:D:195:HIS:HE1	1.56	0.68
1:C:411:MET:HE2	1:C:415:GLU:HG3	1.76	0.68
1:A:29:VAL:HG21	1:A:42:ARG:HG2	1.76	0.68
1:C:62:SER:HA	1:C:75:ILE:O	1.93	0.68
1:C:460:SER:O	1:C:464:ILE:HG13	1.92	0.68
1:E:62:SER:HA	1:E:75:ILE:O	1.93	0.68
1:A:87:THR:HG23	1:F:195:HIS:HE1	1.57	0.68
1:A:460:SER:O	1:A:464:ILE:HG13	1.92	0.68
1:C:499:THR:HG22	1:F:72:TRP:HZ3	1.57	0.68
1:D:17:PHE:HA	1:D:482:TYR:CD2	2.28	0.68
1:F:62:SER:HA	1:F:75:ILE:O	1.93	0.68
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.07	0.68
1:C:87:THR:OG1	1:C:88:PRO:HD3	1.92	0.68
1:C:444:SER:OG	1:C:446:LYS:HG2	1.93	0.68
1:D:29:VAL:HG21	1:D:42:ARG:HG2	1.76	0.68
1:E:444:SER:OG	1:E:446:LYS:HG2	1.93	0.68
4:C:507[B]:NAD:H2D	1:E:459:ARG:NH2	2.07	0.68
1:D:391:HIS:C	4:D:507[A]:NAD:O3D	2.36	0.68
1:F:29:VAL:HG21	1:F:42:ARG:HG2	1.76	0.68
1:C:17:PHE:HA	1:C:482:TYR:CD2	2.28	0.68
1:C:391:HIS:C	4:C:507[A]:NAD:O3D	2.35	0.68
1:B:142:GLU:O	1:B:146:ARG:HG3	1.94	0.68
1:D:444:SER:OG	1:D:446:LYS:HG2	1.93	0.68
1:E:31:ASP:O	1:E:33:LYS:HG2	1.93	0.68
1:A:195:HIS:HE1	1:B:87:THR:HG23	1.59	0.68
1:D:411:MET:HE2	1:D:415:GLU:HG3	1.75	0.68
1:E:32:LEU:HD11	1:E:34:THR:OG1	1.94	0.68
1:F:391:HIS:HD2	4:F:508[A]:NAD:HO2N	1.39	0.68
1:C:142:GLU:O	1:C:146:ARG:HG3	1.94	0.67
1:A:499:THR:HG22	1:D:72:TRP:HZ3	1.60	0.67
1:B:195:HIS:CE1	1:F:87:THR:CG2	2.74	0.67
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD11	1:A:34:THR:OG1	1.94	0.67
1:A:142:GLU:O	1:A:146:ARG:HG3	1.94	0.67
1:B:29:VAL:HG21	1:B:42:ARG:HG2	1.76	0.67
1:D:142:GLU:O	1:D:146:ARG:HG3	1.94	0.67
1:D:62:SER:HA	1:D:75:ILE:O	1.93	0.67
1:E:142:GLU:O	1:E:146:ARG:HG3	1.94	0.67
1:A:281:TRP:HB2	1:A:310:TYR:CD2	2.28	0.67
1:B:31:ASP:O	1:B:33:LYS:HG2	1.93	0.67
1:D:32:LEU:HD11	1:D:34:THR:OG1	1.95	0.67
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.59	0.67
1:A:378:VAL:CG1	3:A:506:AKG:O4	2.39	0.67
1:B:411:MET:HE2	1:B:415:GLU:HG3	1.76	0.67
1:B:417:LEU:HD21	1:F:417:LEU:HD12	1.77	0.67
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.59	0.67
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.59	0.67
1:F:32:LEU:HD11	1:F:34:THR:OG1	1.94	0.67
1:C:260:MET:HE2	1:C:288:PRO:HG3	1.77	0.67
1:F:142:GLU:O	1:F:146:ARG:HG3	1.94	0.67
1:B:32:LEU:HD11	1:B:34:THR:OG1	1.95	0.67
1:B:378:VAL:CG1	3:B:506:AKG:O4	2.39	0.67
1:D:31:ASP:O	1:D:33:LYS:HG2	1.93	0.67
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.59	0.67
1:C:29:VAL:HG21	1:C:42:ARG:HG2	1.76	0.67
1:C:32:LEU:HD11	1:C:34:THR:OG1	1.94	0.67
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.24	0.67
1:D:417:LEU:CD1	1:E:417:LEU:HD21	2.25	0.67
1:E:411:MET:HE2	1:E:415:GLU:HG3	1.75	0.67
1:A:260:MET:HE2	1:A:288:PRO:HG3	1.77	0.66
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.59	0.66
1:B:260:MET:HE2	1:B:288:PRO:HG3	1.77	0.66
1:A:411:MET:HE2	1:A:415:GLU:HG3	1.76	0.66
1:B:72:TRP:HB3	1:E:51:ILE:HD11	1.78	0.66
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.59	0.66
1:C:339:VAL:HG22	1:C:363:ARG:HH21	1.61	0.66
1:E:29:VAL:HG21	1:E:42:ARG:HG2	1.76	0.66
1:D:281:TRP:HB2	1:D:310:TYR:CD2	2.28	0.66
1:A:190:TYR:CE2	1:B:162:VAL:HG11	2.31	0.66
1:D:339:VAL:HG22	1:D:363:ARG:HH21	1.61	0.66
1:F:411:MET:HE2	1:F:415:GLU:HG3	1.76	0.66
1:C:391:HIS:HA	4:C:507[A]:NAD:HO3N	0.84	0.66
1:C:499:THR:HG21	1:F:64:PRO:HG2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:TRP:HB2	1:C:310:TYR:CD2	2.28	0.66
1:F:339:VAL:HG22	1:F:363:ARG:HH21	1.61	0.66
1:D:260:MET:HE2	1:D:288:PRO:HG3	1.77	0.66
1:C:87:THR:HG23	1:D:195:HIS:CE1	2.31	0.65
1:C:79:ARG:HG2	1:C:157:PHE:HB3	1.79	0.65
1:F:411:MET:CE	1:F:415:GLU:HG3	2.26	0.65
1:A:132:ASN:ND2	1:A:134:LYS:HG3	2.12	0.65
1:A:391:HIS:C	4:A:507[A]:NAD:O3D	2.38	0.65
1:A:495:GLU:OE1	1:F:204:SER:OG	2.08	0.65
1:B:66:ARG:H	1:E:501:THR:HG22	1.61	0.65
1:C:72:TRP:HZ3	1:F:499:THR:HG22	1.59	0.65
1:E:260:MET:HE2	1:E:288:PRO:HG3	1.77	0.65
1:F:339:VAL:HG22	1:F:363:ARG:NH2	2.12	0.65
1:A:411:MET:CE	1:A:415:GLU:HG3	2.26	0.65
1:C:87:THR:HG21	1:D:195:HIS:HE1	1.61	0.65
1:D:339:VAL:HG22	1:D:363:ARG:NH2	2.12	0.65
1:E:281:TRP:HB2	1:E:310:TYR:CD2	2.28	0.65
1:E:353:THR:HG23	1:E:354:PRO:HD2	1.79	0.65
1:A:79:ARG:HG2	1:A:157:PHE:HB3	1.79	0.65
1:B:339:VAL:HG22	1:B:363:ARG:NH2	2.12	0.65
1:D:353:THR:HG23	1:D:354:PRO:HD2	1.79	0.65
1:F:260:MET:HE2	1:F:288:PRO:HG3	1.77	0.65
1:C:411:MET:CE	1:C:415:GLU:HG3	2.26	0.65
1:D:411:MET:CE	1:D:415:GLU:HG3	2.26	0.65
1:E:411:MET:CE	1:E:415:GLU:HG3	2.26	0.65
1:F:46:ARG:HG3	1:F:46:ARG:NH1	2.07	0.65
1:A:204:SER:OG	1:B:495:GLU:OE1	2.07	0.65
1:A:339:VAL:HG22	1:A:363:ARG:HH21	1.61	0.65
1:A:339:VAL:HG22	1:A:363:ARG:NH2	2.12	0.65
1:E:79:ARG:HG2	1:E:157:PHE:HB3	1.79	0.65
1:E:339:VAL:HG22	1:E:363:ARG:NH2	2.12	0.65
1:A:353:THR:HG23	1:A:354:PRO:HD2	1.79	0.65
1:B:499:THR:OG1	1:E:147:ARG:NH1	2.29	0.65
1:C:111:MET:HE1	1:C:378:VAL:CG1	2.27	0.65
1:C:339:VAL:HG22	1:C:363:ARG:NH2	2.12	0.65
1:D:132:ASN:ND2	1:D:134:LYS:HG3	2.12	0.65
1:F:132:ASN:ND2	1:F:134:LYS:HG3	2.12	0.64
1:E:111:MET:HE1	1:E:378:VAL:CG1	2.27	0.64
1:C:391:HIS:N	4:C:507[A]:NAD:O3D	2.28	0.64
1:E:339:VAL:HG22	1:E:363:ARG:HH21	1.61	0.64
1:B:132:ASN:ND2	1:B:134:LYS:HG3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLN:HA	1:D:40:GLN:NE2	2.12	0.64
1:A:501:THR:HG22	1:D:66:ARG:H	1.61	0.64
1:C:501:THR:HG22	1:F:66:ARG:H	1.62	0.64
1:F:281:TRP:HB2	1:F:310:TYR:CD2	2.28	0.64
1:B:79:ARG:HG2	1:B:157:PHE:HB3	1.79	0.64
1:D:87:THR:HG21	1:E:195:HIS:HE1	1.62	0.64
1:A:153:ALA:HB1	1:A:187:ILE:CD1	2.25	0.64
1:B:391:HIS:N	4:B:507[A]:NAD:O3D	2.29	0.64
1:B:411:MET:CE	1:B:415:GLU:HG3	2.26	0.64
1:D:46:ARG:HG3	1:D:46:ARG:NH1	2.07	0.64
1:E:132:ASN:ND2	1:E:134:LYS:HG3	2.12	0.64
1:A:40:GLN:NE2	1:A:40:GLN:HA	2.12	0.64
1:B:111:MET:HE1	1:B:378:VAL:CG1	2.27	0.64
1:B:339:VAL:HG22	1:B:363:ARG:HH21	1.61	0.64
1:C:132:ASN:ND2	1:C:134:LYS:HG3	2.12	0.64
1:D:495:GLU:OE1	1:E:204:SER:OG	2.08	0.64
1:F:111:MET:HE1	1:F:378:VAL:CG1	2.27	0.64
1:A:417:LEU:HD21	1:B:417:LEU:HD12	1.80	0.64
1:E:40:GLN:HA	1:E:40:GLN:NE2	2.12	0.64
1:F:353:THR:HG23	1:F:354:PRO:HD2	1.79	0.64
1:C:281:TRP:CB	1:C:310:TYR:HD2	2.11	0.64
1:B:499:THR:HG22	1:E:72:TRP:HZ3	1.62	0.63
1:F:40:GLN:NE2	1:F:40:GLN:HA	2.12	0.63
1:A:107:LEU:HG	1:A:126:LYS:HE2	1.80	0.63
1:B:353:THR:HG23	1:B:354:PRO:HD2	1.79	0.63
1:C:40:GLN:NE2	1:C:40:GLN:HA	2.13	0.63
1:D:111:MET:HE1	1:D:378:VAL:CG1	2.27	0.63
1:F:378:VAL:HG13	3:F:506:AKG:H31	1.81	0.63
1:A:500:PHE:HE2	1:F:185:SER:HB2	1.63	0.63
1:B:46:ARG:HG3	1:B:46:ARG:NH1	2.07	0.63
1:D:79:ARG:HG2	1:D:157:PHE:HB3	1.79	0.63
1:E:378:VAL:HG13	3:E:506:AKG:H31	1.81	0.63
1:B:107:LEU:HG	1:B:126:LYS:HE2	1.80	0.63
1:C:5:ASP:OD2	1:C:332:THR:HB	1.99	0.63
1:C:353:THR:HG23	1:C:354:PRO:HD2	1.79	0.63
1:F:79:ARG:HG2	1:F:157:PHE:HB3	1.79	0.63
1:B:40:GLN:HA	1:B:40:GLN:NE2	2.12	0.63
1:C:107:LEU:HG	1:C:126:LYS:HE2	1.80	0.63
1:A:5:ASP:OD2	1:A:332:THR:HB	1.99	0.63
1:A:111:MET:HE1	1:A:378:VAL:CG1	2.27	0.63
1:B:5:ASP:OD2	1:B:332:THR:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:HG	1:E:126:LYS:HE2	1.80	0.63
1:A:87:THR:HG23	1:F:195:HIS:CE1	2.33	0.63
1:C:393:SER:HB3	4:C:507[A]:NAD:PA	2.39	0.62
1:F:27:LYS:HA	1:F:30:GLU:HB3	1.81	0.62
1:B:27:LYS:HA	1:B:30:GLU:HB3	1.81	0.62
1:E:281:TRP:CB	1:E:310:TYR:HD2	2.11	0.62
1:F:142:GLU:CG	1:F:146:ARG:HD2	2.29	0.62
1:B:153:ALA:HB1	1:B:187:ILE:CD1	2.25	0.62
1:D:5:ASP:OD2	1:D:332:THR:HB	1.99	0.62
1:A:409:LEU:HD11	1:B:409:LEU:HD22	1.81	0.62
1:B:64:PRO:HG2	1:E:499:THR:HG21	1.79	0.62
1:B:281:TRP:CB	1:B:310:TYR:HD2	2.11	0.62
1:D:378:VAL:HG13	3:D:506:AKG:H31	1.81	0.62
1:F:5:ASP:OD2	1:F:332:THR:HB	1.99	0.62
1:F:107:LEU:HG	1:F:126:LYS:HE2	1.80	0.62
1:C:142:GLU:CG	1:C:146:ARG:HD2	2.29	0.62
1:E:5:ASP:OD2	1:E:332:THR:HB	1.99	0.62
1:E:27:LYS:HA	1:E:30:GLU:HB3	1.81	0.62
1:A:378:VAL:HG13	3:A:506:AKG:H31	1.81	0.62
1:C:27:LYS:HA	1:C:30:GLU:HB3	1.81	0.62
1:D:107:LEU:HG	1:D:126:LYS:HE2	1.80	0.62
1:E:142:GLU:CG	1:E:146:ARG:HD2	2.29	0.62
1:D:224:GLU:HA	1:D:227:ILE:HG22	1.82	0.62
1:A:32:LEU:HG	1:A:41:LYS:HG2	1.82	0.62
1:B:391:HIS:HD2	4:B:507[A]:NAD:HO2N	1.46	0.62
1:C:64:PRO:HG2	1:F:499:THR:HG21	1.82	0.62
1:D:27:LYS:HA	1:D:30:GLU:HB3	1.81	0.62
1:A:87:THR:HG21	1:F:195:HIS:HE1	1.64	0.61
1:A:391:HIS:HD2	4:A:507[A]:NAD:HO2N	1.41	0.61
1:F:452:GLY:O	1:F:456:THR:HG23	2.00	0.61
4:A:507[B]:NAD:O1N	4:A:507[B]:NAD:H2B	2.01	0.61
1:B:224:GLU:HA	1:B:227:ILE:HG22	1.82	0.61
1:D:452:GLY:O	1:D:456:THR:HG23	2.00	0.61
1:A:281:TRP:CB	1:A:310:TYR:HD2	2.11	0.61
1:C:378:VAL:HG13	3:C:506:AKG:H31	1.81	0.61
1:C:224:GLU:HA	1:C:227:ILE:HG22	1.82	0.61
1:C:452:GLY:O	1:C:456:THR:HG23	2.00	0.61
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.31	0.61
1:B:51:ILE:HA	1:E:74:VAL:CG2	2.31	0.61
1:B:154:LYS:HD2	1:C:189:HIS:CD2	2.36	0.61
1:B:378:VAL:HG13	3:B:506:AKG:H31	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:GLY:O	1:B:456:THR:HG23	2.00	0.61
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.36	0.61
4:C:507[B]:NAD:O1N	4:C:507[B]:NAD:H2B	2.01	0.61
4:D:507[B]:NAD:O1N	4:D:507[B]:NAD:H2B	2.00	0.61
1:E:32:LEU:HG	1:E:41:LYS:HG2	1.82	0.61
1:F:360:PHE:HD2	1:F:365:ILE:HD12	1.66	0.61
1:B:32:LEU:HG	1:B:41:LYS:HG2	1.82	0.61
1:B:281:TRP:CG	1:B:281:TRP:O	2.54	0.61
4:B:507[B]:NAD:H2B	4:B:507[B]:NAD:O1N	2.00	0.61
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.31	0.61
1:D:32:LEU:HG	1:D:41:LYS:HG2	1.82	0.61
1:F:32:LEU:HG	1:F:41:LYS:HG2	1.82	0.61
1:A:27:LYS:HA	1:A:30:GLU:HB3	1.81	0.61
1:A:233:MET:HE2	1:A:236:LEU:HG	1.83	0.61
1:A:360:PHE:HD2	1:A:365:ILE:HD12	1.66	0.61
1:B:281:TRP:HB2	1:B:310:TYR:CD2	2.28	0.61
1:D:281:TRP:CB	1:D:310:TYR:HD2	2.11	0.61
1:F:281:TRP:CG	1:F:281:TRP:O	2.54	0.61
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.31	0.61
1:E:233:MET:HE2	1:E:236:LEU:HG	1.83	0.61
1:F:224:GLU:HA	1:F:227:ILE:HG22	1.82	0.61
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.36	0.61
1:D:393:SER:HB3	4:D:507[A]:NAD:PA	2.41	0.61
1:E:224:GLU:HA	1:E:227:ILE:HG22	1.82	0.61
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.31	0.60
1:D:360:PHE:HD2	1:D:365:ILE:HD12	1.66	0.60
1:E:252:PHE:CZ	1:E:291:LEU:HD13	2.36	0.60
1:A:281:TRP:O	1:A:281:TRP:CG	2.54	0.60
1:F:233:MET:HE2	1:F:236:LEU:HG	1.83	0.60
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.36	0.60
1:C:281:TRP:CG	1:C:281:TRP:O	2.54	0.60
1:C:360:PHE:HD2	1:C:365:ILE:HD12	1.66	0.60
1:D:33:LYS:HA	1:D:41:LYS:NZ	2.16	0.60
1:D:94:ARG:HH21	1:D:168:ASN:HD21	1.49	0.60
4:E:507[B]:NAD:H2B	4:E:507[B]:NAD:O1N	2.00	0.60
1:A:224:GLU:HA	1:A:227:ILE:HG22	1.82	0.60
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.36	0.60
1:E:219:VAL:HG22	1:E:373:LEU:CD1	2.30	0.60
4:F:508[B]:NAD:O1N	4:F:508[B]:NAD:H2B	2.01	0.60
1:A:33:LYS:HA	1:A:41:LYS:NZ	2.16	0.60
1:A:69:ASP:O	1:A:71:SER:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:CG	1:A:146:ARG:HD2	2.29	0.60
1:B:69:ASP:O	1:B:71:SER:N	2.35	0.60
1:B:233:MET:HE2	1:B:236:LEU:HG	1.83	0.60
1:D:281:TRP:CG	1:D:281:TRP:O	2.54	0.60
1:E:452:GLY:O	1:E:456:THR:HG23	2.00	0.60
1:F:94:ARG:HH21	1:F:168:ASN:HD21	1.50	0.60
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.36	0.60
1:B:33:LYS:HA	1:B:41:LYS:NZ	2.16	0.60
1:C:69:ASP:O	1:C:71:SER:N	2.35	0.60
1:E:281:TRP:CG	1:E:281:TRP:O	2.54	0.60
1:F:393:SER:HB3	4:F:508[A]:NAD:PA	2.42	0.60
1:A:452:GLY:O	1:A:456:THR:HG23	2.00	0.60
1:C:32:LEU:HG	1:C:41:LYS:HG2	1.82	0.60
1:C:33:LYS:HA	1:C:41:LYS:NZ	2.16	0.60
1:D:69:ASP:O	1:D:71:SER:N	2.35	0.60
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.31	0.60
1:E:94:ARG:HH21	1:E:168:ASN:HD21	1.49	0.60
1:A:94:ARG:HH21	1:A:168:ASN:HD21	1.50	0.60
1:A:136:TYR:HB3	1:A:140:ASP:CB	2.32	0.60
1:B:360:PHE:HD2	1:B:365:ILE:HD12	1.66	0.60
1:C:87:THR:CG2	1:D:195:HIS:CE1	2.82	0.60
1:E:258:HIS:HD2	1:E:261:ARG:NH1	2.00	0.60
1:F:258:HIS:HD2	1:F:261:ARG:NH1	2.00	0.60
1:E:33:LYS:HA	1:E:41:LYS:NZ	2.16	0.59
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.59
1:F:153:ALA:HB1	1:F:187:ILE:CD1	2.25	0.59
1:C:136:TYR:HB3	1:C:140:ASP:CB	2.32	0.59
1:E:69:ASP:O	1:E:71:SER:N	2.35	0.59
1:E:393:SER:HB3	4:E:507[A]:NAD:PA	2.42	0.59
1:F:69:ASP:O	1:F:71:SER:N	2.35	0.59
1:A:219:VAL:HG22	1:A:373:LEU:CD1	2.30	0.59
1:B:136:TYR:HB3	1:B:140:ASP:CB	2.32	0.59
1:B:142:GLU:CG	1:B:146:ARG:HD2	2.29	0.59
1:D:233:MET:HE2	1:D:236:LEU:HG	1.83	0.59
1:E:360:PHE:HD2	1:E:365:ILE:HD12	1.66	0.59
1:C:276:SER:N	4:C:508:NAD:N3A	2.51	0.59
1:C:421:PHE:CD2	1:C:421:PHE:N	2.70	0.59
1:C:195:HIS:CE1	1:E:87:THR:HG21	2.35	0.59
1:C:233:MET:HE2	1:C:236:LEU:HG	1.83	0.59
1:D:153:ALA:HB1	1:D:187:ILE:CD1	2.25	0.59
1:D:459:ARG:NH2	4:E:507[B]:NAD:H6N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LYS:HA	1:F:41:LYS:NZ	2.16	0.59
1:A:459:ARG:NH2	4:F:508[B]:NAD:H6N	2.18	0.59
1:E:178:TRP:O	1:E:182:THR:HG23	2.03	0.59
1:E:247:PHE:CZ	1:E:270:CYS:HB2	2.38	0.59
1:F:421:PHE:CD2	1:F:421:PHE:N	2.70	0.59
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.00	0.59
4:A:507[B]:NAD:H6N	1:B:459:ARG:NH2	2.18	0.59
1:B:178:TRP:O	1:B:182:THR:HG23	2.03	0.59
1:C:178:TRP:O	1:C:182:THR:HG23	2.03	0.59
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.00	0.59
1:C:500:PHE:HE2	1:D:185:SER:HB2	1.68	0.59
1:D:219:VAL:HG22	1:D:373:LEU:CD1	2.30	0.59
1:B:421:PHE:CD2	1:B:421:PHE:N	2.70	0.59
1:E:391:HIS:C	4:E:507[A]:NAD:H4D	2.28	0.59
1:A:178:TRP:O	1:A:182:THR:HG23	2.03	0.59
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.38	0.59
1:B:74:VAL:CG2	1:E:51:ILE:HA	2.32	0.59
1:B:258:HIS:HD2	1:B:261:ARG:NH1	2.00	0.59
1:D:276:SER:N	4:D:508:NAD:N3A	2.51	0.59
1:D:421:PHE:N	1:D:421:PHE:CD2	2.70	0.59
1:A:238:MET:SD	1:A:342:LYS:CB	2.91	0.58
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.38	0.58
1:D:238:MET:SD	1:D:342:LYS:CB	2.91	0.58
1:D:258:HIS:HD2	1:D:261:ARG:NH1	2.00	0.58
1:E:238:MET:SD	1:E:342:LYS:CB	2.91	0.58
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.38	0.58
1:F:281:TRP:CB	1:F:310:TYR:HD2	2.11	0.58
1:A:185:SER:HB2	1:B:500:PHE:HE2	1.67	0.58
1:C:185:SER:HB2	1:E:500:PHE:HE2	1.68	0.58
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.68	0.58
1:D:142:GLU:CG	1:D:146:ARG:HD2	2.29	0.58
1:F:276:SER:N	4:F:507:NAD:N3A	2.51	0.58
1:A:195:HIS:CE1	1:B:87:THR:HG23	2.37	0.58
1:C:247:PHE:CZ	1:C:270:CYS:HB2	2.38	0.58
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.68	0.58
1:F:178:TRP:O	1:F:182:THR:HG23	2.03	0.58
1:A:276:SER:N	4:A:508:NAD:N3A	2.51	0.58
1:B:185:SER:HB2	1:F:500:PHE:HE2	1.69	0.58
1:B:276:SER:N	4:B:508:NAD:N3A	2.51	0.58
1:C:92:GLY:HA2	1:C:166:ALA:O	2.04	0.58
1:D:92:GLY:HA2	1:D:166:ALA:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.69	0.58
1:E:136:TYR:HB3	1:E:140:ASP:CB	2.32	0.58
1:F:136:TYR:HB3	1:F:140:ASP:CB	2.32	0.58
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.68	0.58
1:B:437:GLN:O	1:B:440:ILE:HG22	2.04	0.58
1:C:437:GLN:O	1:C:440:ILE:HG22	2.04	0.58
4:C:507[B]:NAD:H6N	1:E:459:ARG:NH2	2.18	0.58
1:E:92:GLY:HA2	1:E:166:ALA:O	2.04	0.58
1:F:437:GLN:O	1:F:440:ILE:HG22	2.04	0.58
1:A:437:GLN:O	1:A:440:ILE:HG22	2.04	0.58
1:B:51:ILE:HD11	1:E:72:TRP:HB3	1.84	0.58
1:C:238:MET:SD	1:C:342:LYS:CB	2.92	0.58
1:C:459:ARG:NH2	4:D:507[B]:NAD:H6N	2.18	0.58
1:D:258:HIS:CD2	1:D:261:ARG:NH1	2.72	0.58
1:E:421:PHE:CD2	1:E:421:PHE:N	2.70	0.58
1:B:258:HIS:CD2	1:B:261:ARG:NH1	2.72	0.58
1:B:395:GLY:HA3	1:B:399:PHE:CZ	2.39	0.58
4:B:507[B]:NAD:H6N	1:F:459:ARG:NH2	2.18	0.58
1:D:136:TYR:HB3	1:D:140:ASP:CB	2.32	0.58
1:D:247:PHE:CZ	1:D:270:CYS:HB2	2.38	0.58
1:E:91:GLY:HA3	1:E:125:ALA:O	2.04	0.58
1:F:92:GLY:HA2	1:F:166:ALA:O	2.04	0.58
1:F:258:HIS:CD2	1:F:261:ARG:NH1	2.72	0.58
1:D:66:ARG:HG2	1:D:70:GLY:O	2.04	0.58
1:D:178:TRP:O	1:D:182:THR:HG23	2.03	0.58
1:B:54:PRO:HG3	1:E:74:VAL:HG11	1.84	0.58
1:B:238:MET:SD	1:B:342:LYS:CB	2.91	0.58
1:C:91:GLY:HA3	1:C:125:ALA:O	2.04	0.58
1:C:233:MET:HA	1:C:236:LEU:HB2	1.86	0.58
1:C:258:HIS:CD2	1:C:261:ARG:NH1	2.72	0.58
1:D:395:GLY:HA3	1:D:399:PHE:CZ	2.39	0.58
1:E:258:HIS:CD2	1:E:261:ARG:NH1	2.72	0.58
1:E:276:SER:N	4:E:508:NAD:N3A	2.51	0.58
1:F:238:MET:SD	1:F:342:LYS:CB	2.91	0.58
1:A:258:HIS:CD2	1:A:261:ARG:NH1	2.72	0.57
1:B:91:GLY:HA3	1:B:125:ALA:O	2.04	0.57
1:D:437:GLN:O	1:D:440:ILE:HG22	2.04	0.57
1:E:395:GLY:HA3	1:E:399:PHE:CZ	2.39	0.57
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.69	0.57
1:F:395:GLY:HA3	1:F:399:PHE:CZ	2.39	0.57
1:A:66:ARG:HG2	1:A:70:GLY:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:MET:HA	1:E:236:LEU:HB2	1.86	0.57
1:A:395:GLY:HA3	1:A:399:PHE:CZ	2.39	0.57
1:B:94:ARG:HH21	1:B:168:ASN:HD21	1.50	0.57
1:C:409:LEU:HD22	1:D:409:LEU:HD11	1.86	0.57
1:E:66:ARG:HG2	1:E:70:GLY:O	2.04	0.57
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.87	0.57
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.87	0.57
1:D:233:MET:HA	1:D:236:LEU:HB2	1.86	0.57
1:E:41:LYS:O	1:E:45:VAL:HG23	2.05	0.57
1:A:92:GLY:HA2	1:A:166:ALA:O	2.04	0.57
1:A:233:MET:HA	1:A:236:LEU:HB2	1.86	0.57
1:F:219:VAL:HG22	1:F:373:LEU:CD1	2.30	0.57
1:B:219:VAL:HG22	1:B:373:LEU:CD1	2.30	0.57
1:B:250:GLN:O	1:B:325:ALA:HB3	2.05	0.57
1:C:94:ARG:HH21	1:C:168:ASN:HD21	1.50	0.57
1:E:153:ALA:HB1	1:E:187:ILE:CD1	2.25	0.57
1:A:391:HIS:N	4:A:507[A]:NAD:O3D	2.33	0.57
1:B:233:MET:HA	1:B:236:LEU:HB2	1.86	0.57
1:C:41:LYS:O	1:C:45:VAL:HG23	2.05	0.57
1:C:66:ARG:HG2	1:C:70:GLY:O	2.04	0.57
1:D:91:GLY:HA3	1:D:125:ALA:O	2.04	0.57
1:F:233:MET:HA	1:F:236:LEU:HB2	1.86	0.57
1:A:91:GLY:HA3	1:A:125:ALA:O	2.04	0.57
1:B:142:GLU:HG2	1:B:146:ARG:CD	2.33	0.57
1:C:37:THR:HG21	1:C:41:LYS:HE3	1.87	0.57
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.57
1:A:421:PHE:N	1:A:421:PHE:CD2	2.70	0.57
1:B:391:HIS:HA	4:B:507[A]:NAD:HO3N	0.74	0.57
1:F:41:LYS:O	1:F:45:VAL:HG23	2.05	0.57
1:B:92:GLY:HA2	1:B:166:ALA:O	2.04	0.57
1:C:250:GLN:O	1:C:325:ALA:HB3	2.05	0.57
1:C:395:GLY:HA3	1:C:399:PHE:CZ	2.39	0.57
1:D:250:GLN:O	1:D:325:ALA:HB3	2.05	0.57
1:B:66:ARG:HG2	1:B:70:GLY:O	2.04	0.56
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.69	0.56
1:C:72:TRP:HB3	1:F:51:ILE:HD11	1.86	0.56
1:E:437:GLN:O	1:E:440:ILE:HG22	2.04	0.56
1:F:33:LYS:HD3	1:F:41:LYS:HZ3	1.69	0.56
1:F:91:GLY:HA3	1:F:125:ALA:O	2.04	0.56
1:B:41:LYS:O	1:B:45:VAL:HG23	2.05	0.56
1:B:139:GLU:OE2	1:B:143:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:THR:HG21	1:D:41:LYS:HE3	1.87	0.56
1:D:41:LYS:O	1:D:45:VAL:HG23	2.05	0.56
1:E:37:THR:HG21	1:E:41:LYS:HE3	1.87	0.56
1:E:250:GLN:O	1:E:325:ALA:HB3	2.05	0.56
1:F:66:ARG:HG2	1:F:70:GLY:O	2.04	0.56
1:A:37:THR:HG21	1:A:41:LYS:HE3	1.87	0.56
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.87	0.56
1:C:153:ALA:HB1	1:C:187:ILE:CD1	2.25	0.56
1:C:409:LEU:HD11	1:E:409:LEU:HD22	1.87	0.56
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.87	0.56
1:E:139:GLU:OE2	1:E:143:LYS:HE3	2.06	0.56
1:F:29:VAL:HG13	1:F:41:LYS:HB3	1.87	0.56
1:F:254:ASN:HB3	4:F:507:NAD:O2N	2.06	0.56
1:C:139:GLU:OE2	1:C:143:LYS:HE3	2.06	0.56
1:F:139:GLU:OE2	1:F:143:LYS:HE3	2.06	0.56
1:A:41:LYS:O	1:A:45:VAL:HG23	2.05	0.56
1:B:117:VAL:HG21	1:B:371:LEU:HD13	1.87	0.56
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.41	0.56
1:C:29:VAL:HG13	1:C:41:LYS:HB3	1.87	0.56
1:C:118:VAL:O	1:C:118:VAL:HG12	2.06	0.56
1:D:139:GLU:OE2	1:D:143:LYS:HE3	2.06	0.56
1:D:337:PRO:HD3	1:D:359:ILE:HD13	1.88	0.56
1:E:254:ASN:HB3	4:E:508:NAD:O2N	2.06	0.56
1:F:117:VAL:HG21	1:F:371:LEU:HD13	1.87	0.56
1:B:393:SER:HB3	4:B:507[A]:NAD:PA	2.45	0.56
1:B:421:PHE:HE1	1:F:421:PHE:CE1	2.21	0.56
1:C:238:MET:HE1	1:C:320:ASP:HB3	1.88	0.56
1:C:254:ASN:HB3	4:C:508:NAD:O2N	2.06	0.56
1:A:29:VAL:HG13	1:A:41:LYS:HB3	1.87	0.56
1:A:142:GLU:HG2	1:A:146:ARG:CD	2.33	0.56
1:A:250:GLN:O	1:A:325:ALA:HB3	2.05	0.56
1:D:118:VAL:O	1:D:118:VAL:HG12	2.06	0.56
1:F:9:PHE:CE1	1:F:107:LEU:HD13	2.34	0.56
1:F:37:THR:HG21	1:F:41:LYS:HE3	1.87	0.56
1:F:39:GLU:O	1:F:42:ARG:HB2	2.06	0.56
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.41	0.56
1:B:37:THR:HG21	1:B:41:LYS:HE3	1.87	0.56
1:C:66:ARG:H	1:F:501:THR:HG22	1.71	0.56
1:F:250:GLN:O	1:F:325:ALA:HB3	2.05	0.56
1:B:29:VAL:HG13	1:B:41:LYS:HB3	1.87	0.56
1:C:391:HIS:HD2	4:C:507[A]:NAD:HO2N	1.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:HG21	1:D:371:LEU:HD13	1.87	0.56
1:D:304:PHE:CD1	1:D:305:PRO:HD2	2.41	0.56
1:B:238:MET:HE1	1:B:320:ASP:HB3	1.88	0.56
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.88	0.56
1:D:254:ASN:HB3	4:D:508:NAD:O2N	2.06	0.56
1:B:316:GLU:CD	1:B:338:ARG:HH11	2.14	0.55
1:D:421:PHE:N	1:D:421:PHE:HD2	2.04	0.55
1:E:421:PHE:N	1:E:421:PHE:HD2	2.04	0.55
1:F:316:GLU:CD	1:F:338:ARG:HH11	2.14	0.55
1:A:421:PHE:N	1:A:421:PHE:HD2	2.04	0.55
1:C:117:VAL:HG21	1:C:371:LEU:HD13	1.87	0.55
1:C:219:VAL:HG22	1:C:373:LEU:CD1	2.30	0.55
1:C:236:LEU:HD13	1:C:342:LYS:HB3	1.88	0.55
1:C:304:PHE:CD1	1:C:305:PRO:HD2	2.41	0.55
1:A:39:GLU:O	1:A:42:ARG:HB2	2.06	0.55
1:A:238:MET:HE1	1:A:320:ASP:HB3	1.88	0.55
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.88	0.55
1:E:117:VAL:HG21	1:E:371:LEU:HD13	1.87	0.55
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.87	0.55
1:A:139:GLU:OE2	1:A:143:LYS:HE3	2.06	0.55
1:A:236:LEU:HD13	1:A:342:LYS:HB3	1.88	0.55
1:A:254:ASN:HB3	4:A:508:NAD:O2N	2.06	0.55
1:A:316:GLU:CD	1:A:338:ARG:HH11	2.14	0.55
1:E:29:VAL:HG13	1:E:41:LYS:HB3	1.87	0.55
1:F:107:LEU:HB3	1:F:126:LYS:CG	2.30	0.55
1:F:236:LEU:HD13	1:F:342:LYS:HB3	1.88	0.55
1:A:35:ARG:O	1:A:37:THR:HG22	2.07	0.55
1:A:118:VAL:O	1:A:118:VAL:HG12	2.06	0.55
1:B:118:VAL:O	1:B:118:VAL:HG12	2.06	0.55
1:C:39:GLU:O	1:C:42:ARG:HB2	2.06	0.55
1:D:9:PHE:CE1	1:D:107:LEU:HD13	2.34	0.55
1:D:87:THR:HG23	1:E:195:HIS:HE1	1.70	0.55
1:E:337:PRO:HD3	1:E:359:ILE:HD13	1.88	0.55
1:F:238:MET:HE1	1:F:320:ASP:HB3	1.88	0.55
1:A:147:ARG:NH1	1:D:501:THR:OXT	2.40	0.55
1:B:35:ARG:O	1:B:37:THR:HG22	2.07	0.55
1:B:254:ASN:HB3	4:B:508:NAD:O2N	2.06	0.55
1:C:250:GLN:OE1	1:C:315:LEU:HD21	2.07	0.55
1:D:29:VAL:HG13	1:D:41:LYS:HB3	1.88	0.55
1:D:112:THR:HG22	1:D:124:GLY:CA	2.32	0.55
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HH11	1:A:46:ARG:CG	2.18	0.55
1:A:436:PHE:CZ	1:F:409:LEU:HD12	2.42	0.55
1:D:316:GLU:CD	1:D:338:ARG:HH11	2.15	0.55
1:E:316:GLU:CD	1:E:338:ARG:HH11	2.14	0.55
1:F:369:PRO:HG2	1:F:478:ARG:HA	1.89	0.55
1:F:462:ARG:NH2	1:F:466:ARG:HH22	2.00	0.55
1:A:117:VAL:HG21	1:A:371:LEU:HD13	1.87	0.55
1:C:24:VAL:HG11	1:C:483:VAL:HG13	1.89	0.55
1:C:316:GLU:CD	1:C:338:ARG:HH11	2.14	0.55
1:E:118:VAL:O	1:E:118:VAL:HG12	2.06	0.55
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.41	0.55
1:B:39:GLU:O	1:B:42:ARG:HB2	2.06	0.55
1:B:46:ARG:HH11	1:B:46:ARG:CG	2.18	0.55
1:B:425:GLY:O	1:B:427:THR:N	2.40	0.55
1:D:35:ARG:O	1:D:37:THR:HG22	2.07	0.55
1:E:250:GLN:OE1	1:E:315:LEU:HD21	2.07	0.55
1:F:118:VAL:O	1:F:118:VAL:HG12	2.06	0.55
1:F:122:PHE:HZ	1:F:385:ILE:HG21	1.72	0.55
1:A:72:TRP:HZ3	1:D:499:THR:HG22	1.71	0.55
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.89	0.55
1:C:74:VAL:CG2	1:F:51:ILE:HA	2.37	0.55
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.89	0.55
1:E:39:GLU:O	1:E:42:ARG:HB2	2.06	0.55
1:E:236:LEU:HD13	1:E:342:LYS:HB3	1.88	0.55
1:E:425:GLY:O	1:E:427:THR:N	2.40	0.55
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.05	0.55
1:F:425:GLY:O	1:F:427:THR:N	2.40	0.55
1:A:87:THR:O	1:A:89:CYS:N	2.40	0.54
1:B:87:THR:O	1:B:89:CYS:N	2.40	0.54
1:C:51:ILE:HD11	1:F:72:TRP:HB3	1.88	0.54
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.42	0.54
1:C:421:PHE:N	1:C:421:PHE:HD2	2.04	0.54
1:F:24:VAL:HG11	1:F:483:VAL:HG13	1.89	0.54
1:F:35:ARG:O	1:F:37:THR:HG22	2.07	0.54
1:F:95:TYR:OH	1:F:145:THR:HG22	2.07	0.54
1:F:337:PRO:HD3	1:F:359:ILE:HD13	1.88	0.54
1:B:421:PHE:N	1:B:421:PHE:HD2	2.04	0.54
1:C:19:ARG:HD2	1:C:479:THR:HG21	1.89	0.54
1:C:425:GLY:O	1:C:427:THR:N	2.40	0.54
1:D:46:ARG:HH11	1:D:46:ARG:CG	2.18	0.54
1:D:95:TYR:OH	1:D:145:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LEU:HD13	1:D:342:LYS:HB3	1.88	0.54
1:D:238:MET:HE1	1:D:320:ASP:HB3	1.88	0.54
1:D:250:GLN:OE1	1:D:315:LEU:HD21	2.07	0.54
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.42	0.54
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.42	0.54
1:A:369:PRO:HG2	1:A:478:ARG:HA	1.89	0.54
1:A:462:ARG:NH2	1:A:466:ARG:HH22	2.00	0.54
1:B:250:GLN:OE1	1:B:315:LEU:HD21	2.07	0.54
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.88	0.54
4:B:507[A]:NAD:O5D	4:B:507[A]:NAD:H6N	2.08	0.54
1:C:122:PHE:HZ	1:C:385:ILE:HG21	1.72	0.54
1:E:87:THR:O	1:E:89:CYS:N	2.40	0.54
1:E:238:MET:HE1	1:E:320:ASP:HB3	1.88	0.54
1:A:19:ARG:HD2	1:A:479:THR:HG21	1.89	0.54
1:A:250:GLN:OE1	1:A:315:LEU:HD21	2.07	0.54
1:B:122:PHE:HZ	1:B:385:ILE:HG21	1.72	0.54
1:B:157:PHE:CE1	1:E:155:LYS:HD2	2.42	0.54
1:B:369:PRO:HG2	1:B:478:ARG:HA	1.89	0.54
1:C:35:ARG:O	1:C:37:THR:HG22	2.07	0.54
1:C:233:MET:HE1	1:C:343:ILE:HD11	1.89	0.54
1:C:369:PRO:HG2	1:C:478:ARG:HA	1.89	0.54
1:E:107:LEU:HB3	1:E:126:LYS:CG	2.30	0.54
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.42	0.54
1:F:29:VAL:HA	1:F:45:VAL:HG21	1.90	0.54
1:F:250:GLN:OE1	1:F:315:LEU:HD21	2.07	0.54
1:B:498:VAL:HB	1:E:72:TRP:CZ2	2.43	0.54
1:D:87:THR:O	1:D:89:CYS:N	2.40	0.54
1:D:142:GLU:HG2	1:D:146:ARG:CD	2.33	0.54
1:D:425:GLY:O	1:D:427:THR:N	2.40	0.54
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.05	0.54
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.42	0.54
1:F:391:HIS:C	4:F:508[A]:NAD:H4D	2.33	0.54
1:A:87:THR:O	1:A:88:PRO:C	2.50	0.54
1:A:339:VAL:N	1:A:363:ARG:NH2	2.56	0.54
1:A:409:LEU:HD12	1:B:436:PHE:CZ	2.43	0.54
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.42	0.54
1:C:33:LYS:HD3	1:C:41:LYS:HZ3	1.72	0.54
1:D:339:VAL:N	1:D:363:ARG:NH2	2.56	0.54
4:E:507[A]:NAD:H6N	4:E:507[A]:NAD:O5D	2.08	0.54
1:A:459:ARG:NH2	4:F:508[B]:NAD:C6N	2.71	0.54
1:B:55:CYS:O	1:E:62:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.06	0.54
4:B:507[B]:NAD:C6N	1:F:459:ARG:NH2	2.71	0.54
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.05	0.54
1:C:310:TYR:CD1	1:C:311:GLU:N	2.75	0.54
4:C:507[B]:NAD:C6N	1:E:459:ARG:NH2	2.71	0.54
1:D:19:ARG:HD2	1:D:479:THR:HG21	1.89	0.54
1:F:112:THR:HG22	1:F:124:GLY:CA	2.32	0.54
1:F:233:MET:HE1	1:F:343:ILE:HD11	1.90	0.54
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.26	0.54
1:C:318:ASP:HA	1:C:340:LYS:HG3	1.90	0.54
1:C:459:ARG:NH2	4:D:507[B]:NAD:C6N	2.71	0.54
4:C:507[A]:NAD:H6N	4:C:507[A]:NAD:O5D	2.08	0.54
1:D:39:GLU:O	1:D:42:ARG:HB2	2.06	0.54
1:F:34:THR:HG21	1:F:44:ARG:NH1	2.23	0.54
4:F:508[A]:NAD:H6N	4:F:508[A]:NAD:O5D	2.08	0.54
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.89	0.54
1:A:29:VAL:HA	1:A:45:VAL:HG21	1.90	0.54
1:A:34:THR:HG21	1:A:44:ARG:NH1	2.23	0.54
1:A:425:GLY:O	1:A:427:THR:N	2.40	0.54
4:A:507[A]:NAD:O5D	4:A:507[A]:NAD:H6N	2.08	0.54
4:A:507[B]:NAD:C6N	1:B:459:ARG:NH2	2.71	0.54
1:B:189:HIS:CD2	1:C:154:LYS:HD2	2.43	0.54
4:C:507[B]:NAD:N3A	1:E:488:LYS:HB3	2.23	0.54
1:D:459:ARG:NH2	4:E:507[B]:NAD:C6N	2.71	0.54
1:E:19:ARG:HD2	1:E:479:THR:HG21	1.89	0.54
1:E:35:ARG:O	1:E:37:THR:HG22	2.07	0.54
1:E:142:GLU:HG2	1:E:146:ARG:CD	2.34	0.54
1:E:303:GLY:N	1:E:309:ILE:HD11	2.23	0.54
1:F:87:THR:O	1:F:89:CYS:N	2.40	0.54
1:F:421:PHE:N	1:F:421:PHE:HD2	2.04	0.54
1:A:95:TYR:OH	1:A:145:THR:HG22	2.07	0.54
4:A:507[B]:NAD:N3A	1:B:488:LYS:HB3	2.23	0.54
1:B:5:ASP:HB2	1:B:333:LYS:HE2	1.90	0.54
1:B:236:LEU:CD1	1:B:342:LYS:HB3	2.38	0.54
1:C:87:THR:O	1:C:89:CYS:N	2.40	0.54
1:C:95:TYR:OH	1:C:145:THR:HG22	2.07	0.54
1:F:303:GLY:N	1:F:309:ILE:HD11	2.23	0.54
1:B:339:VAL:N	1:B:363:ARG:NH2	2.56	0.53
1:D:233:MET:HE1	1:D:343:ILE:HD11	1.90	0.53
1:D:318:ASP:HA	1:D:340:LYS:HG3	1.90	0.53
4:D:507[A]:NAD:O5D	4:D:507[A]:NAD:H6N	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ASP:HB2	1:E:333:LYS:HE2	1.90	0.53
1:E:95:TYR:OH	1:E:145:THR:HG22	2.07	0.53
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.26	0.53
1:E:462:ARG:HE	1:E:466:ARG:NH2	2.06	0.53
1:F:87:THR:O	1:F:88:PRO:C	2.50	0.53
1:A:122:PHE:HZ	1:A:385:ILE:HG21	1.72	0.53
1:A:162:VAL:HG11	1:F:190:TYR:CE2	2.43	0.53
1:A:233:MET:HE1	1:A:343:ILE:HD11	1.90	0.53
1:A:447:ASP:O	1:A:451:SER:HB3	2.08	0.53
3:A:506:AKG:C1	4:A:508:NAD:H5N	2.39	0.53
1:B:19:ARG:HD2	1:B:479:THR:HG21	1.89	0.53
1:B:236:LEU:HD13	1:B:342:LYS:HB3	1.88	0.53
1:B:318:ASP:HA	1:B:340:LYS:HG3	1.90	0.53
4:B:507[B]:NAD:N3A	1:F:488:LYS:HB3	2.23	0.53
1:D:17:PHE:HA	1:D:482:TYR:HD2	1.73	0.53
1:E:122:PHE:HZ	1:E:385:ILE:HG21	1.72	0.53
1:F:236:LEU:CD1	1:F:342:LYS:HB3	2.38	0.53
1:A:189:HIS:CD2	1:E:154:LYS:HD2	2.43	0.53
1:B:33:LYS:HA	1:B:41:LYS:HZ1	1.73	0.53
1:B:195:HIS:CE1	1:F:87:THR:HG21	2.39	0.53
1:B:447:ASP:O	1:B:451:SER:HB3	2.08	0.53
1:C:34:THR:HG21	1:C:44:ARG:NH1	2.23	0.53
1:C:236:LEU:CD1	1:C:342:LYS:HB3	2.38	0.53
1:D:258:HIS:HA	1:D:261:ARG:HB2	1.91	0.53
1:E:369:PRO:HG2	1:E:478:ARG:HA	1.89	0.53
1:A:17:PHE:HA	1:A:482:TYR:HD2	1.73	0.53
1:A:107:LEU:HB3	1:A:126:LYS:CG	2.30	0.53
1:A:236:LEU:CD1	1:A:342:LYS:HB3	2.38	0.53
1:A:258:HIS:HA	1:A:261:ARG:HB2	1.91	0.53
1:A:462:ARG:HE	1:A:466:ARG:NH2	2.06	0.53
1:A:499:THR:CG2	1:D:64:PRO:HG2	2.39	0.53
1:B:233:MET:HE1	1:B:343:ILE:HD11	1.90	0.53
1:B:319:CYS:O	1:B:341:ALA:HA	2.09	0.53
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.89	0.53
1:E:112:THR:HG22	1:E:124:GLY:CA	2.32	0.53
1:E:239:THR:HG23	1:E:240:PRO:N	2.23	0.53
1:F:274:GLY:CA	1:F:314:ILE:HG13	2.39	0.53
1:F:339:VAL:N	1:F:363:ARG:NH2	2.56	0.53
1:B:34:THR:HG21	1:B:44:ARG:NH1	2.23	0.53
1:B:56:ASN:HD22	1:B:84:HIS:CD2	2.27	0.53
1:B:117:VAL:HG23	1:B:485:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASP:O	1:C:451:SER:HB3	2.08	0.53
1:D:29:VAL:HA	1:D:45:VAL:HG21	1.90	0.53
1:D:34:THR:HG21	1:D:44:ARG:NH1	2.23	0.53
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.06	0.53
1:D:282:ASN:HD21	1:D:284:ASP:HB2	1.74	0.53
1:D:303:GLY:N	1:D:309:ILE:HD11	2.23	0.53
1:D:319:CYS:O	1:D:341:ALA:HA	2.09	0.53
1:D:369:PRO:HG2	1:D:478:ARG:HA	1.89	0.53
1:D:447:ASP:O	1:D:451:SER:HB3	2.08	0.53
1:E:233:MET:HE1	1:E:343:ILE:HD11	1.89	0.53
1:E:236:LEU:CD1	1:E:342:LYS:HB3	2.38	0.53
1:E:447:ASP:O	1:E:451:SER:HB3	2.08	0.53
1:F:5:ASP:HB2	1:F:333:LYS:HE2	1.90	0.53
1:A:239:THR:HG23	1:A:240:PRO:N	2.23	0.53
1:A:274:GLY:CA	1:A:314:ILE:HG13	2.39	0.53
1:C:112:THR:HG22	1:C:124:GLY:CA	2.32	0.53
1:C:258:HIS:CD2	1:C:261:ARG:HH11	2.26	0.53
1:C:274:GLY:CA	1:C:314:ILE:HG13	2.39	0.53
1:D:5:ASP:HB2	1:D:333:LYS:HE2	1.90	0.53
1:D:274:GLY:CA	1:D:314:ILE:HG13	2.39	0.53
1:D:391:HIS:C	4:D:507[A]:NAD:H4D	2.33	0.53
1:A:319:CYS:O	1:A:341:ALA:HA	2.09	0.53
1:B:95:TYR:OH	1:B:145:THR:HG22	2.07	0.53
1:C:56:ASN:HD22	1:C:84:HIS:CD2	2.27	0.53
1:C:142:GLU:HG2	1:C:146:ARG:CD	2.33	0.53
1:C:379:THR:O	1:C:382:TYR:HB3	2.09	0.53
1:C:488:LYS:HB3	4:D:507[B]:NAD:N3A	2.23	0.53
1:D:122:PHE:HZ	1:D:385:ILE:HG21	1.72	0.53
1:D:462:ARG:HE	1:D:466:ARG:NH2	2.06	0.53
1:D:488:LYS:HB3	4:E:507[B]:NAD:N3A	2.23	0.53
1:E:339:VAL:N	1:E:363:ARG:NH2	2.56	0.53
1:E:379:THR:O	1:E:382:TYR:HB3	2.09	0.53
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.74	0.53
1:F:56:ASN:HD22	1:F:84:HIS:CD2	2.27	0.53
1:F:310:TYR:CD1	1:F:311:GLU:N	2.75	0.53
1:F:462:ARG:HE	1:F:466:ARG:NH2	2.07	0.53
1:A:488:LYS:HB3	4:F:508[B]:NAD:N3A	2.23	0.53
1:B:258:HIS:HA	1:B:261:ARG:HB2	1.91	0.53
1:B:274:GLY:CA	1:B:314:ILE:HG13	2.39	0.53
1:D:310:TYR:CD1	1:D:311:GLU:N	2.75	0.53
1:D:379:THR:O	1:D:382:TYR:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ARG:NH2	1:E:478:ARG:HD2	2.24	0.53
1:E:258:HIS:HA	1:E:261:ARG:HB2	1.91	0.53
1:E:282:ASN:HD21	1:E:284:ASP:HB2	1.74	0.53
1:E:360:PHE:CD2	1:E:365:ILE:HD12	2.44	0.53
1:F:282:ASN:HD21	1:F:284:ASP:HB2	1.74	0.53
3:F:506:AKG:C1	4:F:507:NAD:H5N	2.39	0.53
1:A:5:ASP:HB2	1:A:333:LYS:HE2	1.90	0.53
1:A:9:PHE:CE1	1:A:107:LEU:HD13	2.34	0.53
1:A:19:ARG:NH2	1:A:478:ARG:HD2	2.24	0.53
1:B:340:LYS:N	1:B:363:ARG:HH22	2.05	0.53
1:B:360:PHE:CD2	1:B:365:ILE:HD12	2.44	0.53
1:C:162:VAL:HG11	1:D:190:TYR:CE2	2.44	0.53
1:C:360:PHE:CD2	1:C:365:ILE:HD12	2.44	0.53
1:D:107:LEU:HB3	1:D:126:LYS:CG	2.30	0.53
1:D:239:THR:HG23	1:D:240:PRO:N	2.23	0.53
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.26	0.53
1:E:29:VAL:HA	1:E:45:VAL:HG21	1.90	0.53
1:E:40:GLN:HA	1:E:43:ASN:HD22	1.74	0.53
1:E:48:ILE:O	1:E:52:ILE:HG13	2.09	0.53
1:E:319:CYS:O	1:E:341:ALA:HA	2.09	0.53
1:F:19:ARG:NH2	1:F:478:ARG:HD2	2.24	0.53
1:F:258:HIS:HA	1:F:261:ARG:HB2	1.91	0.53
1:A:379:THR:O	1:A:382:TYR:HB3	2.09	0.53
1:B:348:ALA:HB3	1:B:351:PRO:HG3	1.91	0.53
1:C:19:ARG:NH2	1:C:478:ARG:HD2	2.24	0.53
1:C:29:VAL:HA	1:C:45:VAL:HG21	1.90	0.53
1:C:200:GLY:HA2	1:C:211:ARG:HD3	1.91	0.53
1:C:239:THR:HG23	1:C:240:PRO:N	2.23	0.53
1:F:447:ASP:O	1:F:451:SER:HB3	2.09	0.53
1:A:201:LYS:NZ	1:A:388:ASN:HD21	2.05	0.52
1:B:282:ASN:HD21	1:B:284:ASP:HB2	1.74	0.52
1:B:418:GLU:HG2	1:B:428:ILE:HG12	1.91	0.52
1:C:46:ARG:HH11	1:C:46:ARG:CG	2.18	0.52
1:C:117:VAL:HG23	1:C:485:ALA:HB2	1.91	0.52
1:C:339:VAL:N	1:C:363:ARG:NH2	2.56	0.52
1:C:418:GLU:HG2	1:C:428:ILE:HG12	1.91	0.52
3:C:506:AKG:C1	4:C:508:NAD:H5N	2.39	0.52
1:D:40:GLN:HA	1:D:43:ASN:HD22	1.74	0.52
3:E:506:AKG:C1	4:E:508:NAD:H5N	2.39	0.52
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.31	0.52
1:F:418:GLU:HG2	1:F:428:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:O	1:A:338:ARG:NH2	2.43	0.52
1:B:107:LEU:HB3	1:B:126:LYS:CG	2.30	0.52
1:B:334:SER:O	1:B:338:ARG:NH2	2.43	0.52
1:C:48:ILE:O	1:C:52:ILE:HG13	2.09	0.52
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.36	0.52
1:C:258:HIS:HA	1:C:261:ARG:HB2	1.91	0.52
1:C:260:MET:HE2	1:C:288:PRO:CG	2.40	0.52
1:C:303:GLY:N	1:C:309:ILE:HD11	2.23	0.52
1:D:108:ALA:O	1:D:111:MET:HB2	2.09	0.52
1:E:9:PHE:CE1	1:E:107:LEU:HD13	2.34	0.52
1:E:34:THR:HG21	1:E:44:ARG:NH1	2.23	0.52
1:E:117:VAL:HG23	1:E:485:ALA:HB2	1.91	0.52
1:F:19:ARG:HD2	1:F:479:THR:HG21	1.89	0.52
1:A:56:ASN:HD22	1:A:84:HIS:CD2	2.27	0.52
1:A:318:ASP:HA	1:A:340:LYS:HG3	1.90	0.52
1:A:348:ALA:HB3	1:A:351:PRO:HG3	1.91	0.52
1:B:435:GLU:H	1:B:435:GLU:CD	2.18	0.52
1:C:5:ASP:HB2	1:C:333:LYS:HE2	1.90	0.52
1:C:435:GLU:CD	1:C:435:GLU:H	2.18	0.52
1:D:87:THR:HG23	1:E:195:HIS:CE1	2.44	0.52
1:D:236:LEU:CD1	1:D:342:LYS:HB3	2.38	0.52
3:D:506:AKG:C1	4:D:508:NAD:H5N	2.39	0.52
1:F:318:ASP:HA	1:F:340:LYS:HG3	1.90	0.52
1:A:48:ILE:O	1:A:52:ILE:HG13	2.09	0.52
1:E:260:MET:HE2	1:E:288:PRO:CG	2.40	0.52
1:E:348:ALA:HB3	1:E:351:PRO:HG3	1.91	0.52
1:F:108:ALA:O	1:F:111:MET:HB2	2.09	0.52
1:F:258:HIS:CD2	1:F:261:ARG:HH11	2.26	0.52
1:F:379:THR:O	1:F:382:TYR:HB3	2.09	0.52
1:A:108:ALA:O	1:A:111:MET:HB2	2.09	0.52
1:B:462:ARG:HE	1:B:466:ARG:NH2	2.06	0.52
3:B:506:AKG:C1	4:B:508:NAD:H5N	2.39	0.52
1:C:66:ARG:NH1	1:C:70:GLY:HA2	2.25	0.52
1:C:108:ALA:O	1:C:111:MET:HB2	2.09	0.52
1:D:56:ASN:HD22	1:D:84:HIS:CD2	2.27	0.52
1:D:246:THR:N	1:D:320:ASP:OD1	2.43	0.52
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.31	0.52
1:E:318:ASP:HA	1:E:340:LYS:HG3	1.90	0.52
1:A:246:THR:N	1:A:320:ASP:OD1	2.43	0.52
1:C:462:ARG:HE	1:C:466:ARG:NH2	2.06	0.52
1:F:200:GLY:HA2	1:F:211:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH1	1:A:70:GLY:HA2	2.25	0.52
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.26	0.52
1:B:379:THR:O	1:B:382:TYR:HB3	2.09	0.52
1:D:19:ARG:NH2	1:D:478:ARG:HD2	2.24	0.52
1:D:48:ILE:O	1:D:52:ILE:HG13	2.09	0.52
1:D:117:VAL:HG23	1:D:485:ALA:HB2	1.91	0.52
1:E:33:LYS:HD3	1:E:41:LYS:HZ3	1.74	0.52
1:F:48:ILE:O	1:F:52:ILE:HG13	2.09	0.52
1:F:319:CYS:O	1:F:341:ALA:HA	2.09	0.52
1:A:117:VAL:HG23	1:A:485:ALA:HB2	1.91	0.52
1:A:200:GLY:HA2	1:A:211:ARG:HD3	1.91	0.52
1:B:44:ARG:NH1	1:B:494:ASN:HD21	2.08	0.52
1:C:246:THR:N	1:C:320:ASP:OD1	2.43	0.52
1:E:66:ARG:NH1	1:E:70:GLY:HA2	2.25	0.52
1:E:250:GLN:CD	1:E:315:LEU:HD21	2.35	0.52
1:E:413:VAL:O	1:E:417:LEU:HG	2.10	0.52
1:F:44:ARG:CZ	1:F:494:ASN:HD21	2.23	0.52
1:F:46:ARG:HH11	1:F:46:ARG:CG	2.18	0.52
1:F:66:ARG:NH1	1:F:70:GLY:HA2	2.25	0.52
1:F:260:MET:HE2	1:F:288:PRO:CG	2.40	0.52
1:A:44:ARG:NH1	1:A:494:ASN:HD21	2.08	0.52
1:A:51:ILE:HD11	1:D:72:TRP:HB3	1.92	0.52
1:A:112:THR:HG22	1:A:124:GLY:CA	2.32	0.52
1:A:339:VAL:H	1:A:363:ARG:NH2	2.08	0.52
1:B:29:VAL:HA	1:B:45:VAL:HG21	1.90	0.52
1:B:66:ARG:NH1	1:B:70:GLY:HA2	2.25	0.52
1:B:108:ALA:O	1:B:111:MET:HB2	2.09	0.52
1:B:282:ASN:ND2	1:B:282:ASN:C	2.68	0.52
1:D:418:GLU:HG2	1:D:428:ILE:HG12	1.91	0.52
1:E:274:GLY:CA	1:E:314:ILE:HG13	2.39	0.52
1:F:413:VAL:O	1:F:417:LEU:HG	2.10	0.52
1:A:40:GLN:HA	1:A:43:ASN:HD22	1.74	0.52
1:A:260:MET:HE2	1:A:288:PRO:CG	2.40	0.52
1:B:48:ILE:O	1:B:52:ILE:HG13	2.09	0.52
1:B:200:GLY:HA2	1:B:211:ARG:HD3	1.91	0.52
1:B:239:THR:HG23	1:B:240:PRO:N	2.23	0.52
1:B:246:THR:N	1:B:320:ASP:OD1	2.43	0.52
1:C:339:VAL:H	1:C:363:ARG:NH2	2.08	0.52
1:D:413:VAL:O	1:D:417:LEU:HG	2.10	0.52
1:F:117:VAL:HG23	1:F:485:ALA:HB2	1.91	0.52
1:F:246:THR:N	1:F:320:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HG2	1:A:380:VAL:HG12	1.93	0.51
1:A:360:PHE:CD2	1:A:365:ILE:HD12	2.44	0.51
1:A:413:VAL:O	1:A:417:LEU:HG	2.10	0.51
1:B:339:VAL:H	1:B:363:ARG:NH2	2.09	0.51
1:C:44:ARG:NH1	1:C:494:ASN:HD21	2.08	0.51
1:C:334:SER:O	1:C:338:ARG:NH2	2.43	0.51
1:D:250:GLN:CD	1:D:315:LEU:HD21	2.35	0.51
1:D:435:GLU:CD	1:D:435:GLU:H	2.18	0.51
1:E:200:GLY:HA2	1:E:211:ARG:HD3	1.91	0.51
1:E:282:ASN:ND2	1:E:282:ASN:C	2.68	0.51
1:E:418:GLU:HG2	1:E:428:ILE:HG12	1.91	0.51
1:F:142:GLU:HG2	1:F:146:ARG:CD	2.33	0.51
1:F:239:THR:HG23	1:F:240:PRO:N	2.23	0.51
1:A:282:ASN:HD21	1:A:284:ASP:HB2	1.74	0.51
1:A:418:GLU:HG2	1:A:428:ILE:HG12	1.91	0.51
1:B:44:ARG:CZ	1:B:494:ASN:HD21	2.23	0.51
1:B:250:GLN:CD	1:B:315:LEU:HD21	2.35	0.51
1:C:44:ARG:CZ	1:C:494:ASN:HD21	2.23	0.51
1:C:252:PHE:HD2	1:C:295:LYS:HE3	1.76	0.51
1:C:282:ASN:HD21	1:C:284:ASP:HB2	1.74	0.51
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.46	0.51
1:E:108:ALA:O	1:E:111:MET:HB2	2.09	0.51
1:E:339:VAL:H	1:E:363:ARG:NH2	2.09	0.51
1:F:334:SER:O	1:F:338:ARG:NH2	2.43	0.51
1:F:348:ALA:HB3	1:F:351:PRO:HG3	1.91	0.51
1:F:360:PHE:CD2	1:F:365:ILE:HD12	2.44	0.51
1:A:250:GLN:CD	1:A:315:LEU:HD21	2.35	0.51
1:A:435:GLU:CD	1:A:435:GLU:H	2.18	0.51
1:B:19:ARG:NH2	1:B:478:ARG:HD2	2.24	0.51
1:B:40:GLN:HA	1:B:43:ASN:HD22	1.74	0.51
1:B:87:THR:O	1:B:88:PRO:C	2.50	0.51
1:B:138:ASP:HA	1:B:141:LEU:HD12	1.93	0.51
1:B:310:TYR:CD1	1:B:311:GLU:N	2.75	0.51
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.71	0.51
1:D:44:ARG:NH1	1:D:494:ASN:HD21	2.08	0.51
1:D:348:ALA:HB3	1:D:351:PRO:HG3	1.91	0.51
1:E:44:ARG:NH1	1:E:494:ASN:HD21	2.08	0.51
1:E:146:ARG:HE	1:E:182:THR:HG22	1.76	0.51
1:E:246:THR:N	1:E:320:ASP:OD1	2.43	0.51
1:F:435:GLU:CD	1:F:435:GLU:H	2.18	0.51
1:A:146:ARG:HE	1:A:182:THR:HG22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HD2	1:A:295:LYS:HE3	1.76	0.51
1:A:346:GLU:HB3	1:A:370:ASP:HB3	1.93	0.51
1:B:190:TYR:CE2	1:F:162:VAL:HG11	2.45	0.51
1:B:417:LEU:HD21	1:F:417:LEU:HD11	1.90	0.51
1:C:348:ALA:HB3	1:C:351:PRO:HG3	1.91	0.51
1:D:33:LYS:HD3	1:D:41:LYS:HZ3	1.75	0.51
1:D:334:SER:O	1:D:338:ARG:NH2	2.43	0.51
1:E:56:ASN:HD22	1:E:84:HIS:CD2	2.27	0.51
1:F:489:VAL:O	1:F:493:TYR:HD1	1.94	0.51
1:A:195:HIS:HE1	1:B:87:THR:HG21	1.72	0.51
1:A:333:LYS:HB2	1:A:355:GLN:HB3	1.93	0.51
1:A:417:LEU:CD2	1:B:417:LEU:CD1	2.88	0.51
1:B:417:LEU:CD2	1:F:417:LEU:HD13	2.41	0.51
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.74	0.51
1:C:211:ARG:HG2	1:C:380:VAL:HG12	1.93	0.51
1:C:319:CYS:O	1:C:341:ALA:HA	2.09	0.51
1:C:421:PHE:HE1	1:E:421:PHE:HE1	1.59	0.51
1:D:66:ARG:NH1	1:D:70:GLY:HA2	2.25	0.51
1:D:90:LYS:HD2	1:D:122:PHE:CE1	2.46	0.51
1:D:200:GLY:HA2	1:D:211:ARG:HD3	1.91	0.51
1:E:66:ARG:HG3	1:E:72:TRP:CE2	2.46	0.51
1:E:334:SER:O	1:E:338:ARG:NH2	2.43	0.51
1:F:346:GLU:HB3	1:F:370:ASP:HB3	1.93	0.51
1:B:9:PHE:CE1	1:B:107:LEU:HD13	2.34	0.51
1:B:17:PHE:HA	1:B:482:TYR:HD2	1.73	0.51
1:B:66:ARG:HG3	1:B:72:TRP:CE2	2.46	0.51
1:B:72:TRP:CZ2	1:E:498:VAL:HB	2.45	0.51
1:C:138:ASP:HA	1:C:141:LEU:HD12	1.93	0.51
1:D:260:MET:HE2	1:D:288:PRO:CG	2.39	0.51
1:D:333:LYS:HB2	1:D:355:GLN:HB3	1.93	0.51
1:D:339:VAL:H	1:D:363:ARG:NH2	2.08	0.51
1:D:489:VAL:O	1:D:493:TYR:HD1	1.94	0.51
1:E:59:LEU:CD2	1:E:61:LEU:HD11	2.41	0.51
1:E:87:THR:O	1:E:88:PRO:C	2.50	0.51
1:E:310:TYR:CD1	1:E:311:GLU:N	2.75	0.51
1:E:435:GLU:H	1:E:435:GLU:CD	2.18	0.51
1:F:44:ARG:NH1	1:F:494:ASN:HD21	2.08	0.51
1:F:59:LEU:CD2	1:F:61:LEU:HD11	2.41	0.51
1:F:211:ARG:HG2	1:F:380:VAL:HG12	1.93	0.51
1:F:339:VAL:H	1:F:363:ARG:NH2	2.08	0.51
1:A:138:ASP:HA	1:A:141:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG11	1:E:54:PRO:HG3	1.92	0.51
1:B:421:PHE:CE1	1:F:421:PHE:CE1	2.99	0.51
1:C:282:ASN:ND2	1:C:282:ASN:C	2.68	0.51
1:C:346:GLU:HB3	1:C:370:ASP:HB3	1.93	0.51
1:C:413:VAL:O	1:C:417:LEU:HG	2.10	0.51
1:D:138:ASP:HA	1:D:141:LEU:HD12	1.93	0.51
1:F:90:LYS:HD2	1:F:122:PHE:CE1	2.46	0.51
1:F:250:GLN:CD	1:F:315:LEU:HD21	2.35	0.51
1:A:44:ARG:CZ	1:A:494:ASN:HD21	2.23	0.51
1:A:87:THR:CG2	1:F:195:HIS:CE1	2.85	0.51
1:D:252:PHE:HD2	1:D:295:LYS:HE3	1.76	0.51
1:E:346:GLU:HB3	1:E:370:ASP:HB3	1.93	0.51
1:F:146:ARG:HE	1:F:182:THR:HG22	1.76	0.51
1:A:59:LEU:CD2	1:A:61:LEU:HD11	2.41	0.51
1:A:210:GLY:O	1:A:214:ALA:HB2	2.11	0.51
1:A:282:ASN:ND2	1:A:282:ASN:C	2.68	0.51
1:A:401:TYR:CG	1:B:443:ALA:HB2	2.46	0.51
1:B:62:SER:HB3	1:E:55:CYS:O	2.11	0.51
1:B:303:GLY:N	1:B:309:ILE:HD11	2.23	0.51
1:B:346:GLU:HB3	1:B:370:ASP:HB3	1.93	0.51
1:B:413:VAL:O	1:B:417:LEU:HG	2.10	0.51
1:E:138:ASP:HA	1:E:141:LEU:HD12	1.93	0.51
1:F:210:GLY:O	1:F:214:ALA:HB2	2.11	0.51
1:F:315:LEU:HD11	1:F:330:GLN:HB3	1.93	0.51
1:B:17:PHE:CE1	1:B:486:ILE:HG12	2.46	0.51
1:B:59:LEU:CD2	1:B:61:LEU:HD11	2.41	0.51
1:B:211:ARG:HG2	1:B:380:VAL:HG12	1.93	0.51
1:B:260:MET:HE2	1:B:288:PRO:CG	2.39	0.51
1:B:416:SER:HB3	1:F:430:ILE:CD1	2.41	0.51
1:C:17:PHE:HA	1:C:482:TYR:HD2	1.73	0.51
1:F:333:LYS:HB2	1:F:355:GLN:HB3	1.93	0.51
1:F:340:LYS:N	1:F:363:ARG:HH22	2.05	0.51
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.46	0.50
1:C:393:SER:HB3	4:C:507[B]:NAD:PA	2.51	0.50
4:C:507[B]:NAD:C6N	1:E:459:ARG:HH21	2.24	0.50
1:D:59:LEU:CD2	1:D:61:LEU:HD11	2.41	0.50
1:E:44:ARG:CZ	1:E:494:ASN:HD21	2.23	0.50
1:E:61:LEU:HD23	1:E:151:GLU:HB3	1.93	0.50
1:E:169:MET:HE2	4:E:508:NAD:H3D	1.93	0.50
1:E:210:GLY:O	1:E:214:ALA:HB2	2.11	0.50
1:E:315:LEU:HD11	1:E:330:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:VAL:O	1:E:493:TYR:HD1	1.94	0.50
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.46	0.50
1:F:252:PHE:HD2	1:F:295:LYS:HE3	1.76	0.50
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.93	0.50
1:A:417:LEU:CD1	1:F:417:LEU:HD21	2.40	0.50
1:B:146:ARG:HE	1:B:182:THR:HG22	1.76	0.50
1:B:210:GLY:O	1:B:214:ALA:HB2	2.11	0.50
1:B:252:PHE:HD2	1:B:295:LYS:HE3	1.75	0.50
1:B:489:VAL:O	1:B:493:TYR:HD1	1.94	0.50
1:C:9:PHE:CE1	1:C:107:LEU:HD13	2.34	0.50
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.93	0.50
1:C:146:ARG:HE	1:C:182:THR:HG22	1.76	0.50
1:D:360:PHE:CD2	1:D:365:ILE:HD12	2.44	0.50
1:D:409:LEU:HD22	1:E:409:LEU:HD11	1.92	0.50
1:E:17:PHE:CE1	1:E:486:ILE:HG12	2.46	0.50
1:E:90:LYS:HD2	1:E:122:PHE:CE1	2.46	0.50
1:E:333:LYS:HB2	1:E:355:GLN:HB3	1.93	0.50
1:A:90:LYS:HD2	1:A:122:PHE:CE1	2.46	0.50
1:C:17:PHE:CE1	1:C:486:ILE:HG12	2.46	0.50
1:C:87:THR:O	1:C:88:PRO:C	2.50	0.50
1:C:250:GLN:CD	1:C:315:LEU:HD21	2.35	0.50
1:D:44:ARG:CZ	1:D:494:ASN:HD21	2.23	0.50
1:D:146:ARG:HE	1:D:182:THR:HG22	1.76	0.50
1:D:346:GLU:HB3	1:D:370:ASP:HB3	1.93	0.50
1:A:84:HIS:C	1:A:86:ARG:N	2.69	0.50
1:A:489:VAL:O	1:A:493:TYR:HD1	1.94	0.50
4:B:507[B]:NAD:C6N	1:F:459:ARG:HH21	2.24	0.50
1:C:66:ARG:HG3	1:C:72:TRP:CE2	2.46	0.50
1:D:66:ARG:HG3	1:D:72:TRP:CE2	2.46	0.50
1:D:87:THR:O	1:D:88:PRO:C	2.50	0.50
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.31	0.50
1:E:252:PHE:HD2	1:E:295:LYS:HE3	1.76	0.50
1:F:282:ASN:ND2	1:F:282:ASN:C	2.68	0.50
1:F:443:ALA:HB1	1:F:447:ASP:HB2	1.94	0.50
1:A:459:ARG:HH21	4:F:508[B]:NAD:C6N	2.24	0.50
1:B:443:ALA:HB1	1:B:447:ASP:HB2	1.94	0.50
1:C:169:MET:HE2	4:C:508:NAD:H3D	1.93	0.50
1:C:489:VAL:O	1:C:493:TYR:HD1	1.94	0.50
1:D:445:GLU:O	1:D:449:VAL:HG23	2.12	0.50
1:E:94:ARG:HE	1:E:168:ASN:ND2	2.10	0.50
1:F:66:ARG:HG3	1:F:72:TRP:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HE2	4:B:508:NAD:H3D	1.93	0.50
1:C:90:LYS:HD2	1:C:122:PHE:CE1	2.46	0.50
1:C:333:LYS:HB2	1:C:355:GLN:HB3	1.93	0.50
1:D:61:LEU:HD23	1:D:151:GLU:HB3	1.93	0.50
1:D:459:ARG:HH21	4:E:507[B]:NAD:C6N	2.24	0.50
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.93	0.50
1:E:230:ALA:O	1:E:231:SER:C	2.55	0.50
1:A:315:LEU:HD11	1:A:330:GLN:HB3	1.93	0.50
1:C:59:LEU:CD2	1:C:61:LEU:HD11	2.41	0.50
1:D:222:GLY:HA3	1:D:373:LEU:HD23	1.94	0.50
1:E:17:PHE:HA	1:E:482:TYR:HD2	1.73	0.50
1:E:211:ARG:HG2	1:E:380:VAL:HG12	1.92	0.50
1:E:222:GLY:HA3	1:E:373:LEU:HD23	1.94	0.50
1:E:281:TRP:O	1:E:282:ASN:C	2.55	0.50
1:A:33:LYS:HA	1:A:41:LYS:HZ1	1.76	0.50
1:A:94:ARG:HE	1:A:168:ASN:ND2	2.10	0.50
1:A:230:ALA:O	1:A:231:SER:C	2.55	0.50
1:B:84:HIS:C	1:B:86:ARG:N	2.69	0.50
1:B:230:ALA:O	1:B:231:SER:C	2.55	0.50
1:B:445:GLU:O	1:B:449:VAL:HG23	2.12	0.50
1:C:340:LYS:N	1:C:363:ARG:HH22	2.05	0.50
1:C:459:ARG:HH21	4:D:507[B]:NAD:C6N	2.24	0.50
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.71	0.50
1:E:462:ARG:NH2	1:E:466:ARG:HH22	2.00	0.50
1:F:230:ALA:O	1:F:231:SER:C	2.55	0.50
1:A:14:GLU:O	1:A:17:PHE:HB3	2.12	0.50
1:B:61:LEU:HD23	1:B:151:GLU:HB3	1.93	0.50
1:B:90:LYS:HD2	1:B:122:PHE:CE1	2.46	0.50
1:B:94:ARG:HE	1:B:168:ASN:ND2	2.10	0.50
1:C:61:LEU:HD23	1:C:151:GLU:HB3	1.93	0.50
1:D:84:HIS:C	1:D:86:ARG:N	2.69	0.50
1:E:84:HIS:C	1:E:86:ARG:N	2.69	0.50
1:F:61:LEU:HD23	1:F:151:GLU:HB3	1.93	0.50
1:F:248:ALA:O	1:F:322:LEU:HD12	2.12	0.50
1:A:445:GLU:O	1:A:449:VAL:HG23	2.12	0.49
1:C:14:GLU:O	1:C:17:PHE:HB3	2.12	0.49
1:C:230:ALA:O	1:C:231:SER:C	2.55	0.49
1:C:281:TRP:CH2	1:C:283:PRO:HG3	2.47	0.49
1:C:362:GLU:C	1:C:364:ASN:H	2.20	0.49
1:C:462:ARG:NH2	1:C:466:ARG:HH22	2.00	0.49
1:D:14:GLU:O	1:D:17:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:GLY:O	1:D:214:ALA:HB2	2.11	0.49
1:D:421:PHE:HE1	1:E:421:PHE:HE1	1.60	0.49
1:E:248:ALA:O	1:E:322:LEU:HD12	2.12	0.49
1:F:94:ARG:HE	1:F:168:ASN:ND2	2.10	0.49
1:A:2:ASP:OD2	1:A:5:ASP:HB3	2.13	0.49
1:A:38:GLN:OE1	1:A:40:GLN:HB2	2.12	0.49
1:A:281:TRP:CH2	1:A:283:PRO:HG3	2.48	0.49
1:B:112:THR:HG22	1:B:124:GLY:CA	2.32	0.49
1:C:51:ILE:HA	1:F:74:VAL:CG2	2.42	0.49
1:C:61:LEU:HD12	1:C:61:LEU:N	2.27	0.49
1:C:210:GLY:O	1:C:214:ALA:HB2	2.11	0.49
1:D:248:ALA:O	1:D:322:LEU:HD12	2.12	0.49
1:F:38:GLN:OE1	1:F:40:GLN:HB2	2.12	0.49
1:F:169:MET:HE2	4:F:507:NAD:H3D	1.93	0.49
1:F:281:TRP:CH2	1:F:283:PRO:HG3	2.48	0.49
1:A:169:MET:HE2	4:A:508:NAD:H3D	1.93	0.49
4:A:507[B]:NAD:C6N	1:B:459:ARG:HH21	2.24	0.49
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.93	0.49
1:B:107:LEU:CB	1:B:126:LYS:HG2	2.31	0.49
1:B:462:ARG:NH2	1:B:466:ARG:HH22	2.00	0.49
1:D:93:ILE:HD11	1:D:165:PRO:HB3	1.94	0.49
1:D:169:MET:HE2	4:D:508:NAD:H3D	1.93	0.49
1:E:93:ILE:HD11	1:E:165:PRO:HB3	1.94	0.49
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.93	0.49
1:B:222:GLY:HA3	1:B:373:LEU:CD2	2.42	0.49
1:D:94:ARG:HE	1:D:168:ASN:ND2	2.10	0.49
1:D:211:ARG:HG2	1:D:380:VAL:HG12	1.93	0.49
1:E:38:GLN:OE1	1:E:40:GLN:HB2	2.12	0.49
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.71	0.49
1:F:94:ARG:CZ	1:F:107:LEU:HD21	2.42	0.49
1:A:248:ALA:O	1:A:322:LEU:HD12	2.12	0.49
1:A:281:TRP:O	1:A:282:ASN:C	2.55	0.49
1:B:94:ARG:CZ	1:B:107:LEU:HD21	2.42	0.49
1:D:2:ASP:OD2	1:D:5:ASP:HB3	2.13	0.49
1:E:46:ARG:HH11	1:E:46:ARG:CG	2.18	0.49
1:E:94:ARG:CZ	1:E:107:LEU:HD21	2.42	0.49
1:F:93:ILE:HD11	1:F:165:PRO:HB3	1.94	0.49
1:F:344:ILE:HD12	1:F:367:VAL:HG22	1.95	0.49
1:B:2:ASP:OD2	1:B:5:ASP:HB3	2.13	0.49
1:B:38:GLN:OE1	1:B:40:GLN:HB2	2.12	0.49
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HD11	1:B:330:GLN:HB3	1.93	0.49
1:C:443:ALA:HB1	1:C:447:ASP:HB2	1.94	0.49
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.13	0.49
1:D:230:ALA:O	1:D:231:SER:C	2.55	0.49
1:E:222:GLY:HA3	1:E:373:LEU:CD2	2.43	0.49
1:E:281:TRP:CH2	1:E:283:PRO:HG3	2.48	0.49
1:E:362:GLU:C	1:E:364:ASN:H	2.20	0.49
1:A:66:ARG:HG3	1:A:72:TRP:CE2	2.46	0.49
1:A:94:ARG:CZ	1:A:107:LEU:HD21	2.42	0.49
1:B:14:GLU:O	1:B:17:PHE:HB3	2.13	0.49
1:B:147:ARG:NH1	1:E:499:THR:OG1	2.43	0.49
1:B:147:ARG:NH1	1:E:500:PHE:CD1	2.80	0.49
1:B:391:HIS:C	4:B:507[A]:NAD:H4D	2.38	0.49
1:B:499:THR:HG21	1:E:64:PRO:HG2	1.93	0.49
1:E:2:ASP:OD2	1:E:5:ASP:HB3	2.13	0.49
1:F:138:ASP:HA	1:F:141:LEU:HD12	1.93	0.49
1:F:362:GLU:C	1:F:364:ASN:N	2.70	0.49
1:B:253:GLY:HA3	4:B:508:NAD:H4B	1.95	0.49
1:C:38:GLN:OE1	1:C:40:GLN:HB2	2.12	0.49
1:C:391:HIS:C	4:C:507[A]:NAD:H4D	2.38	0.49
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.94	0.49
1:D:61:LEU:N	1:D:61:LEU:HD12	2.27	0.49
1:D:315:LEU:HD11	1:D:330:GLN:HB3	1.93	0.49
1:E:14:GLU:O	1:E:17:PHE:HB3	2.12	0.49
1:E:344:ILE:HD12	1:E:367:VAL:HG22	1.95	0.49
1:F:2:ASP:OD2	1:F:5:ASP:HB3	2.13	0.49
1:F:14:GLU:O	1:F:17:PHE:HB3	2.12	0.49
1:F:281:TRP:O	1:F:282:ASN:C	2.55	0.49
1:A:64:PRO:HG2	1:D:499:THR:CG2	2.37	0.49
1:A:362:GLU:C	1:A:364:ASN:N	2.71	0.49
1:B:222:GLY:HA3	1:B:373:LEU:HD23	1.94	0.49
1:C:315:LEU:HD11	1:C:330:GLN:HB3	1.93	0.49
1:D:189:HIS:CD2	1:F:154:LYS:HD2	2.48	0.49
1:F:222:GLY:HA3	1:F:373:LEU:HD23	1.94	0.49
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.31	0.49
1:B:362:GLU:C	1:B:364:ASN:H	2.20	0.49
1:C:94:ARG:CZ	1:C:107:LEU:HD21	2.42	0.49
1:C:248:ALA:O	1:C:322:LEU:HD12	2.12	0.49
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.93	0.49
1:D:94:ARG:CZ	1:D:107:LEU:HD21	2.42	0.49
1:E:61:LEU:HD12	1:E:61:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.13	0.49
1:E:331:LEU:HD12	1:E:352:THR:HG22	1.95	0.49
1:F:61:LEU:HD12	1:F:61:LEU:N	2.27	0.49
1:A:61:LEU:N	1:A:61:LEU:HD12	2.27	0.48
1:A:93:ILE:HD11	1:A:165:PRO:HB3	1.94	0.48
1:B:333:LYS:HB2	1:B:355:GLN:HB3	1.93	0.48
1:C:281:TRP:O	1:C:282:ASN:C	2.55	0.48
1:D:38:GLN:OE1	1:D:40:GLN:HB2	2.12	0.48
1:D:362:GLU:C	1:D:364:ASN:H	2.20	0.48
1:F:150:MET:SD	1:F:186:THR:HG21	2.53	0.48
1:F:222:GLY:HA3	1:F:373:LEU:CD2	2.43	0.48
1:F:313:SER:CB	1:F:316:GLU:HB2	2.42	0.48
1:A:61:LEU:HD23	1:A:151:GLU:HB3	1.93	0.48
1:A:222:GLY:HA3	1:A:373:LEU:HD23	1.94	0.48
1:A:303:GLY:N	1:A:309:ILE:HD11	2.23	0.48
1:B:93:ILE:HD11	1:B:165:PRO:HB3	1.94	0.48
1:B:248:ALA:O	1:B:322:LEU:HD12	2.12	0.48
1:C:2:ASP:OD2	1:C:5:ASP:HB3	2.13	0.48
1:C:84:HIS:C	1:C:86:ARG:N	2.69	0.48
1:C:93:ILE:HD11	1:C:165:PRO:HB3	1.94	0.48
1:C:222:GLY:HA3	1:C:373:LEU:CD2	2.42	0.48
1:E:362:GLU:C	1:E:364:ASN:N	2.71	0.48
1:F:445:GLU:O	1:F:449:VAL:HG23	2.12	0.48
1:A:222:GLY:HA3	1:A:373:LEU:CD2	2.42	0.48
1:A:289:LYS:HG2	1:A:293:ASP:OD1	2.14	0.48
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.13	0.48
1:C:150:MET:SD	1:C:186:THR:HG21	2.53	0.48
1:C:253:GLY:HA3	4:C:508:NAD:H4B	1.95	0.48
1:C:331:LEU:HD12	1:C:352:THR:HG22	1.95	0.48
1:C:353:THR:HG22	1:C:355:GLN:H	1.79	0.48
1:D:281:TRP:CH2	1:D:283:PRO:HG3	2.48	0.48
1:E:445:GLU:O	1:E:449:VAL:HG23	2.12	0.48
1:F:331:LEU:HD12	1:F:352:THR:HG22	1.95	0.48
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.13	0.48
1:A:443:ALA:HB1	1:A:447:ASP:HB2	1.94	0.48
1:B:289:LYS:HG2	1:B:293:ASP:OD1	2.14	0.48
1:C:222:GLY:HA3	1:C:373:LEU:HD23	1.94	0.48
1:D:59:LEU:HD23	1:D:61:LEU:HD11	1.96	0.48
1:D:222:GLY:HA3	1:D:373:LEU:CD2	2.42	0.48
1:D:281:TRP:O	1:D:282:ASN:C	2.55	0.48
1:D:443:ALA:HB1	1:D:447:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:ALA:HB1	1:E:447:ASP:HB2	1.94	0.48
1:F:90:LYS:HZ3	1:F:164:VAL:HG12	1.77	0.48
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.13	0.48
1:F:362:GLU:C	1:F:364:ASN:H	2.20	0.48
1:B:275:GLU:OE1	1:B:275:GLU:HA	2.14	0.48
1:B:331:LEU:HD12	1:B:352:THR:HG22	1.95	0.48
1:C:74:VAL:HG11	1:F:54:PRO:HG3	1.96	0.48
1:C:94:ARG:HE	1:C:168:ASN:ND2	2.10	0.48
1:D:289:LYS:HG2	1:D:293:ASP:OD1	2.13	0.48
1:D:349:ASN:C	1:D:351:PRO:HD3	2.39	0.48
1:F:253:GLY:HA3	4:F:507:NAD:H4B	1.95	0.48
1:F:353:THR:HG22	1:F:355:GLN:H	1.79	0.48
1:A:40:GLN:HA	1:A:40:GLN:HE21	1.79	0.48
1:A:59:LEU:HD23	1:A:61:LEU:HD11	1.96	0.48
1:A:391:HIS:C	4:A:507[A]:NAD:H4D	2.38	0.48
1:B:59:LEU:HD23	1:B:61:LEU:HD11	1.96	0.48
1:B:281:TRP:O	1:B:282:ASN:C	2.55	0.48
1:B:344:ILE:HD12	1:B:367:VAL:HG22	1.95	0.48
1:D:344:ILE:HD12	1:D:367:VAL:HG22	1.95	0.48
1:D:362:GLU:C	1:D:364:ASN:N	2.71	0.48
1:E:350:GLY:N	1:E:351:PRO:HD3	2.29	0.48
1:F:136:TYR:CD1	1:F:136:TYR:N	2.82	0.48
1:A:136:TYR:CD1	1:A:136:TYR:N	2.82	0.48
1:A:150:MET:SD	1:A:186:THR:HG21	2.53	0.48
1:B:61:LEU:N	1:B:61:LEU:HD12	2.27	0.48
1:B:281:TRP:CH2	1:B:283:PRO:HG3	2.48	0.48
1:B:350:GLY:N	1:B:351:PRO:HD3	2.29	0.48
1:C:136:TYR:N	1:C:136:TYR:CD1	2.82	0.48
1:C:369:PRO:CG	1:C:478:ARG:HA	2.44	0.48
1:D:82:HIS:CG	1:D:112:THR:HG21	2.48	0.48
1:D:275:GLU:OE1	1:D:275:GLU:HA	2.14	0.48
1:D:340:LYS:N	1:D:363:ARG:HH22	2.05	0.48
1:F:275:GLU:C	4:F:507:NAD:C2A	2.87	0.48
1:F:349:ASN:C	1:F:351:PRO:HD3	2.39	0.48
1:A:349:ASN:C	1:A:351:PRO:HD3	2.39	0.48
1:A:499:THR:OG1	1:D:147:ARG:NH1	2.43	0.48
1:B:150:MET:SD	1:B:186:THR:HG21	2.53	0.48
1:B:257:LEU:O	1:B:260:MET:HB3	2.14	0.48
1:C:59:LEU:HD23	1:C:61:LEU:HD11	1.96	0.48
1:C:344:ILE:CG2	1:C:367:VAL:HG13	2.44	0.48
1:D:282:ASN:ND2	1:D:282:ASN:C	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:GLY:N	1:D:351:PRO:HD3	2.29	0.48
1:F:350:GLY:N	1:F:351:PRO:HD3	2.29	0.48
1:F:369:PRO:CG	1:F:478:ARG:HA	2.44	0.48
1:A:287:ASP:OD1	1:A:290:GLU:HG3	2.14	0.48
1:A:344:ILE:HD12	1:A:367:VAL:HG22	1.95	0.48
1:C:289:LYS:HG2	1:C:293:ASP:OD1	2.13	0.48
1:C:349:ASN:C	1:C:351:PRO:HD3	2.39	0.48
1:D:462:ARG:NH2	1:D:466:ARG:HH22	2.00	0.48
1:A:257:LEU:O	1:A:260:MET:HB3	2.14	0.48
1:A:344:ILE:CG2	1:A:367:VAL:HG13	2.44	0.48
1:A:362:GLU:C	1:A:364:ASN:H	2.20	0.48
1:A:456:THR:HG21	1:F:396:ARG:HE	1.78	0.48
1:B:136:TYR:N	1:B:136:TYR:CD1	2.82	0.48
1:B:282:ASN:ND2	1:B:284:ASP:N	2.60	0.48
1:B:344:ILE:CG2	1:B:367:VAL:HG13	2.44	0.48
1:C:287:ASP:OD1	1:C:290:GLU:HG3	2.14	0.48
1:C:445:GLU:O	1:C:449:VAL:HG23	2.12	0.48
1:D:287:ASP:OD1	1:D:290:GLU:HG3	2.14	0.48
1:D:331:LEU:HD12	1:D:352:THR:HG22	1.95	0.48
1:D:353:THR:HG22	1:D:355:GLN:H	1.79	0.48
1:F:17:PHE:HA	1:F:482:TYR:HD2	1.73	0.48
1:F:84:HIS:C	1:F:86:ARG:N	2.69	0.48
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.96	0.48
1:A:253:GLY:HA3	4:A:508:NAD:H4B	1.95	0.47
1:A:275:GLU:C	4:A:508:NAD:C2A	2.87	0.47
1:A:310:TYR:CD1	1:A:311:GLU:N	2.75	0.47
1:B:287:ASP:OD1	1:B:290:GLU:HG3	2.14	0.47
1:C:275:GLU:OE1	1:C:275:GLU:HA	2.14	0.47
1:D:150:MET:SD	1:D:186:THR:HG21	2.53	0.47
1:D:275:GLU:C	4:D:508:NAD:C2A	2.87	0.47
1:D:313:SER:CB	1:D:316:GLU:HB2	2.42	0.47
1:D:469:MET:O	1:D:471:TYR:N	2.47	0.47
1:E:289:LYS:HG2	1:E:293:ASP:OD1	2.13	0.47
1:E:333:LYS:HE2	1:E:333:LYS:HB3	1.65	0.47
1:E:344:ILE:CG2	1:E:367:VAL:HG13	2.44	0.47
1:E:369:PRO:CG	1:E:478:ARG:HA	2.44	0.47
1:F:282:ASN:ND2	1:F:284:ASP:N	2.60	0.47
1:A:94:ARG:CZ	1:A:169:MET:HE3	2.44	0.47
1:A:331:LEU:HD12	1:A:352:THR:HG22	1.95	0.47
1:B:72:TRP:CH2	1:E:499:THR:HG22	2.49	0.47
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASP:O	1:D:3:ARG:C	2.58	0.47
1:E:349:ASN:C	1:E:351:PRO:HD3	2.39	0.47
1:E:353:THR:HG22	1:E:355:GLN:H	1.79	0.47
1:F:2:ASP:O	1:F:3:ARG:C	2.57	0.47
1:A:369:PRO:CG	1:A:478:ARG:HA	2.44	0.47
1:B:94:ARG:CZ	1:B:169:MET:HE3	2.44	0.47
1:B:333:LYS:HE2	1:B:333:LYS:HB3	1.65	0.47
1:C:107:LEU:HB3	1:C:126:LYS:CG	2.29	0.47
1:C:275:GLU:C	4:C:508:NAD:C2A	2.87	0.47
1:C:344:ILE:HD12	1:C:367:VAL:HG22	1.95	0.47
1:D:94:ARG:CZ	1:D:169:MET:HE3	2.45	0.47
1:D:252:PHE:CE1	1:D:291:LEU:HD13	2.49	0.47
1:E:59:LEU:HD23	1:E:61:LEU:HD11	1.96	0.47
1:E:252:PHE:CE1	1:E:291:LEU:HD13	2.49	0.47
1:E:275:GLU:C	4:E:508:NAD:C2A	2.87	0.47
1:F:252:PHE:CE1	1:F:291:LEU:HD13	2.49	0.47
1:F:257:LEU:O	1:F:260:MET:HB3	2.14	0.47
1:F:289:LYS:HG2	1:F:293:ASP:OD1	2.14	0.47
1:F:469:MET:O	1:F:471:TYR:N	2.47	0.47
1:C:252:PHE:CE1	1:C:291:LEU:HD13	2.49	0.47
1:C:469:MET:O	1:C:471:TYR:N	2.47	0.47
1:E:275:GLU:OE1	1:E:275:GLU:HA	2.14	0.47
1:F:275:GLU:OE1	1:F:275:GLU:HA	2.14	0.47
1:F:344:ILE:CG2	1:F:367:VAL:HG13	2.44	0.47
1:A:470:LYS:HE3	1:A:471:TYR:OH	2.15	0.47
1:B:33:LYS:HD3	1:B:41:LYS:NZ	2.30	0.47
1:C:456:THR:HG21	1:D:396:ARG:HE	1.80	0.47
1:D:33:LYS:HD3	1:D:41:LYS:NZ	2.30	0.47
1:D:136:TYR:N	1:D:136:TYR:CD1	2.82	0.47
1:E:82:HIS:CG	1:E:112:THR:HG21	2.48	0.47
1:E:94:ARG:CZ	1:E:169:MET:HE3	2.45	0.47
1:A:275:GLU:OE1	1:A:275:GLU:HA	2.14	0.47
1:B:275:GLU:C	4:B:508:NAD:C2A	2.87	0.47
1:B:353:THR:HG22	1:B:355:GLN:H	1.79	0.47
1:B:369:PRO:CG	1:B:478:ARG:HA	2.44	0.47
1:C:470:LYS:HE3	1:C:471:TYR:CZ	2.50	0.47
1:D:393:SER:HB3	4:D:507[B]:NAD:PA	2.54	0.47
1:D:470:LYS:HE3	1:D:471:TYR:OH	2.15	0.47
1:E:150:MET:SD	1:E:186:THR:HG21	2.53	0.47
1:E:287:ASP:OD1	1:E:290:GLU:HG3	2.14	0.47
1:A:252:PHE:CE1	1:A:291:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:N	1:A:363:ARG:HH22	2.05	0.47
1:A:470:LYS:HE3	1:A:471:TYR:CZ	2.50	0.47
1:B:313:SER:CB	1:B:316:GLU:HB2	2.42	0.47
1:B:349:ASN:C	1:B:351:PRO:HD3	2.39	0.47
1:B:470:LYS:HE3	1:B:471:TYR:CZ	2.50	0.47
1:B:470:LYS:HE3	1:B:471:TYR:OH	2.15	0.47
1:C:33:LYS:HD3	1:C:41:LYS:NZ	2.30	0.47
1:C:333:LYS:HE2	1:C:333:LYS:HB3	1.65	0.47
1:C:350:GLY:N	1:C:351:PRO:HD3	2.29	0.47
1:C:393:SER:HB3	4:C:507[A]:NAD:O3	2.15	0.47
1:C:417:LEU:CD2	1:E:417:LEU:CD1	2.91	0.47
1:D:154:LYS:HD2	1:F:189:HIS:CD2	2.50	0.47
1:D:220:PHE:HZ	1:D:266:PHE:CD2	2.33	0.47
1:D:257:LEU:O	1:D:260:MET:HB3	2.14	0.47
1:D:344:ILE:CG2	1:D:367:VAL:HG13	2.44	0.47
1:D:500:PHE:CE2	1:E:185:SER:HB2	2.44	0.47
1:E:136:TYR:N	1:E:136:TYR:CD1	2.82	0.47
1:E:253:GLY:HA3	4:E:508:NAD:H4B	1.95	0.47
1:E:257:LEU:O	1:E:260:MET:HB3	2.14	0.47
1:F:199:THR:HA	1:F:384:GLN:OE1	2.15	0.47
1:A:350:GLY:N	1:A:351:PRO:HD3	2.29	0.47
1:B:2:ASP:O	1:B:3:ARG:C	2.58	0.47
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.96	0.47
1:C:199:THR:HA	1:C:384:GLN:OE1	2.15	0.47
1:C:220:PHE:HZ	1:C:266:PHE:CD2	2.33	0.47
1:C:257:LEU:O	1:C:260:MET:HB3	2.14	0.47
1:A:33:LYS:HD3	1:A:41:LYS:HZ3	1.79	0.47
1:A:33:LYS:HD3	1:A:41:LYS:NZ	2.30	0.47
1:A:51:ILE:HA	1:D:74:VAL:CG2	2.45	0.47
1:A:313:SER:CB	1:A:316:GLU:HB2	2.42	0.47
1:A:469:MET:O	1:A:471:TYR:N	2.47	0.47
1:B:72:TRP:HZ3	1:E:499:THR:CG2	2.21	0.47
1:B:199:THR:HA	1:B:384:GLN:OE1	2.15	0.47
1:B:252:PHE:CE1	1:B:291:LEU:HD13	2.49	0.47
1:C:72:TRP:CZ2	1:F:498:VAL:HB	2.49	0.47
1:E:199:THR:HA	1:E:384:GLN:OE1	2.15	0.47
1:E:220:PHE:HZ	1:E:266:PHE:CD2	2.33	0.47
1:F:59:LEU:HD23	1:F:61:LEU:HD11	1.96	0.47
1:F:94:ARG:CZ	1:F:169:MET:HE3	2.44	0.47
1:A:53:LYS:O	1:A:82:HIS:HE1	1.98	0.47
1:B:64:PRO:HG2	1:E:499:THR:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HZ	1:B:266:PHE:CD2	2.33	0.47
1:D:253:GLY:HA3	4:D:508:NAD:H4B	1.95	0.47
1:E:469:MET:O	1:E:471:TYR:N	2.47	0.47
1:F:246:THR:HG22	1:F:320:ASP:H	1.80	0.47
1:A:2:ASP:O	1:A:3:ARG:C	2.58	0.46
1:A:353:THR:HG22	1:A:355:GLN:H	1.79	0.46
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.50	0.46
1:B:174:ARG:NE	1:B:178:TRP:CH2	2.83	0.46
1:C:174:ARG:NE	1:C:178:TRP:CH2	2.83	0.46
1:D:470:LYS:HE3	1:D:471:TYR:CZ	2.50	0.46
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.96	0.46
1:E:331:LEU:CD1	1:E:344:ILE:HD13	2.46	0.46
1:F:53:LYS:O	1:F:82:HIS:HE1	1.98	0.46
1:F:220:PHE:HZ	1:F:266:PHE:CD2	2.33	0.46
1:F:331:LEU:CD1	1:F:344:ILE:HD13	2.46	0.46
1:A:489:VAL:O	1:A:489:VAL:HG12	2.15	0.46
1:D:53:LYS:O	1:D:82:HIS:HE1	1.98	0.46
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.96	0.46
1:D:406:ASN:HD22	1:D:406:ASN:HA	1.60	0.46
1:D:432:PRO:CB	1:D:436:PHE:HD2	2.28	0.46
1:E:40:GLN:HA	1:E:40:GLN:HE21	1.79	0.46
1:E:470:LYS:HE3	1:E:471:TYR:CZ	2.50	0.46
1:F:201:LYS:HZ3	1:F:388:ASN:HD21	1.62	0.46
1:F:393:SER:HB3	4:F:508[B]:NAD:PA	2.55	0.46
1:F:470:LYS:HE3	1:F:471:TYR:CZ	2.50	0.46
1:A:190:TYR:CD2	1:B:162:VAL:CG1	2.99	0.46
1:A:199:THR:HA	1:A:384:GLN:OE1	2.15	0.46
1:B:469:MET:O	1:B:471:TYR:N	2.47	0.46
1:C:331:LEU:CD1	1:C:344:ILE:HD13	2.46	0.46
1:D:369:PRO:CG	1:D:478:ARG:HA	2.44	0.46
1:E:174:ARG:NE	1:E:178:TRP:CH2	2.84	0.46
1:E:470:LYS:HE3	1:E:471:TYR:OH	2.15	0.46
1:F:33:LYS:HD3	1:F:41:LYS:NZ	2.30	0.46
1:F:331:LEU:HD22	1:F:339:VAL:HG11	1.98	0.46
1:A:174:ARG:NE	1:A:178:TRP:CH2	2.84	0.46
1:A:416:SER:HB3	1:B:430:ILE:HA	1.97	0.46
1:A:500:PHE:O	1:A:500:PHE:HD1	1.99	0.46
1:B:489:VAL:O	1:B:489:VAL:HG12	2.15	0.46
1:C:94:ARG:CZ	1:C:169:MET:HE3	2.44	0.46
1:C:470:LYS:HE3	1:C:471:TYR:OH	2.15	0.46
1:D:199:THR:HA	1:D:384:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG11	4:D:508:NAD:O4D	2.16	0.46
1:E:500:PHE:O	1:E:500:PHE:HD1	1.99	0.46
1:F:470:LYS:HE3	1:F:471:TYR:OH	2.15	0.46
1:F:500:PHE:O	1:F:500:PHE:HD1	1.99	0.46
1:A:246:THR:HG22	1:A:320:ASP:H	1.80	0.46
1:A:282:ASN:ND2	1:A:284:ASP:N	2.60	0.46
1:B:33:LYS:HA	1:B:33:LYS:HD3	1.72	0.46
1:B:246:THR:HG22	1:B:320:ASP:H	1.80	0.46
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.96	0.46
1:C:396:ARG:HE	1:E:456:THR:HG21	1.80	0.46
1:C:421:PHE:HE1	1:D:421:PHE:HE1	1.63	0.46
1:C:500:PHE:O	1:C:500:PHE:HD1	1.99	0.46
1:E:2:ASP:O	1:E:3:ARG:C	2.58	0.46
1:E:53:LYS:O	1:E:82:HIS:HE1	1.98	0.46
1:E:255:VAL:HG11	4:E:508:NAD:O4D	2.16	0.46
1:F:40:GLN:HA	1:F:40:GLN:HE21	1.79	0.46
1:F:489:VAL:O	1:F:489:VAL:HG12	2.15	0.46
1:A:82:HIS:CG	1:A:112:THR:HG21	2.48	0.46
1:A:255:VAL:HG11	4:A:508:NAD:O4D	2.16	0.46
1:B:417:LEU:HD22	1:F:417:LEU:HD13	1.98	0.46
1:C:238:MET:SD	1:C:342:LYS:HB2	2.56	0.46
1:D:9:PHE:CZ	1:D:328:GLU:HG2	2.51	0.46
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.71	0.46
1:D:331:LEU:HD22	1:D:339:VAL:HG11	1.98	0.46
1:E:38:GLN:HB2	1:E:39:GLU:H	1.59	0.46
1:E:315:LEU:HA	1:E:322:LEU:HD21	1.98	0.46
1:F:255:VAL:HG11	4:F:507:NAD:O4D	2.16	0.46
1:A:238:MET:SD	1:A:342:LYS:HB2	2.56	0.46
1:A:331:LEU:CD1	1:A:344:ILE:HD13	2.46	0.46
1:C:9:PHE:CZ	1:C:328:GLU:HG2	2.51	0.46
1:C:155:LYS:HD2	1:F:157:PHE:CE1	2.51	0.46
1:C:362:GLU:C	1:C:364:ASN:N	2.71	0.46
1:D:174:ARG:NE	1:D:178:TRP:CH2	2.84	0.46
1:E:313:SER:CB	1:E:316:GLU:HB2	2.42	0.46
1:E:393:SER:HB3	4:E:507[B]:NAD:PA	2.55	0.46
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.96	0.46
1:A:168:ASN:ND2	1:A:169:MET:H	2.14	0.46
1:A:315:LEU:HA	1:A:322:LEU:HD21	1.98	0.46
1:B:38:GLN:HB2	1:B:39:GLU:H	1.59	0.46
1:B:90:LYS:HD2	1:B:122:PHE:CD1	2.51	0.46
1:B:331:LEU:CD1	1:B:344:ILE:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:C	1:B:364:ASN:N	2.71	0.46
1:C:40:GLN:HA	1:C:40:GLN:HE21	1.79	0.46
1:C:53:LYS:O	1:C:82:HIS:HE1	1.98	0.46
1:C:82:HIS:CG	1:C:112:THR:HG21	2.48	0.46
1:D:90:LYS:HD2	1:D:122:PHE:CD1	2.51	0.46
1:D:282:ASN:HD21	1:D:284:ASP:CB	2.29	0.46
1:E:33:LYS:HD3	1:E:41:LYS:NZ	2.30	0.46
1:E:246:THR:HG22	1:E:320:ASP:H	1.80	0.46
1:F:90:LYS:HD2	1:F:122:PHE:CD1	2.51	0.46
1:B:498:VAL:HB	1:E:72:TRP:CH2	2.51	0.46
1:C:2:ASP:O	1:C:3:ARG:C	2.58	0.46
1:D:168:ASN:ND2	1:D:169:MET:H	2.14	0.46
1:D:246:THR:HG22	1:D:320:ASP:H	1.80	0.46
1:E:9:PHE:CZ	1:E:328:GLU:HG2	2.51	0.46
1:E:238:MET:SD	1:E:342:LYS:HB2	2.56	0.46
1:F:10:PHE:O	1:F:14:GLU:HB2	2.16	0.46
1:A:10:PHE:O	1:A:14:GLU:HB2	2.16	0.46
1:A:220:PHE:HZ	1:A:266:PHE:CD2	2.33	0.46
1:A:500:PHE:CD1	1:D:147:ARG:NH1	2.84	0.46
1:B:53:LYS:O	1:B:82:HIS:HE1	1.98	0.46
1:B:61:LEU:HD23	1:B:151:GLU:CB	2.46	0.46
1:D:238:MET:SD	1:D:342:LYS:HB2	2.56	0.46
1:E:282:ASN:ND2	1:E:284:ASP:N	2.60	0.46
1:F:238:MET:SD	1:F:342:LYS:HB2	2.56	0.46
1:A:61:LEU:HD23	1:A:151:GLU:CB	2.46	0.45
1:A:282:ASN:HD21	1:A:284:ASP:CB	2.29	0.45
1:B:255:VAL:HG11	4:B:508:NAD:O4D	2.16	0.45
1:B:500:PHE:HD1	1:B:500:PHE:O	1.99	0.45
1:C:255:VAL:HG11	4:C:508:NAD:O4D	2.16	0.45
1:D:10:PHE:O	1:D:14:GLU:HB2	2.16	0.45
1:D:40:GLN:HA	1:D:40:GLN:HE21	1.79	0.45
1:D:61:LEU:HD23	1:D:151:GLU:CB	2.46	0.45
1:D:87:THR:CG2	1:E:195:HIS:CE1	2.91	0.45
1:D:315:LEU:HA	1:D:322:LEU:HD21	1.98	0.45
1:D:457:MET:HA	1:D:457:MET:CE	2.42	0.45
1:E:10:PHE:O	1:E:14:GLU:HB2	2.16	0.45
1:F:287:ASP:OD1	1:F:290:GLU:HG3	2.14	0.45
1:F:336:ALA:O	1:F:339:VAL:HG13	2.16	0.45
1:A:9:PHE:CZ	1:A:328:GLU:HG2	2.51	0.45
1:A:409:LEU:HD22	1:F:409:LEU:HD11	1.96	0.45
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD23	1:C:151:GLU:CB	2.46	0.45
1:C:90:LYS:HD2	1:C:122:PHE:CD1	2.51	0.45
1:C:489:VAL:O	1:C:489:VAL:HG12	2.15	0.45
1:D:298:HIS:O	1:D:299:GLY:C	2.60	0.45
1:E:8:ASN:OD1	1:E:11:LYS:HG3	2.16	0.45
1:E:61:LEU:HD23	1:E:151:GLU:CB	2.46	0.45
1:E:379:THR:HG22	1:E:383:PHE:CZ	2.52	0.45
1:A:336:ALA:O	1:A:339:VAL:HG13	2.16	0.45
1:A:443:ALA:HB2	1:F:401:TYR:CD2	2.51	0.45
1:B:225:ASN:O	1:B:465:MET:HE1	2.17	0.45
1:B:331:LEU:HD22	1:B:339:VAL:HG11	1.98	0.45
1:C:282:ASN:ND2	1:C:284:ASP:N	2.60	0.45
1:C:298:HIS:O	1:C:299:GLY:C	2.59	0.45
1:C:495:GLU:OE1	1:D:204:SER:OG	2.11	0.45
1:D:225:ASN:O	1:D:465:MET:HE1	2.17	0.45
1:E:168:ASN:ND2	1:E:169:MET:H	2.14	0.45
1:E:386:LEU:HD12	1:E:386:LEU:HA	1.80	0.45
1:F:174:ARG:NE	1:F:178:TRP:CH2	2.84	0.45
1:F:315:LEU:HA	1:F:322:LEU:HD21	1.98	0.45
1:A:8:ASN:OD1	1:A:11:LYS:HG3	2.16	0.45
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.99	0.45
1:A:90:LYS:HD2	1:A:122:PHE:CD1	2.51	0.45
1:A:321:ILE:HG23	1:A:343:ILE:HG22	1.99	0.45
1:A:379:THR:HG22	1:A:383:PHE:CZ	2.52	0.45
1:A:393:SER:HB3	4:A:507[A]:NAD:PA	2.57	0.45
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.71	0.45
1:B:238:MET:SD	1:B:342:LYS:HB2	2.56	0.45
1:B:298:HIS:O	1:B:299:GLY:C	2.60	0.45
1:C:8:ASN:OD1	1:C:11:LYS:HG3	2.17	0.45
1:C:168:ASN:ND2	1:C:169:MET:H	2.14	0.45
1:D:321:ILE:HG23	1:D:343:ILE:HG22	1.99	0.45
1:D:489:VAL:O	1:D:489:VAL:HG12	2.15	0.45
1:E:336:ALA:O	1:E:339:VAL:HG13	2.16	0.45
1:F:9:PHE:CZ	1:F:328:GLU:HG2	2.51	0.45
1:B:10:PHE:HA	1:B:106:ALA:HB2	1.99	0.45
1:B:10:PHE:O	1:B:14:GLU:HB2	2.16	0.45
1:B:33:LYS:HD3	1:B:41:LYS:HZ3	1.81	0.45
1:B:185:SER:HB2	1:F:500:PHE:CE2	2.51	0.45
1:B:379:THR:HG22	1:B:383:PHE:CZ	2.52	0.45
1:C:282:ASN:HD21	1:C:284:ASP:CB	2.29	0.45
1:D:8:ASN:OD1	1:D:11:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ALA:O	1:D:339:VAL:HG13	2.16	0.45
1:D:500:PHE:O	1:D:500:PHE:HD1	1.99	0.45
1:E:282:ASN:HD21	1:E:284:ASP:CB	2.29	0.45
1:F:61:LEU:HD23	1:F:151:GLU:CB	2.46	0.45
1:A:154:LYS:HD2	1:E:189:HIS:CD2	2.51	0.45
1:B:282:ASN:HD21	1:B:284:ASP:CB	2.29	0.45
1:B:315:LEU:HA	1:B:322:LEU:HD21	1.98	0.45
1:E:469:MET:O	1:E:470:LYS:C	2.60	0.45
1:A:195:HIS:CE1	1:B:87:THR:CG2	2.90	0.45
1:B:8:ASN:OD1	1:B:11:LYS:HG3	2.17	0.45
1:B:336:ALA:O	1:B:339:VAL:HG13	2.16	0.45
1:B:416:SER:HB3	1:F:430:ILE:HD13	1.99	0.45
1:C:246:THR:HG22	1:C:320:ASP:H	1.80	0.45
1:C:370:ASP:HB2	1:C:374:ASN:ND2	2.20	0.45
1:E:90:LYS:HD2	1:E:122:PHE:CD1	2.51	0.45
1:E:331:LEU:HD22	1:E:339:VAL:HG11	1.98	0.45
1:E:340:LYS:N	1:E:363:ARG:HH22	2.05	0.45
1:E:377:GLY:O	1:E:381:SER:HB2	2.17	0.45
1:E:489:VAL:O	1:E:489:VAL:HG12	2.15	0.45
1:F:379:THR:HG22	1:F:383:PHE:CZ	2.52	0.45
1:A:225:ASN:O	1:A:465:MET:HE1	2.17	0.45
1:A:263:LEU:HA	1:A:263:LEU:HD23	1.82	0.45
1:A:331:LEU:HD22	1:A:339:VAL:HG11	1.98	0.45
1:A:377:GLY:O	1:A:381:SER:HB2	2.17	0.45
1:B:9:PHE:CZ	1:B:328:GLU:HG2	2.51	0.45
1:B:401:TYR:CG	1:F:443:ALA:HB2	2.51	0.45
1:C:107:LEU:CB	1:C:126:LYS:HG2	2.31	0.45
1:C:379:THR:HG22	1:C:383:PHE:CZ	2.52	0.45
1:E:282:ASN:H	1:E:307:ALA:HB1	1.82	0.45
1:E:393:SER:HB3	4:E:507[A]:NAD:O1A	2.17	0.45
1:F:115:CYS:HB3	1:F:120:VAL:O	2.17	0.45
1:F:398:THR:O	1:F:399:PHE:C	2.60	0.45
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.71	0.45
1:A:232:TYR:CE2	1:A:465:MET:HG2	2.52	0.45
1:B:469:MET:O	1:B:470:LYS:C	2.60	0.45
1:C:486:ILE:O	1:C:490:PHE:HB2	2.17	0.45
1:D:10:PHE:HA	1:D:106:ALA:HB2	1.99	0.45
1:E:115:CYS:HB3	1:E:120:VAL:O	2.17	0.45
1:F:8:ASN:OD1	1:F:11:LYS:HG3	2.16	0.45
1:F:230:ALA:O	1:F:234:SER:N	2.49	0.45
1:A:67:ARG:NH1	1:A:136:TYR:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:H	1:A:307:ALA:HB1	1.82	0.45
1:B:64:PRO:HG2	1:E:499:THR:CG2	2.44	0.45
1:D:115:CYS:HB3	1:D:120:VAL:O	2.17	0.45
1:E:24:VAL:O	1:E:25:GLU:C	2.60	0.45
1:F:10:PHE:HA	1:F:106:ALA:HB2	1.99	0.45
1:F:282:ASN:HD21	1:F:284:ASP:CB	2.29	0.45
1:F:469:MET:O	1:F:470:LYS:C	2.60	0.45
1:A:112:THR:HB	1:A:124:GLY:H	1.82	0.44
1:C:67:ARG:NH1	1:C:136:TYR:HA	2.32	0.44
1:C:225:ASN:O	1:C:465:MET:HE1	2.17	0.44
1:D:4:GLU:O	1:D:5:ASP:CB	2.65	0.44
1:D:112:THR:HB	1:D:124:GLY:H	1.82	0.44
1:D:417:LEU:CD1	1:E:417:LEU:CD2	2.94	0.44
1:E:321:ILE:HG23	1:E:343:ILE:HG22	1.99	0.44
1:F:112:THR:HB	1:F:124:GLY:H	1.82	0.44
1:F:225:ASN:O	1:F:465:MET:HE1	2.17	0.44
1:F:377:GLY:O	1:F:381:SER:HB2	2.17	0.44
1:A:24:VAL:O	1:A:25:GLU:C	2.60	0.44
1:A:298:HIS:O	1:A:299:GLY:C	2.60	0.44
1:A:469:MET:O	1:A:470:LYS:C	2.60	0.44
1:A:486:ILE:O	1:A:490:PHE:HB2	2.17	0.44
1:A:499:THR:HG23	1:A:501:THR:N	2.33	0.44
1:B:4:GLU:O	1:B:5:ASP:CB	2.65	0.44
1:B:67:ARG:NH1	1:B:136:TYR:HA	2.32	0.44
1:B:79:ARG:HD2	1:B:127:ALA:HB2	2.00	0.44
1:B:168:ASN:ND2	1:B:169:MET:H	2.14	0.44
1:B:232:TYR:CE2	1:B:465:MET:HG2	2.52	0.44
1:C:10:PHE:O	1:C:14:GLU:HB2	2.16	0.44
1:C:24:VAL:O	1:C:25:GLU:C	2.60	0.44
1:C:313:SER:CB	1:C:316:GLU:HB2	2.42	0.44
1:C:321:ILE:HG23	1:C:343:ILE:HG22	1.99	0.44
1:C:331:LEU:HD22	1:C:339:VAL:HG11	1.98	0.44
1:D:486:ILE:O	1:D:490:PHE:HB2	2.18	0.44
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.99	0.44
1:E:90:LYS:HZ3	1:E:164:VAL:HG12	1.82	0.44
1:F:386:LEU:HA	1:F:386:LEU:HD12	1.80	0.44
1:B:282:ASN:H	1:B:307:ALA:HB1	1.82	0.44
1:C:227:ILE:HA	1:C:233:MET:SD	2.57	0.44
1:C:315:LEU:HA	1:C:322:LEU:HD21	1.98	0.44
1:C:500:PHE:CD1	1:F:147:ARG:NH1	2.86	0.44
1:E:225:ASN:O	1:E:465:MET:HE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:LEU:HD23	1:E:263:LEU:HA	1.82	0.44
1:F:67:ARG:NH1	1:F:136:TYR:HA	2.32	0.44
1:F:227:ILE:HG13	1:F:233:MET:SD	2.58	0.44
1:F:282:ASN:H	1:F:307:ALA:HB1	1.82	0.44
1:A:4:GLU:O	1:A:5:ASP:CB	2.65	0.44
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.18	0.44
1:A:398:THR:O	1:A:399:PHE:C	2.60	0.44
1:B:112:THR:HB	1:B:124:GLY:H	1.82	0.44
1:C:62:SER:HB3	1:F:55:CYS:O	2.17	0.44
1:C:87:THR:HG21	1:D:195:HIS:CE1	2.48	0.44
1:C:115:CYS:HB3	1:C:120:VAL:O	2.17	0.44
1:C:232:TYR:CE2	1:C:465:MET:HG2	2.52	0.44
1:C:377:GLY:O	1:C:381:SER:HB2	2.17	0.44
1:C:432:PRO:CB	1:C:436:PHE:HD2	2.28	0.44
1:D:24:VAL:O	1:D:25:GLU:C	2.60	0.44
1:D:67:ARG:NH1	1:D:136:TYR:HA	2.32	0.44
1:D:227:ILE:HG13	1:D:233:MET:SD	2.58	0.44
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.52	0.44
1:D:282:ASN:H	1:D:307:ALA:HB1	1.82	0.44
1:D:331:LEU:CD1	1:D:344:ILE:HD13	2.46	0.44
1:D:368:ILE:HA	1:D:369:PRO:HD3	1.85	0.44
1:E:4:GLU:O	1:E:5:ASP:CB	2.65	0.44
1:E:79:ARG:HD2	1:E:127:ALA:HB2	2.00	0.44
1:F:486:ILE:O	1:F:490:PHE:HB2	2.18	0.44
1:F:499:THR:HG23	1:F:501:THR:N	2.33	0.44
1:A:227:ILE:HG13	1:A:233:MET:SD	2.58	0.44
1:A:354:PRO:O	1:A:357:ASP:HB2	2.18	0.44
1:B:24:VAL:O	1:B:25:GLU:C	2.60	0.44
1:B:227:ILE:HG13	1:B:233:MET:SD	2.58	0.44
1:B:294:PHE:CE2	1:B:298:HIS:CE1	3.06	0.44
1:C:67:ARG:HH12	1:C:136:TYR:HA	1.83	0.44
1:C:185:SER:HB2	1:E:500:PHE:CE2	2.51	0.44
1:C:469:MET:O	1:C:470:LYS:C	2.60	0.44
4:C:508:NAD:O2N	4:C:508:NAD:N7N	2.47	0.44
1:E:67:ARG:NH1	1:E:136:TYR:HA	2.32	0.44
1:E:227:ILE:HA	1:E:233:MET:SD	2.57	0.44
1:E:232:TYR:CE2	1:E:465:MET:HG2	2.52	0.44
1:F:168:ASN:ND2	1:F:169:MET:H	2.14	0.44
1:F:263:LEU:HD23	1:F:263:LEU:HA	1.82	0.44
1:A:115:CYS:HB3	1:A:120:VAL:O	2.17	0.44
1:B:82:HIS:CG	1:B:112:THR:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:CYS:HB3	1:B:120:VAL:O	2.17	0.44
1:B:227:ILE:HA	1:B:233:MET:SD	2.57	0.44
1:B:398:THR:O	1:B:399:PHE:C	2.60	0.44
1:B:486:ILE:O	1:B:490:PHE:HB2	2.18	0.44
1:C:4:GLU:O	1:C:5:ASP:CB	2.65	0.44
1:C:84:HIS:O	1:C:86:ARG:N	2.51	0.44
1:C:336:ALA:O	1:C:339:VAL:HG13	2.16	0.44
1:D:227:ILE:HA	1:D:233:MET:SD	2.57	0.44
1:D:377:GLY:O	1:D:381:SER:HB2	2.17	0.44
1:E:112:THR:HB	1:E:124:GLY:H	1.82	0.44
1:F:37:THR:HG21	1:F:41:LYS:HG3	2.00	0.44
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.52	0.44
1:F:298:HIS:O	1:F:299:GLY:C	2.60	0.44
1:F:321:ILE:HG23	1:F:343:ILE:HG22	1.99	0.44
1:F:354:PRO:O	1:F:357:ASP:HB2	2.18	0.44
1:A:333:LYS:HE2	1:A:333:LYS:HB3	1.65	0.44
1:D:235:ILE:H	1:D:235:ILE:HG13	1.69	0.44
1:D:282:ASN:ND2	1:D:284:ASP:N	2.60	0.44
1:D:379:THR:HG22	1:D:383:PHE:CZ	2.52	0.44
1:D:469:MET:O	1:D:470:LYS:C	2.60	0.44
1:E:371:LEU:HG	1:E:482:TYR:CE1	2.53	0.44
1:E:473:LEU:HD12	1:E:480:ALA:HB2	2.00	0.44
1:F:4:GLU:O	1:F:5:ASP:CB	2.65	0.44
1:F:24:VAL:O	1:F:25:GLU:C	2.60	0.44
1:F:432:PRO:CB	1:F:436:PHE:HD2	2.28	0.44
1:A:67:ARG:HH12	1:A:136:TYR:HA	1.83	0.44
1:A:172:GLY:H	1:A:175:GLU:HG2	1.83	0.44
1:A:281:TRP:CG	1:A:310:TYR:HD2	2.36	0.44
1:A:371:LEU:HG	1:A:482:TYR:CE1	2.53	0.44
1:B:377:GLY:O	1:B:381:SER:HB2	2.17	0.44
1:B:420:LYS:NZ	1:F:425:GLY:O	2.46	0.44
1:C:172:GLY:H	1:C:175:GLU:HG2	1.83	0.44
1:C:206:GLY:HA2	4:C:507[A]:NAD:H5N	2.00	0.44
1:D:371:LEU:HG	1:D:482:TYR:CE1	2.53	0.44
1:E:219:VAL:HG13	1:E:373:LEU:HD11	2.00	0.44
1:A:227:ILE:HA	1:A:233:MET:SD	2.57	0.44
1:A:406:ASN:HD22	1:A:406:ASN:HA	1.60	0.44
1:A:499:THR:OG1	1:D:147:ARG:NH2	2.51	0.44
1:B:355:GLN:OE1	1:B:355:GLN:HA	2.18	0.44
1:C:200:GLY:H	1:C:384:GLN:NE2	2.16	0.44
1:C:294:PHE:CE2	1:C:298:HIS:CE1	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:CD2	4:D:507[A]:NAD:HO2N	2.12	0.44
1:E:298:HIS:O	1:E:299:GLY:C	2.60	0.44
1:E:354:PRO:O	1:E:357:ASP:HB2	2.18	0.44
1:A:200:GLY:H	1:A:384:GLN:NE2	2.16	0.43
1:B:457:MET:HA	1:B:457:MET:CE	2.42	0.43
1:B:499:THR:HG23	1:B:501:THR:N	2.33	0.43
1:C:371:LEU:HG	1:C:482:TYR:CE1	2.53	0.43
1:D:79:ARG:HD2	1:D:127:ALA:HB2	2.00	0.43
1:E:465:MET:O	1:E:466:ARG:C	2.61	0.43
1:F:82:HIS:CG	1:F:112:THR:HG21	2.48	0.43
1:F:473:LEU:HD12	1:F:480:ALA:HB2	2.00	0.43
1:A:37:THR:HG21	1:A:41:LYS:HG3	2.00	0.43
1:A:79:ARG:HD2	1:A:127:ALA:HB2	2.00	0.43
1:B:25:GLU:OE1	1:B:46:ARG:NE	2.51	0.43
1:B:67:ARG:HH12	1:B:136:TYR:HA	1.83	0.43
1:B:219:VAL:HG13	1:B:373:LEU:HD11	2.00	0.43
1:B:354:PRO:O	1:B:357:ASP:HB2	2.18	0.43
1:B:420:LYS:HZ2	1:F:428:ILE:HG23	1.83	0.43
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.99	0.43
1:C:242:PHE:O	1:C:268:ALA:HA	2.18	0.43
1:C:398:THR:O	1:C:399:PHE:C	2.60	0.43
1:D:294:PHE:CE2	1:D:298:HIS:CE1	3.06	0.43
1:D:398:THR:O	1:D:399:PHE:C	2.60	0.43
1:E:172:GLY:H	1:E:175:GLU:HG2	1.83	0.43
1:E:230:ALA:O	1:E:234:SER:N	2.49	0.43
1:E:242:PHE:O	1:E:268:ALA:HA	2.18	0.43
1:E:294:PHE:CE2	1:E:298:HIS:CE1	3.06	0.43
1:E:355:GLN:OE1	1:E:355:GLN:HA	2.18	0.43
1:E:398:THR:O	1:E:399:PHE:C	2.60	0.43
1:F:79:ARG:HD2	1:F:127:ALA:HB2	2.00	0.43
1:F:200:GLY:H	1:F:384:GLN:NE2	2.16	0.43
1:F:227:ILE:HA	1:F:233:MET:SD	2.57	0.43
1:A:25:GLU:OE1	1:A:46:ARG:NE	2.51	0.43
1:A:84:HIS:O	1:A:86:ARG:N	2.51	0.43
1:B:172:GLY:H	1:B:175:GLU:HG2	1.83	0.43
1:C:37:THR:HG21	1:C:41:LYS:HG3	2.00	0.43
1:C:79:ARG:HD2	1:C:127:ALA:HB2	2.00	0.43
1:C:94:ARG:HE	1:C:168:ASN:HD22	1.66	0.43
1:C:146:ARG:NE	1:C:182:THR:HG22	2.33	0.43
1:C:190:TYR:CE2	1:E:162:VAL:HG11	2.54	0.43
1:C:401:TYR:CG	1:E:443:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:507[A]:NAD:N6A	1:E:120:VAL:O	2.49	0.43
1:D:200:GLY:H	1:D:384:GLN:NE2	2.16	0.43
1:D:242:PHE:O	1:D:268:ALA:HA	2.18	0.43
1:D:355:GLN:OE1	1:D:355:GLN:HA	2.18	0.43
1:D:500:PHE:HE2	1:E:185:SER:CB	2.29	0.43
1:E:227:ILE:HG13	1:E:233:MET:SD	2.58	0.43
1:F:25:GLU:OE1	1:F:46:ARG:NE	2.51	0.43
1:F:94:ARG:HE	1:F:168:ASN:HD22	1.66	0.43
1:F:371:LEU:HG	1:F:482:TYR:CE1	2.53	0.43
1:B:66:ARG:HG3	1:B:72:TRP:CD2	2.54	0.43
1:B:321:ILE:HG23	1:B:343:ILE:HG22	1.99	0.43
1:C:219:VAL:HG13	1:C:373:LEU:HD11	2.00	0.43
1:C:227:ILE:HG13	1:C:233:MET:SD	2.58	0.43
1:C:394:TYR:CE1	1:C:448:ILE:HG13	2.54	0.43
1:D:37:THR:HG21	1:D:41:LYS:HG3	2.00	0.43
1:D:499:THR:HG23	1:D:501:THR:N	2.33	0.43
1:E:94:ARG:HE	1:E:168:ASN:HD22	1.66	0.43
1:E:146:ARG:NE	1:E:182:THR:HG22	2.33	0.43
1:A:94:ARG:HE	1:A:168:ASN:HD22	1.67	0.43
1:A:230:ALA:O	1:A:234:SER:N	2.49	0.43
1:A:294:PHE:CE2	1:A:298:HIS:CE1	3.06	0.43
1:A:396:ARG:HE	1:B:456:THR:HG21	1.83	0.43
1:A:473:LEU:HD12	1:A:480:ALA:HB2	2.00	0.43
1:C:473:LEU:HD12	1:C:480:ALA:HB2	2.00	0.43
1:D:84:HIS:O	1:D:86:ARG:N	2.51	0.43
1:D:354:PRO:O	1:D:357:ASP:HB2	2.18	0.43
1:E:200:GLY:H	1:E:384:GLN:NE2	2.16	0.43
1:E:394:TYR:CE1	1:E:448:ILE:HG13	2.54	0.43
1:E:457:MET:HA	1:E:457:MET:CE	2.42	0.43
1:E:499:THR:HG23	1:E:501:THR:N	2.33	0.43
1:F:84:HIS:O	1:F:86:ARG:N	2.51	0.43
1:F:146:ARG:NE	1:F:182:THR:HG22	2.33	0.43
1:A:190:TYR:CD2	1:B:162:VAL:HG11	2.52	0.43
1:A:394:TYR:CE1	1:A:448:ILE:HG13	2.54	0.43
1:A:499:THR:CB	1:D:64:PRO:HG2	2.49	0.43
1:B:4:GLU:O	1:B:5:ASP:HB3	2.19	0.43
1:C:5:ASP:OD1	1:C:353:THR:HG21	2.19	0.43
1:C:112:THR:HB	1:C:124:GLY:H	1.82	0.43
1:C:354:PRO:O	1:C:357:ASP:HB2	2.18	0.43
1:D:25:GLU:OE1	1:D:46:ARG:NE	2.52	0.43
1:D:465:MET:O	1:D:466:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:THR:HG21	1:E:41:LYS:HG3	2.00	0.43
1:F:355:GLN:OE1	1:F:355:GLN:HA	2.18	0.43
1:A:5:ASP:OD1	1:A:353:THR:HG21	2.19	0.43
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.48	0.43
1:A:500:PHE:CE2	1:F:185:SER:HB2	2.48	0.43
1:B:57:HIS:HE1	1:E:151:GLU:OE1	2.02	0.43
1:B:266:PHE:CD1	1:B:266:PHE:N	2.87	0.43
1:D:57:HIS:CD2	1:D:84:HIS:NE2	2.87	0.43
1:D:67:ARG:HH12	1:D:136:TYR:HA	1.83	0.43
1:D:172:GLY:H	1:D:175:GLU:HG2	1.83	0.43
1:D:230:ALA:O	1:D:234:SER:N	2.49	0.43
1:E:66:ARG:HG3	1:E:72:TRP:CD2	2.54	0.43
1:E:486:ILE:O	1:E:490:PHE:HB2	2.18	0.43
1:F:219:VAL:HG13	1:F:373:LEU:HD11	2.00	0.43
1:F:235:ILE:H	1:F:235:ILE:HG13	1.69	0.43
1:F:281:TRP:CG	1:F:310:TYR:HD2	2.36	0.43
1:B:370:ASP:CB	1:B:374:ASN:HD21	2.21	0.43
1:B:396:ARG:HE	1:F:456:THR:HG21	1.84	0.43
1:B:501:THR:HG22	1:E:66:ARG:H	1.83	0.43
1:C:266:PHE:N	1:C:266:PHE:CD1	2.87	0.43
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.83	0.43
1:C:499:THR:HG22	1:F:72:TRP:CH2	2.53	0.43
1:C:499:THR:HG23	1:C:501:THR:N	2.33	0.43
1:D:394:TYR:CE1	1:D:448:ILE:HG13	2.54	0.43
1:E:84:HIS:O	1:E:86:ARG:N	2.51	0.43
1:E:219:VAL:O	1:E:223:ILE:HG13	2.19	0.43
1:F:67:ARG:HH12	1:F:136:TYR:HA	1.83	0.43
1:F:242:PHE:O	1:F:268:ALA:HA	2.18	0.43
1:F:394:TYR:CE1	1:F:448:ILE:HG13	2.54	0.43
1:A:408:HIS:HB3	1:B:436:PHE:HB2	2.01	0.43
1:B:238:MET:SD	1:B:342:LYS:HB3	2.59	0.43
1:B:393:SER:HB3	4:B:507[B]:NAD:PA	2.57	0.43
1:C:499:THR:CG2	1:F:64:PRO:HG2	2.44	0.43
1:D:162:VAL:HG11	1:E:190:TYR:CE2	2.53	0.43
1:D:420:LYS:HZ3	1:D:420:LYS:HG2	1.69	0.43
1:E:25:GLU:OE1	1:E:46:ARG:NE	2.51	0.43
4:E:508:NAD:O2N	4:E:508:NAD:N7N	2.47	0.43
1:F:57:HIS:CD2	1:F:84:HIS:NE2	2.87	0.43
1:F:294:PHE:CE2	1:F:298:HIS:CE1	3.06	0.43
1:A:86:ARG:CZ	4:F:508[A]:NAD:C4N	2.97	0.43
1:A:146:ARG:NE	1:A:182:THR:HG22	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASP:OD1	1:B:353:THR:HG21	2.19	0.43
1:B:200:GLY:H	1:B:384:GLN:NE2	2.16	0.43
1:B:230:ALA:O	1:B:234:SER:N	2.49	0.43
1:B:242:PHE:CD1	1:B:263:LEU:HD22	2.54	0.43
1:C:23:ILE:HD12	1:C:479:THR:OG1	2.19	0.43
1:C:355:GLN:OE1	1:C:355:GLN:HA	2.18	0.43
1:C:370:ASP:CB	1:C:374:ASN:HD21	2.21	0.43
1:D:242:PHE:CD1	1:D:263:LEU:HD22	2.54	0.43
1:D:473:LEU:HD12	1:D:480:ALA:HB2	2.00	0.43
1:E:23:ILE:HD12	1:E:479:THR:OG1	2.19	0.43
1:E:238:MET:SD	1:E:342:LYS:HB3	2.59	0.43
1:F:238:MET:SD	1:F:342:LYS:HB3	2.59	0.43
1:A:23:ILE:HD12	1:A:479:THR:OG1	2.19	0.42
1:A:219:VAL:O	1:A:223:ILE:HG13	2.19	0.42
1:B:57:HIS:CD2	1:B:84:HIS:NE2	2.87	0.42
1:B:432:PRO:CB	1:B:436:PHE:HD2	2.28	0.42
1:C:5:ASP:HB2	1:C:333:LYS:NZ	2.34	0.42
1:C:224:GLU:HB2	1:C:242:PHE:HE2	1.84	0.42
1:C:281:TRP:CG	1:C:310:TYR:HD2	2.36	0.42
4:C:507[A]:NAD:C4N	1:E:86:ARG:CZ	2.97	0.42
1:D:23:ILE:HD12	1:D:479:THR:OG1	2.19	0.42
1:D:66:ARG:HG3	1:D:72:TRP:CD2	2.54	0.42
1:E:5:ASP:HB2	1:E:333:LYS:NZ	2.34	0.42
1:E:186:THR:HG22	1:E:187:ILE:N	2.34	0.42
1:E:281:TRP:CG	1:E:310:TYR:HD2	2.36	0.42
1:F:66:ARG:HG3	1:F:72:TRP:CD2	2.54	0.42
4:F:507:NAD:O2N	4:F:507:NAD:N7N	2.47	0.42
1:A:185:SER:HB2	1:B:500:PHE:CE2	2.51	0.42
1:A:201:LYS:HZ3	1:A:388:ASN:HD21	1.68	0.42
1:A:242:PHE:CD1	1:A:263:LEU:HD22	2.54	0.42
1:B:37:THR:HG21	1:B:41:LYS:HG3	2.00	0.42
1:B:40:GLN:HA	1:B:40:GLN:HE21	1.79	0.42
1:B:229:ASN:O	1:B:230:ALA:C	2.62	0.42
1:B:371:LEU:HG	1:B:482:TYR:CE1	2.53	0.42
1:C:4:GLU:O	1:C:5:ASP:HB3	2.19	0.42
1:C:25:GLU:OE1	1:C:46:ARG:NE	2.51	0.42
1:C:219:VAL:O	1:C:223:ILE:HG13	2.19	0.42
1:C:238:MET:SD	1:C:342:LYS:HB3	2.59	0.42
1:D:4:GLU:O	1:D:5:ASP:HB3	2.19	0.42
1:D:5:ASP:OD1	1:D:353:THR:HG21	2.19	0.42
1:E:33:LYS:HA	1:E:41:LYS:HZ1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ASP:HB2	1:F:333:LYS:NZ	2.34	0.42
1:F:219:VAL:O	1:F:223:ILE:HG13	2.19	0.42
1:A:224:GLU:HB2	1:A:242:PHE:HE2	1.84	0.42
1:A:401:TYR:CE2	1:B:443:ALA:N	2.87	0.42
1:B:23:ILE:CD1	1:B:473:LEU:HD21	2.47	0.42
1:B:84:HIS:O	1:B:86:ARG:N	2.51	0.42
1:B:146:ARG:NE	1:B:182:THR:HG22	2.34	0.42
1:B:421:PHE:CZ	1:F:421:PHE:HD1	2.37	0.42
1:C:86:ARG:NH2	4:D:507[A]:NAD:C5N	2.83	0.42
1:C:157:PHE:CE1	1:F:155:LYS:HD2	2.55	0.42
1:C:406:ASN:HD22	1:C:406:ASN:HA	1.60	0.42
1:D:38:GLN:HB2	1:D:39:GLU:H	1.59	0.42
1:E:242:PHE:CD1	1:E:263:LEU:HD22	2.54	0.42
1:F:242:PHE:CD1	1:F:263:LEU:HD22	2.54	0.42
1:F:266:PHE:N	1:F:266:PHE:CD1	2.87	0.42
1:A:4:GLU:O	1:A:5:ASP:HB3	2.19	0.42
1:A:219:VAL:HG13	1:A:373:LEU:HD11	2.00	0.42
1:A:242:PHE:HB2	1:A:266:PHE:O	2.20	0.42
1:A:266:PHE:N	1:A:266:PHE:CD1	2.87	0.42
1:A:392:VAL:HG13	1:B:386:LEU:HD21	2.02	0.42
1:B:23:ILE:HD12	1:B:479:THR:OG1	2.19	0.42
1:B:84:HIS:C	1:B:86:ARG:H	2.28	0.42
1:B:186:THR:HG22	1:B:187:ILE:N	2.35	0.42
1:B:204:SER:OG	1:F:495:GLU:OE1	2.18	0.42
1:B:242:PHE:O	1:B:268:ALA:HA	2.18	0.42
1:B:394:TYR:CE1	1:B:448:ILE:HG13	2.54	0.42
4:B:507[A]:NAD:C5N	1:F:86:ARG:NH2	2.83	0.42
1:C:29:VAL:CA	1:C:45:VAL:HG21	2.50	0.42
1:C:33:LYS:HA	1:C:33:LYS:HD3	1.72	0.42
1:C:282:ASN:H	1:C:307:ALA:HB1	1.82	0.42
1:D:29:VAL:CA	1:D:45:VAL:HG21	2.50	0.42
1:D:146:ARG:NE	1:D:182:THR:HG22	2.33	0.42
1:D:281:TRP:CG	1:D:310:TYR:HD2	2.36	0.42
1:E:5:ASP:OD1	1:E:353:THR:HG21	2.19	0.42
1:E:266:PHE:CD1	1:E:266:PHE:N	2.87	0.42
1:F:4:GLU:O	1:F:5:ASP:HB3	2.19	0.42
1:F:242:PHE:HB2	1:F:266:PHE:O	2.20	0.42
1:F:406:ASN:HD22	1:F:406:ASN:HA	1.60	0.42
1:A:66:ARG:HG3	1:A:72:TRP:CD2	2.54	0.42
1:A:386:LEU:HD21	1:F:392:VAL:HG13	2.00	0.42
1:B:5:ASP:HB2	1:B:333:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TRP:CG	1:B:310:TYR:HD2	2.36	0.42
4:B:507[A]:NAD:C4N	1:F:86:ARG:CZ	2.97	0.42
1:C:57:HIS:CD2	1:C:84:HIS:NE2	2.87	0.42
1:C:66:ARG:HG3	1:C:72:TRP:CD2	2.54	0.42
1:C:242:PHE:CD1	1:C:263:LEU:HD22	2.54	0.42
1:C:465:MET:O	1:C:466:ARG:C	2.61	0.42
1:D:86:ARG:NH2	4:E:507[A]:NAD:C5N	2.82	0.42
1:D:224:GLU:HB2	1:D:242:PHE:HE2	1.84	0.42
1:D:229:ASN:O	1:D:230:ALA:C	2.62	0.42
1:E:57:HIS:CD2	1:E:84:HIS:NE2	2.87	0.42
1:E:242:PHE:HB2	1:E:266:PHE:O	2.20	0.42
1:A:110:LEU:O	1:A:114:LYS:HB2	2.20	0.42
1:A:229:ASN:O	1:A:230:ALA:C	2.62	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.91	0.42
1:B:412:SER:O	1:B:413:VAL:C	2.63	0.42
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.83	0.42
1:F:158:ILE:HG13	1:F:165:PRO:CD	2.50	0.42
1:A:57:HIS:CD2	1:A:84:HIS:NE2	2.87	0.42
1:A:242:PHE:O	1:A:268:ALA:HA	2.18	0.42
1:A:274:GLY:N	1:A:314:ILE:HG13	2.35	0.42
1:B:158:ILE:HG13	1:B:165:PRO:CD	2.50	0.42
1:B:274:GLY:N	1:B:314:ILE:HG13	2.35	0.42
1:B:473:LEU:HD12	1:B:480:ALA:HB2	2.00	0.42
1:D:5:ASP:HB2	1:D:333:LYS:NZ	2.34	0.42
1:D:158:ILE:HG13	1:D:165:PRO:CD	2.50	0.42
1:D:238:MET:SD	1:D:342:LYS:HB3	2.59	0.42
1:E:370:ASP:HB2	1:E:374:ASN:ND2	2.20	0.42
1:E:393:SER:CB	4:E:507[A]:NAD:PA	3.07	0.42
1:F:5:ASP:OD1	1:F:353:THR:HG21	2.19	0.42
1:F:84:HIS:C	1:F:86:ARG:H	2.28	0.42
1:F:172:GLY:H	1:F:175:GLU:HG2	1.83	0.42
1:F:186:THR:HG22	1:F:187:ILE:N	2.35	0.42
1:A:158:ILE:HG13	1:A:165:PRO:CD	2.50	0.42
1:A:432:PRO:CB	1:A:436:PHE:HD2	2.28	0.42
1:A:443:ALA:HB2	1:F:401:TYR:CG	2.55	0.42
1:B:219:VAL:O	1:B:223:ILE:HG13	2.19	0.42
1:C:84:HIS:C	1:C:86:ARG:H	2.28	0.42
1:C:235:ILE:H	1:C:235:ILE:HG13	1.69	0.42
1:D:86:ARG:CZ	4:E:507[A]:NAD:C4N	2.97	0.42
1:D:428:ILE:HD13	1:D:428:ILE:H	1.84	0.42
1:E:42:ARG:O	1:E:46:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.84	0.42
1:F:23:ILE:HD12	1:F:479:THR:OG1	2.19	0.42
1:F:32:LEU:CD1	1:F:44:ARG:HH11	2.33	0.42
1:F:229:ASN:O	1:F:230:ALA:C	2.62	0.42
1:F:274:GLY:N	1:F:314:ILE:HG13	2.35	0.42
1:F:282:ASN:HD21	1:F:284:ASP:H	1.66	0.42
1:A:5:ASP:HB2	1:A:333:LYS:NZ	2.34	0.42
1:A:29:VAL:HG22	1:A:42:ARG:HA	2.02	0.42
1:A:465:MET:O	1:A:466:ARG:C	2.61	0.42
4:A:507[A]:NAD:C5N	1:B:86:ARG:NH2	2.83	0.42
1:B:15:GLY:O	1:B:16:PHE:C	2.63	0.42
1:B:224:GLU:HB2	1:B:242:PHE:HE2	1.84	0.42
1:B:242:PHE:HB2	1:B:266:PHE:O	2.20	0.42
1:B:298:HIS:C	1:B:300:THR:N	2.76	0.42
1:B:406:ASN:HB3	1:B:440:ILE:HD11	2.02	0.42
1:C:32:LEU:CD1	1:C:44:ARG:HH11	2.33	0.42
1:C:86:ARG:CZ	4:D:507[A]:NAD:C4N	2.97	0.42
1:C:120:VAL:O	4:D:507[A]:NAD:N6A	2.49	0.42
1:D:32:LEU:CD1	1:D:44:ARG:HH11	2.33	0.42
1:E:32:LEU:CD1	1:E:44:ARG:HH11	2.33	0.42
1:F:110:LEU:HD23	1:F:110:LEU:HA	1.87	0.42
1:F:224:GLU:HB2	1:F:242:PHE:HE2	1.84	0.42
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.72	0.42
1:C:38:GLN:HB2	1:C:39:GLU:H	1.59	0.42
1:C:186:THR:HG22	1:C:187:ILE:N	2.34	0.42
1:D:32:LEU:HD11	1:D:44:ARG:HH11	1.85	0.42
1:D:33:LYS:HA	1:D:33:LYS:HD3	1.72	0.42
1:D:186:THR:HG22	1:D:187:ILE:N	2.35	0.42
1:D:450:HIS:CE1	5:D:514:HOH:O	2.72	0.42
1:E:33:LYS:HA	1:E:33:LYS:HD3	1.72	0.42
1:E:229:ASN:O	1:E:230:ALA:C	2.62	0.42
1:E:321:ILE:HG23	1:E:343:ILE:CG2	2.50	0.42
1:F:29:VAL:HG22	1:F:42:ARG:HA	2.02	0.42
1:F:110:LEU:O	1:F:114:LYS:HB2	2.20	0.42
1:F:321:ILE:HG23	1:F:343:ILE:CG2	2.50	0.42
1:A:370:ASP:CB	1:A:374:ASN:HD21	2.21	0.41
1:A:406:ASN:HB3	1:A:440:ILE:HD11	2.02	0.41
4:A:507[A]:NAD:C4N	1:B:86:ARG:CZ	2.97	0.41
1:B:32:LEU:CD1	1:B:44:ARG:HH11	2.33	0.41
1:D:266:PHE:N	1:D:266:PHE:CD1	2.87	0.41
1:D:321:ILE:HG23	1:D:343:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:ASN:HB3	1:D:440:ILE:HD11	2.02	0.41
1:E:30:GLU:O	1:E:31:ASP:C	2.63	0.41
1:E:158:ILE:HG13	1:E:165:PRO:CD	2.50	0.41
1:E:201:LYS:HZ3	1:E:388:ASN:HD21	1.67	0.41
1:F:30:GLU:O	1:F:31:ASP:C	2.63	0.41
1:F:42:ARG:O	1:F:46:ARG:N	2.53	0.41
1:F:113:TYR:HB2	1:F:371:LEU:HD21	2.02	0.41
1:F:336:ALA:N	1:F:337:PRO:CD	2.83	0.41
1:A:32:LEU:CD1	1:A:44:ARG:HH11	2.33	0.41
1:A:147:ARG:NH1	1:D:500:PHE:CD1	2.88	0.41
1:A:186:THR:HG22	1:A:187:ILE:N	2.35	0.41
1:B:5:ASP:CB	1:B:333:LYS:HE2	2.51	0.41
1:C:401:TYR:CD2	1:E:443:ALA:HB2	2.55	0.41
1:D:110:LEU:O	1:D:114:LYS:HB2	2.20	0.41
1:D:276:SER:N	4:D:508:NAD:C2A	2.84	0.41
1:D:294:PHE:CD2	1:D:298:HIS:ND1	2.88	0.41
1:E:67:ARG:HH12	1:E:136:TYR:HA	1.83	0.41
1:F:15:GLY:O	1:F:16:PHE:C	2.63	0.41
1:F:239:THR:HG23	1:F:240:PRO:O	2.20	0.41
1:A:32:LEU:HD11	1:A:44:ARG:HH11	1.85	0.41
1:A:86:ARG:NH2	4:F:508[A]:NAD:C5N	2.83	0.41
1:A:239:THR:HG23	1:A:240:PRO:O	2.20	0.41
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.50	0.41
1:A:321:ILE:HA	1:A:343:ILE:O	2.20	0.41
1:A:498:VAL:HB	1:D:72:TRP:CZ2	2.55	0.41
1:B:94:ARG:HE	1:B:168:ASN:HD22	1.67	0.41
1:C:30:GLU:O	1:C:31:ASP:C	2.63	0.41
1:C:229:ASN:O	1:C:230:ALA:C	2.62	0.41
1:C:274:GLY:N	1:C:314:ILE:HG13	2.35	0.41
1:D:13:VAL:HA	1:D:16:PHE:CD1	2.55	0.41
1:D:32:LEU:CD1	1:D:44:ARG:NH1	2.83	0.41
1:D:219:VAL:HG13	1:D:373:LEU:HD11	2.00	0.41
1:D:219:VAL:O	1:D:223:ILE:HG13	2.19	0.41
1:D:242:PHE:HB2	1:D:266:PHE:O	2.20	0.41
1:D:274:GLY:N	1:D:314:ILE:HG13	2.35	0.41
1:D:286:ILE:HD12	1:D:286:ILE:N	2.35	0.41
1:D:336:ALA:N	1:D:337:PRO:CD	2.83	0.41
1:D:412:SER:O	1:D:413:VAL:C	2.63	0.41
1:E:4:GLU:O	1:E:5:ASP:HB3	2.19	0.41
1:E:5:ASP:HB2	1:E:333:LYS:CE	2.50	0.41
1:E:276:SER:N	4:E:508:NAD:C2A	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ALA:N	1:E:337:PRO:CD	2.83	0.41
1:E:393:SER:HB3	4:E:507[A]:NAD:O3	2.20	0.41
1:E:412:SER:O	1:E:413:VAL:C	2.63	0.41
1:F:298:HIS:C	1:F:300:THR:N	2.76	0.41
1:A:42:ARG:O	1:A:46:ARG:N	2.53	0.41
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.56	0.41
1:A:276:SER:N	4:A:508:NAD:C2A	2.84	0.41
1:B:3:ARG:HB2	1:B:4:GLU:H	1.72	0.41
1:B:13:VAL:HA	1:B:16:PHE:CD1	2.55	0.41
1:B:239:THR:HG23	1:B:240:PRO:O	2.20	0.41
1:B:246:THR:CG2	1:B:319:CYS:HA	2.51	0.41
1:B:282:ASN:C	1:B:282:ASN:HD22	2.29	0.41
1:C:13:VAL:HA	1:C:16:PHE:CD1	2.55	0.41
1:C:175:GLU:HA	1:C:178:TRP:CE3	2.56	0.41
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.87	0.41
1:D:432:PRO:HB3	1:D:436:PHE:CD2	2.48	0.41
1:F:32:LEU:HD11	1:F:44:ARG:HH11	1.85	0.41
1:F:32:LEU:CD1	1:F:44:ARG:NH1	2.84	0.41
1:F:276:SER:N	4:F:507:NAD:C2A	2.84	0.41
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.48	0.41
1:A:246:THR:CG2	1:A:319:CYS:HA	2.51	0.41
1:A:336:ALA:N	1:A:337:PRO:CD	2.83	0.41
1:A:457:MET:HA	1:A:457:MET:CE	2.42	0.41
1:B:32:LEU:CD1	1:B:44:ARG:NH1	2.84	0.41
1:B:321:ILE:HG23	1:B:343:ILE:CG2	2.50	0.41
1:C:5:ASP:HB2	1:C:333:LYS:CE	2.50	0.41
1:C:5:ASP:CB	1:C:333:LYS:HE2	2.51	0.41
1:C:230:ALA:O	1:C:234:SER:N	2.49	0.41
1:C:294:PHE:CD2	1:C:298:HIS:ND1	2.88	0.41
4:C:507[A]:NAD:C5N	1:E:86:ARG:NH2	2.83	0.41
1:E:286:ILE:N	1:E:286:ILE:HD12	2.35	0.41
1:E:298:HIS:C	1:E:300:THR:N	2.76	0.41
1:E:321:ILE:HA	1:E:343:ILE:O	2.20	0.41
1:E:331:LEU:HD13	1:E:344:ILE:HD13	2.03	0.41
1:F:246:THR:CG2	1:F:319:CYS:HA	2.51	0.41
1:F:406:ASN:HB3	1:F:440:ILE:HD11	2.02	0.41
1:F:412:SER:O	1:F:413:VAL:C	2.63	0.41
1:A:5:ASP:CB	1:A:333:LYS:HE2	2.51	0.41
1:A:84:HIS:C	1:A:86:ARG:H	2.28	0.41
1:B:113:TYR:HB2	1:B:371:LEU:HD21	2.02	0.41
1:B:465:MET:O	1:B:466:ARG:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:HB2	1:C:266:PHE:O	2.20	0.41
1:C:246:THR:CG2	1:C:319:CYS:HA	2.51	0.41
1:C:321:ILE:HA	1:C:343:ILE:O	2.20	0.41
1:D:29:VAL:HG22	1:D:42:ARG:HA	2.02	0.41
1:D:227:ILE:HD11	1:D:245:LYS:HG2	2.03	0.41
1:D:246:THR:CG2	1:D:319:CYS:HA	2.51	0.41
1:E:13:VAL:HA	1:E:16:PHE:CD1	2.55	0.41
1:E:406:ASN:HB3	1:E:440:ILE:HD11	2.02	0.41
1:F:29:VAL:CA	1:F:45:VAL:HG21	2.50	0.41
1:F:38:GLN:HB2	1:F:39:GLU:H	1.59	0.41
1:A:15:GLY:O	1:A:18:ASP:N	2.54	0.41
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.80	0.41
1:A:495:GLU:HB2	1:F:205:GLN:HE21	1.86	0.41
1:B:30:GLU:O	1:B:31:ASP:C	2.63	0.41
1:B:110:LEU:O	1:B:114:LYS:HB2	2.20	0.41
1:B:155:LYS:HD2	1:E:157:PHE:CE1	2.56	0.41
1:B:401:TYR:CD1	1:F:443:ALA:HB2	2.56	0.41
1:B:421:PHE:CZ	1:F:421:PHE:CD1	3.09	0.41
1:C:32:LEU:CD1	1:C:44:ARG:NH1	2.84	0.41
1:C:110:LEU:O	1:C:114:LYS:HB2	2.20	0.41
1:D:42:ARG:O	1:D:46:ARG:N	2.53	0.41
1:D:84:HIS:C	1:D:86:ARG:H	2.28	0.41
1:D:331:LEU:HD13	1:D:344:ILE:HD13	2.03	0.41
3:D:506:AKG:O2	4:D:508:NAD:C6N	2.68	0.41
1:E:32:LEU:HD11	1:E:44:ARG:HH11	1.85	0.41
1:E:110:LEU:O	1:E:114:LYS:HB2	2.20	0.41
1:E:274:GLY:N	1:E:314:ILE:HG13	2.35	0.41
1:E:344:ILE:HB	1:E:367:VAL:HA	2.03	0.41
1:E:420:LYS:HZ3	1:E:420:LYS:HG2	1.66	0.41
1:F:13:VAL:HA	1:F:16:PHE:CD1	2.55	0.41
1:F:33:LYS:HA	1:F:41:LYS:HZ3	1.85	0.41
1:F:167:PRO:HG3	1:F:176:MET:CG	2.51	0.41
1:F:175:GLU:HA	1:F:178:TRP:CE3	2.56	0.41
1:F:294:PHE:CD2	1:F:298:HIS:ND1	2.88	0.41
1:F:302:LEU:HD23	1:F:302:LEU:HA	1.83	0.41
1:F:331:LEU:HD13	1:F:344:ILE:HD13	2.03	0.41
1:F:333:LYS:HE2	1:F:333:LYS:HB3	1.65	0.41
3:F:506:AKG:O2	4:F:507:NAD:C6N	2.68	0.41
1:A:5:ASP:HB2	1:A:333:LYS:CE	2.50	0.41
1:A:238:MET:SD	1:A:342:LYS:HB3	2.59	0.41
1:A:294:PHE:CD2	1:A:298:HIS:ND1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLU:HB2	1:B:242:PHE:CE2	2.56	0.41
1:B:227:ILE:HD11	1:B:245:LYS:HG2	2.03	0.41
1:B:294:PHE:CD2	1:B:298:HIS:ND1	2.88	0.41
4:B:507[A]:NAD:N6A	1:F:120:VAL:O	2.49	0.41
1:C:15:GLY:O	1:C:18:ASP:N	2.54	0.41
1:C:344:ILE:HB	1:C:367:VAL:HA	2.03	0.41
1:C:360:PHE:HB3	1:C:365:ILE:HB	2.03	0.41
1:C:412:SER:O	1:C:413:VAL:C	2.63	0.41
3:C:506:AKG:O2	4:C:508:NAD:C6N	2.68	0.41
1:D:5:ASP:HB2	1:D:333:LYS:CE	2.50	0.41
1:D:33:LYS:HA	1:D:41:LYS:HZ1	1.83	0.41
1:D:370:ASP:HB2	1:D:374:ASN:ND2	2.20	0.41
1:E:32:LEU:CD1	1:E:44:ARG:NH1	2.83	0.41
1:E:84:HIS:C	1:E:86:ARG:H	2.28	0.41
1:E:428:ILE:HD13	1:E:428:ILE:H	1.84	0.41
1:F:23:ILE:CD1	1:F:473:LEU:HD21	2.47	0.41
1:F:465:MET:O	1:F:466:ARG:C	2.61	0.41
1:A:13:VAL:HA	1:A:16:PHE:CD1	2.55	0.41
1:A:15:GLY:O	1:A:16:PHE:C	2.63	0.41
1:A:32:LEU:CD1	1:A:44:ARG:NH1	2.84	0.41
1:A:87:THR:HG21	1:F:195:HIS:CE1	2.51	0.41
1:A:227:ILE:HD11	1:A:245:LYS:HG2	2.03	0.41
1:A:298:HIS:C	1:A:300:THR:N	2.76	0.41
1:A:360:PHE:HB3	1:A:365:ILE:HB	2.03	0.41
1:A:409:LEU:HD12	1:B:436:PHE:HZ	1.83	0.41
1:B:15:GLY:O	1:B:18:ASP:N	2.54	0.41
1:B:32:LEU:HD11	1:B:44:ARG:HH11	1.85	0.41
1:B:42:ARG:O	1:B:46:ARG:N	2.53	0.41
1:B:57:HIS:CE1	1:E:151:GLU:OE1	2.74	0.41
1:B:286:ILE:HD12	1:B:286:ILE:N	2.36	0.41
1:C:29:VAL:HG22	1:C:42:ARG:HA	2.02	0.41
1:C:42:ARG:O	1:C:46:ARG:N	2.53	0.41
1:C:93:ILE:HA	1:C:127:ALA:HB3	2.03	0.41
1:C:158:ILE:HG13	1:C:165:PRO:CD	2.50	0.41
1:C:276:SER:N	4:C:508:NAD:C2A	2.84	0.41
1:C:286:ILE:HD12	1:C:286:ILE:N	2.35	0.41
1:C:417:LEU:CD1	1:D:417:LEU:CD2	2.96	0.41
1:C:498:VAL:HB	1:F:72:TRP:CZ2	2.55	0.41
1:D:94:ARG:HE	1:D:168:ASN:HD22	1.67	0.41
1:D:321:ILE:HA	1:D:343:ILE:O	2.20	0.41
1:D:360:PHE:O	1:D:365:ILE:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:VAL:CA	1:E:45:VAL:HG21	2.50	0.41
1:E:86:ARG:HA	1:E:86:ARG:HD2	1.85	0.41
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.56	0.41
1:E:239:THR:HG23	1:E:240:PRO:O	2.20	0.41
1:E:283:PRO:C	1:E:285:GLY:H	2.29	0.41
1:F:321:ILE:HA	1:F:343:ILE:O	2.20	0.41
1:F:343:ILE:HG12	1:F:366:MET:HE2	2.03	0.41
1:F:413:VAL:O	1:F:416:SER:HB2	2.21	0.41
1:B:26:ASP:HA	1:B:42:ARG:HH12	1.86	0.41
3:B:506:AKG:O2	4:B:508:NAD:C6N	2.68	0.41
1:C:32:LEU:HD11	1:C:44:ARG:HH11	1.85	0.41
1:C:55:CYS:O	1:F:62:SER:HB3	2.21	0.41
1:C:413:VAL:O	1:C:416:SER:HB2	2.21	0.41
1:D:15:GLY:O	1:D:18:ASP:N	2.54	0.41
1:D:26:ASP:HA	1:D:42:ARG:HH12	1.86	0.41
1:D:224:GLU:HB2	1:D:242:PHE:CE2	2.56	0.41
1:D:273:VAL:HG21	1:D:291:LEU:HD11	2.03	0.41
1:D:344:ILE:HB	1:D:367:VAL:HA	2.03	0.41
1:E:5:ASP:CB	1:E:333:LYS:HE2	2.51	0.41
1:E:29:VAL:HG22	1:E:42:ARG:HA	2.02	0.41
1:E:294:PHE:CD2	1:E:298:HIS:ND1	2.88	0.41
1:F:15:GLY:O	1:F:18:ASP:N	2.54	0.41
1:F:360:PHE:HB3	1:F:365:ILE:HB	2.03	0.41
1:A:395:GLY:O	1:A:396:ARG:C	2.65	0.40
1:B:29:VAL:HG22	1:B:42:ARG:HA	2.02	0.40
1:B:321:ILE:HA	1:B:343:ILE:O	2.20	0.40
1:B:385:ILE:CG2	1:B:386:LEU:N	2.85	0.40
1:C:224:GLU:HB2	1:C:242:PHE:CE2	2.56	0.40
1:C:336:ALA:N	1:C:337:PRO:CD	2.83	0.40
1:C:361:LEU:HD23	1:C:361:LEU:HA	1.97	0.40
1:C:499:THR:CB	1:F:64:PRO:HG2	2.51	0.40
1:D:113:TYR:HB2	1:D:371:LEU:HD21	2.02	0.40
1:D:165:PRO:HD2	1:D:197:CYS:O	2.21	0.40
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.56	0.40
1:D:360:PHE:HB3	1:D:365:ILE:HB	2.03	0.40
1:E:15:GLY:O	1:E:18:ASP:N	2.54	0.40
1:E:432:PRO:CB	1:E:436:PHE:HD2	2.28	0.40
1:F:93:ILE:HA	1:F:127:ALA:HB3	2.04	0.40
1:F:286:ILE:HD12	1:F:286:ILE:N	2.36	0.40
1:F:385:ILE:CG2	1:F:386:LEU:N	2.85	0.40
1:A:113:TYR:HB2	1:A:371:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:HE21	1:B:495:GLU:HB2	1.86	0.40
1:B:167:PRO:HG3	1:B:176:MET:CG	2.51	0.40
1:B:276:SER:N	4:B:508:NAD:C2A	2.84	0.40
1:B:360:PHE:HB3	1:B:365:ILE:HB	2.03	0.40
1:C:54:PRO:HG3	1:F:74:VAL:HG11	2.02	0.40
1:C:167:PRO:HG3	1:C:176:MET:CG	2.51	0.40
1:C:343:ILE:HG12	1:C:366:MET:HE2	2.03	0.40
1:C:406:ASN:HB3	1:C:440:ILE:HD11	2.02	0.40
1:D:386:LEU:HD12	1:D:386:LEU:HA	1.80	0.40
1:E:167:PRO:HG3	1:E:176:MET:CG	2.51	0.40
1:E:227:ILE:HD11	1:E:245:LYS:HG2	2.03	0.40
1:E:273:VAL:HG21	1:E:291:LEU:HD11	2.03	0.40
1:E:360:PHE:HB3	1:E:365:ILE:HB	2.03	0.40
1:F:395:GLY:O	1:F:396:ARG:C	2.64	0.40
1:A:26:ASP:HA	1:A:42:ARG:HH12	1.86	0.40
1:A:409:LEU:HD21	1:B:409:LEU:CD2	2.51	0.40
1:B:29:VAL:CA	1:B:45:VAL:HG21	2.50	0.40
1:B:336:ALA:N	1:B:337:PRO:CD	2.83	0.40
1:C:23:ILE:CD1	1:C:473:LEU:HD21	2.47	0.40
1:C:113:TYR:HB2	1:C:371:LEU:HD21	2.02	0.40
1:C:273:VAL:HG21	1:C:291:LEU:HD11	2.03	0.40
1:C:321:ILE:HG23	1:C:343:ILE:CG2	2.50	0.40
1:D:298:HIS:C	1:D:300:THR:N	2.76	0.40
1:D:333:LYS:HE2	1:D:333:LYS:HB3	1.65	0.40
1:E:113:TYR:HB2	1:E:371:LEU:HD21	2.02	0.40
1:E:370:ASP:CB	1:E:374:ASN:HD21	2.21	0.40
1:F:224:GLU:HB2	1:F:242:PHE:CE2	2.56	0.40
1:F:236:LEU:O	1:F:342:LYS:HD2	2.21	0.40
1:F:260:MET:HE2	1:F:288:PRO:CA	2.52	0.40
1:F:346:GLU:OE2	1:F:369:PRO:HA	2.22	0.40
1:A:23:ILE:CD1	1:A:473:LEU:HD21	2.47	0.40
1:A:224:GLU:HB2	1:A:242:PHE:CE2	2.56	0.40
1:A:273:VAL:HG21	1:A:291:LEU:HD11	2.03	0.40
1:A:286:ILE:HD12	1:A:286:ILE:N	2.36	0.40
1:B:165:PRO:HD2	1:B:197:CYS:O	2.21	0.40
1:B:413:VAL:O	1:B:416:SER:HB2	2.21	0.40
1:C:417:LEU:HD21	1:E:417:LEU:HD12	2.01	0.40
1:D:30:GLU:O	1:D:31:ASP:C	2.63	0.40
1:D:395:GLY:O	1:D:396:ARG:C	2.65	0.40
1:E:110:LEU:HD23	1:E:110:LEU:HA	1.87	0.40
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:THR:CG2	1:E:319:CYS:HA	2.51	0.40
1:E:346:GLU:OE2	1:E:369:PRO:HA	2.22	0.40
1:F:273:VAL:HG21	1:F:291:LEU:HD11	2.03	0.40
1:A:331:LEU:HD13	1:A:344:ILE:HD13	2.03	0.40
1:A:344:ILE:HB	1:A:367:VAL:HA	2.03	0.40
1:B:303:GLY:H	1:B:309:ILE:CD1	2.31	0.40
1:C:110:LEU:HD23	1:C:110:LEU:HA	1.87	0.40
1:C:239:THR:HG23	1:C:240:PRO:O	2.20	0.40
1:C:282:ASN:C	1:C:282:ASN:HD22	2.29	0.40
1:D:15:GLY:O	1:D:16:PHE:C	2.63	0.40
1:E:331:LEU:HA	1:E:335:ASN:HD21	1.87	0.40
1:E:413:VAL:O	1:E:416:SER:HB2	2.21	0.40
1:F:26:ASP:HA	1:F:42:ARG:HH12	1.86	0.40

All (3) 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:A:3:ARG:CZ	1:E:298:HIS:NE2[2_556]	2.14	0.06
1:B:309:ILE:CG1	1:C:284:ASP:OD1[2_545]	2.14	0.06
1:B:69:ASP:O	1:C:3:ARG:NH2[2_545]	2.19	0.01

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	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2 15
1	B	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2 15
1	C	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2 15
1	D	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
1	F	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	2	15
All	All	2994/3006 (100%)	2502 (84%)	354 (12%)	138 (5%)	2	15

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	35	ARG
1	A	70	GLY
1	B	5	ASP
1	B	35	ARG
1	B	70	GLY
1	C	5	ASP
1	C	35	ARG
1	C	70	GLY
1	D	5	ASP
1	D	35	ARG
1	D	70	GLY
1	E	5	ASP
1	E	35	ARG
1	E	70	GLY
1	F	5	ASP
1	F	35	ARG
1	F	70	GLY
1	A	34	THR
1	A	230	ALA
1	A	422	GLY
1	A	426	GLY
1	B	34	THR
1	B	230	ALA
1	B	422	GLY
1	B	426	GLY
1	C	34	THR
1	C	230	ALA
1	C	422	GLY
1	C	426	GLY
1	D	34	THR
1	D	230	ALA
1	D	422	GLY
1	D	426	GLY

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Mol	Chain	Res	Type
1	E	34	THR
1	E	230	ALA
1	E	422	GLY
1	E	426	GLY
1	F	34	THR
1	F	230	ALA
1	F	422	GLY
1	F	426	GLY
1	A	38	GLN
1	A	85	GLN
1	A	396	ARG
1	A	470	LYS
1	A	498	VAL
1	B	38	GLN
1	B	396	ARG
1	B	470	LYS
1	B	498	VAL
1	C	38	GLN
1	C	396	ARG
1	C	470	LYS
1	C	498	VAL
1	D	38	GLN
1	D	85	GLN
1	D	396	ARG
1	D	470	LYS
1	D	498	VAL
1	E	38	GLN
1	E	85	GLN
1	E	396	ARG
1	E	470	LYS
1	E	498	VAL
1	F	38	GLN
1	F	396	ARG
1	F	470	LYS
1	F	498	VAL
1	A	25	GLU
1	A	158	ILE
1	A	327	SER
1	A	399	PHE
1	A	414	GLN
1	B	25	GLU
1	B	85	GLN

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Mol	Chain	Res	Type
1	B	158	ILE
1	B	327	SER
1	B	399	PHE
1	B	414	GLN
1	C	25	GLU
1	C	85	GLN
1	C	158	ILE
1	C	327	SER
1	C	399	PHE
1	C	414	GLN
1	D	25	GLU
1	D	158	ILE
1	D	327	SER
1	D	399	PHE
1	D	414	GLN
1	E	25	GLU
1	E	158	ILE
1	E	327	SER
1	E	399	PHE
1	E	414	GLN
1	F	25	GLU
1	F	85	GLN
1	F	158	ILE
1	F	327	SER
1	F	399	PHE
1	F	414	GLN
1	A	37	THR
1	A	71	SER
1	B	37	THR
1	B	71	SER
1	C	37	THR
1	C	71	SER
1	D	37	THR
1	D	71	SER
1	E	37	THR
1	E	71	SER
1	F	37	THR
1	F	71	SER
1	A	133	PRO
1	B	133	PRO
1	C	133	PRO
1	D	133	PRO

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Mol	Chain	Res	Type
1	E	133	PRO
1	F	133	PRO
1	A	251	GLY
1	B	251	GLY
1	C	251	GLY
1	D	251	GLY
1	E	251	GLY
1	F	251	GLY
1	A	309	ILE
1	B	88	PRO
1	B	309	ILE
1	C	309	ILE
1	D	309	ILE
1	E	88	PRO
1	E	309	ILE
1	F	88	PRO
1	F	309	ILE
1	A	88	PRO
1	C	88	PRO
1	D	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	B	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	C	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	D	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	E	417/417 (100%)	353 (85%)	64 (15%)	3	14
1	F	417/417 (100%)	353 (85%)	64 (15%)	3	14
All	All	2502/2502 (100%)	2118 (85%)	384 (15%)	3	14

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	26	ASP
1	A	32	LEU
1	A	38	GLN
1	A	40	GLN
1	A	46	ARG
1	A	61	LEU
1	A	90	LYS
1	A	102	ASP
1	A	107	LEU
1	A	112	THR
1	A	130	LYS
1	A	138	ASP
1	A	145	THR
1	A	162	VAL
1	A	170	SER
1	A	175	GLU
1	A	182	THR
1	A	187	ILE
1	A	211	ARG
1	A	231	SER
1	A	236	LEU
1	A	239	THR
1	A	246	THR
1	A	249	VAL
1	A	255	VAL
1	A	271	VAL
1	A	275	GLU
1	A	280	ILE
1	A	291	LEU
1	A	295	LYS
1	A	308	LYS
1	A	310	TYR
1	A	314	ILE
1	A	316	GLU
1	A	321	ILE
1	A	328	GLU
1	A	330	GLN
1	A	354	PRO
1	A	371	LEU
1	A	373	LEU
1	A	378	VAL
1	A	381	SER

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Mol	Chain	Res	Type
1	A	385	ILE
1	A	386	LEU
1	A	392	VAL
1	A	393	SER
1	A	396	ARG
1	A	402	GLU
1	A	405	SER
1	A	406	ASN
1	A	413	VAL
1	A	421	PHE
1	A	423	LYS
1	A	427	THR
1	A	428	ILE
1	A	437	GLN
1	A	451	SER
1	A	458	GLU
1	A	469	MET
1	A	479	THR
1	A	499	THR
1	A	500	PHE
1	A	501	THR
1	B	3	ARG
1	B	26	ASP
1	B	32	LEU
1	B	38	GLN
1	B	40	GLN
1	B	46	ARG
1	B	61	LEU
1	B	90	LYS
1	B	102	ASP
1	B	107	LEU
1	B	112	THR
1	B	130	LYS
1	B	138	ASP
1	B	145	THR
1	B	162	VAL
1	B	170	SER
1	B	175	GLU
1	B	182	THR
1	B	187	ILE
1	B	211	ARG
1	B	231	SER

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Mol	Chain	Res	Type
1	B	236	LEU
1	B	239	THR
1	B	246	THR
1	B	249	VAL
1	B	255	VAL
1	B	271	VAL
1	B	275	GLU
1	B	280	ILE
1	B	291	LEU
1	B	295	LYS
1	B	308	LYS
1	B	310	TYR
1	B	314	ILE
1	B	316	GLU
1	B	321	ILE
1	B	328	GLU
1	B	330	GLN
1	B	354	PRO
1	B	371	LEU
1	B	373	LEU
1	B	378	VAL
1	B	381	SER
1	B	385	ILE
1	B	386	LEU
1	B	392	VAL
1	B	393	SER
1	B	396	ARG
1	B	402	GLU
1	B	405	SER
1	B	406	ASN
1	B	413	VAL
1	B	421	PHE
1	B	423	LYS
1	B	427	THR
1	B	428	ILE
1	B	437	GLN
1	B	451	SER
1	B	458	GLU
1	B	469	MET
1	B	479	THR
1	B	499	THR
1	B	500	PHE

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Mol	Chain	Res	Type
1	B	501	THR
1	C	3	ARG
1	C	26	ASP
1	C	32	LEU
1	C	38	GLN
1	C	40	GLN
1	C	46	ARG
1	C	61	LEU
1	C	90	LYS
1	C	102	ASP
1	C	107	LEU
1	C	112	THR
1	C	130	LYS
1	C	138	ASP
1	C	145	THR
1	C	162	VAL
1	C	170	SER
1	C	175	GLU
1	C	182	THR
1	C	187	ILE
1	C	211	ARG
1	C	231	SER
1	C	236	LEU
1	C	239	THR
1	C	246	THR
1	C	249	VAL
1	C	255	VAL
1	C	271	VAL
1	C	275	GLU
1	C	280	ILE
1	C	291	LEU
1	C	295	LYS
1	C	308	LYS
1	C	310	TYR
1	C	314	ILE
1	C	316	GLU
1	C	321	ILE
1	C	328	GLU
1	C	330	GLN
1	C	354	PRO
1	C	371	LEU
1	C	373	LEU

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Mol	Chain	Res	Type
1	C	378	VAL
1	C	381	SER
1	C	385	ILE
1	C	386	LEU
1	C	392	VAL
1	C	393	SER
1	C	396	ARG
1	C	402	GLU
1	C	405	SER
1	C	406	ASN
1	C	413	VAL
1	C	421	PHE
1	C	423	LYS
1	C	427	THR
1	C	428	ILE
1	C	437	GLN
1	C	451	SER
1	C	458	GLU
1	C	469	MET
1	C	479	THR
1	C	499	THR
1	C	500	PHE
1	C	501	THR
1	D	3	ARG
1	D	26	ASP
1	D	32	LEU
1	D	38	GLN
1	D	40	GLN
1	D	46	ARG
1	D	61	LEU
1	D	90	LYS
1	D	102	ASP
1	D	107	LEU
1	D	112	THR
1	D	130	LYS
1	D	138	ASP
1	D	145	THR
1	D	162	VAL
1	D	170	SER
1	D	175	GLU
1	D	182	THR
1	D	187	ILE

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Mol	Chain	Res	Type
1	D	211	ARG
1	D	231	SER
1	D	236	LEU
1	D	239	THR
1	D	246	THR
1	D	249	VAL
1	D	255	VAL
1	D	271	VAL
1	D	275	GLU
1	D	280	ILE
1	D	291	LEU
1	D	295	LYS
1	D	308	LYS
1	D	310	TYR
1	D	314	ILE
1	D	316	GLU
1	D	321	ILE
1	D	328	GLU
1	D	330	GLN
1	D	354	PRO
1	D	371	LEU
1	D	373	LEU
1	D	378	VAL
1	D	381	SER
1	D	385	ILE
1	D	386	LEU
1	D	392	VAL
1	D	393	SER
1	D	396	ARG
1	D	402	GLU
1	D	405	SER
1	D	406	ASN
1	D	413	VAL
1	D	421	PHE
1	D	423	LYS
1	D	427	THR
1	D	428	ILE
1	D	437	GLN
1	D	451	SER
1	D	458	GLU
1	D	469	MET
1	D	479	THR

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Mol	Chain	Res	Type
1	D	499	THR
1	D	500	PHE
1	D	501	THR
1	E	3	ARG
1	E	26	ASP
1	E	32	LEU
1	E	38	GLN
1	E	40	GLN
1	E	46	ARG
1	E	61	LEU
1	E	90	LYS
1	E	102	ASP
1	E	107	LEU
1	E	112	THR
1	E	130	LYS
1	E	138	ASP
1	E	145	THR
1	E	162	VAL
1	E	170	SER
1	E	175	GLU
1	E	182	THR
1	E	187	ILE
1	E	211	ARG
1	E	231	SER
1	E	236	LEU
1	E	239	THR
1	E	246	THR
1	E	249	VAL
1	E	255	VAL
1	E	271	VAL
1	E	275	GLU
1	E	280	ILE
1	E	291	LEU
1	E	295	LYS
1	E	308	LYS
1	E	310	TYR
1	E	314	ILE
1	E	316	GLU
1	E	321	ILE
1	E	328	GLU
1	E	330	GLN
1	E	354	PRO

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Mol	Chain	Res	Type
1	E	371	LEU
1	E	373	LEU
1	E	378	VAL
1	E	381	SER
1	E	385	ILE
1	E	386	LEU
1	E	392	VAL
1	E	393	SER
1	E	396	ARG
1	E	402	GLU
1	E	405	SER
1	E	406	ASN
1	E	413	VAL
1	E	421	PHE
1	E	423	LYS
1	E	427	THR
1	E	428	ILE
1	E	437	GLN
1	E	451	SER
1	E	458	GLU
1	E	469	MET
1	E	479	THR
1	E	499	THR
1	E	500	PHE
1	E	501	THR
1	F	3	ARG
1	F	26	ASP
1	F	32	LEU
1	F	38	GLN
1	F	40	GLN
1	F	46	ARG
1	F	61	LEU
1	F	90	LYS
1	F	102	ASP
1	F	107	LEU
1	F	112	THR
1	F	130	LYS
1	F	138	ASP
1	F	145	THR
1	F	162	VAL
1	F	170	SER
1	F	175	GLU

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Mol	Chain	Res	Type
1	F	182	THR
1	F	187	ILE
1	F	211	ARG
1	F	231	SER
1	F	236	LEU
1	F	239	THR
1	F	246	THR
1	F	249	VAL
1	F	255	VAL
1	F	271	VAL
1	F	275	GLU
1	F	280	ILE
1	F	291	LEU
1	F	295	LYS
1	F	308	LYS
1	F	310	TYR
1	F	314	ILE
1	F	316	GLU
1	F	321	ILE
1	F	328	GLU
1	F	330	GLN
1	F	354	PRO
1	F	371	LEU
1	F	373	LEU
1	F	378	VAL
1	F	381	SER
1	F	385	ILE
1	F	386	LEU
1	F	392	VAL
1	F	393	SER
1	F	396	ARG
1	F	402	GLU
1	F	405	SER
1	F	406	ASN
1	F	413	VAL
1	F	421	PHE
1	F	423	LYS
1	F	427	THR
1	F	428	ILE
1	F	437	GLN
1	F	451	SER
1	F	458	GLU

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Mol	Chain	Res	Type
1	F	469	MET
1	F	479	THR
1	F	499	THR
1	F	500	PHE
1	F	501	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	56	ASN
1	A	57	HIS
1	A	82	HIS
1	A	132	ASN
1	A	168	ASN
1	A	189	HIS
1	A	195	HIS
1	A	205	GLN
1	A	209	HIS
1	A	254	ASN
1	A	258	HIS
1	A	264	HIS
1	A	282	ASN
1	A	388	ASN
1	A	391	HIS
1	A	406	ASN
1	A	450	HIS
1	A	463	GLN
1	A	484	ASN
1	A	494	ASN
1	B	43	ASN
1	B	56	ASN
1	B	57	HIS
1	B	82	HIS
1	B	132	ASN
1	B	168	ASN
1	B	189	HIS
1	B	195	HIS
1	B	209	HIS
1	B	254	ASN
1	B	258	HIS
1	B	264	HIS

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	388	ASN
1	B	391	HIS
1	B	406	ASN
1	B	450	HIS
1	B	463	GLN
1	B	484	ASN
1	B	494	ASN
1	C	43	ASN
1	C	56	ASN
1	C	57	HIS
1	C	82	HIS
1	C	132	ASN
1	C	168	ASN
1	C	189	HIS
1	C	195	HIS
1	C	209	HIS
1	C	254	ASN
1	C	258	HIS
1	C	264	HIS
1	C	282	ASN
1	C	388	ASN
1	C	391	HIS
1	C	406	ASN
1	C	450	HIS
1	C	463	GLN
1	C	484	ASN
1	C	494	ASN
1	D	43	ASN
1	D	56	ASN
1	D	57	HIS
1	D	82	HIS
1	D	132	ASN
1	D	168	ASN
1	D	189	HIS
1	D	195	HIS
1	D	205	GLN
1	D	209	HIS
1	D	254	ASN
1	D	258	HIS
1	D	264	HIS
1	D	282	ASN

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Mol	Chain	Res	Type
1	D	388	ASN
1	D	391	HIS
1	D	406	ASN
1	D	408	HIS
1	D	450	HIS
1	D	463	GLN
1	D	484	ASN
1	D	494	ASN
1	E	43	ASN
1	E	56	ASN
1	E	57	HIS
1	E	82	HIS
1	E	132	ASN
1	E	168	ASN
1	E	189	HIS
1	E	195	HIS
1	E	205	GLN
1	E	209	HIS
1	E	254	ASN
1	E	258	HIS
1	E	264	HIS
1	E	282	ASN
1	E	388	ASN
1	E	391	HIS
1	E	406	ASN
1	E	408	HIS
1	E	450	HIS
1	E	463	GLN
1	E	484	ASN
1	E	494	ASN
1	F	43	ASN
1	F	56	ASN
1	F	57	HIS
1	F	82	HIS
1	F	132	ASN
1	F	168	ASN
1	F	189	HIS
1	F	195	HIS
1	F	205	GLN
1	F	209	HIS
1	F	254	ASN
1	F	258	HIS

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Mol	Chain	Res	Type
1	F	264	HIS
1	F	282	ASN
1	F	388	ASN
1	F	391	HIS
1	F	406	ASN
1	F	450	HIS
1	F	463	GLN
1	F	484	ASN
1	F	494	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 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	PO4	F	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.92	0
2	PO4	B	505	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	D	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
4	NAD	D	508	-	46,48,48	2.47	14 (30%)	64,73,73	2.10	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	502	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
2	PO4	C	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
3	AKG	C	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.30	5 (45%)
4	NAD	C	508	-	46,48,48	2.48	15 (32%)	64,73,73	2.09	16 (25%)
4	NAD	E	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	B	508	-	46,48,48	2.47	15 (32%)	64,73,73	2.09	16 (25%)
3	AKG	B	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.30	5 (45%)
4	NAD	E	507[B]	-	46,48,48	2.69	15 (32%)	64,73,73	1.95	17 (26%)
2	PO4	B	504	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	C	507[A]	-	46,48,48	2.58	14 (30%)	64,73,73	2.22	18 (28%)
2	PO4	A	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
2	PO4	E	502	-	4,4,4	1.24	1 (25%)	6,6,6	0.91	0
2	PO4	E	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	C	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)
4	NAD	F	508[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	F	508[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)
3	AKG	D	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.31	5 (45%)
2	PO4	C	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	B	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	A	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
4	NAD	A	508	-	46,48,48	2.47	15 (32%)	64,73,73	2.09	16 (25%)
2	PO4	C	504	-	4,4,4	2.00	1 (25%)	6,6,6	0.90	0
2	PO4	D	505	-	4,4,4	1.98	1 (25%)	6,6,6	0.90	0
4	NAD	F	507	-	46,48,48	2.48	15 (32%)	64,73,73	2.09	16 (25%)
2	PO4	D	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
2	PO4	F	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
2	PO4	C	505	-	4,4,4	1.25	1 (25%)	6,6,6	0.92	0
2	PO4	F	504	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
2	PO4	E	504	-	4,4,4	1.26	1 (25%)	6,6,6	0.91	0
4	NAD	E	508	-	46,48,48	2.48	15 (32%)	64,73,73	2.10	16 (25%)
3	AKG	A	506	-	9,9,9	1.75	2 (22%)	11,11,11	3.30	5 (45%)
3	AKG	F	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.30	5 (45%)
2	PO4	B	503	-	4,4,4	1.26	1 (25%)	6,6,6	0.92	0
2	PO4	E	503	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
4	NAD	A	507[A]	-	46,48,48	2.58	14 (30%)	64,73,73	2.22	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	502	-	4,4,4	1.25	1 (25%)	6,6,6	0.91	0
2	PO4	F	502	-	4,4,4	1.27	1 (25%)	6,6,6	0.92	0
4	NAD	D	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
3	AKG	E	506	-	9,9,9	1.76	2 (22%)	11,11,11	3.29	5 (45%)
4	NAD	A	507[B]	-	46,48,48	2.69	15 (32%)	64,73,73	1.96	17 (26%)
4	NAD	D	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	17 (26%)
2	PO4	A	505	-	4,4,4	1.99	1 (25%)	6,6,6	0.90	0
4	NAD	B	507[A]	-	46,48,48	2.57	14 (30%)	64,73,73	2.21	18 (28%)
4	NAD	B	507[B]	-	46,48,48	2.68	15 (32%)	64,73,73	1.95	18 (28%)

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
4	NAD	D	508	-	-	11/30/62/62	0/5/5/5
4	NAD	C	508	-	-	11/30/62/62	0/5/5/5
4	NAD	E	507[A]	-	-	9/30/62/62	0/5/5/5
3	AKG	C	506	-	-	4/9/9/9	-
4	NAD	B	508	-	-	11/30/62/62	0/5/5/5
3	AKG	B	506	-	-	4/9/9/9	-
4	NAD	E	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	C	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	C	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	F	508[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	F	508[B]	-	-	10/30/62/62	0/5/5/5
3	AKG	D	506	-	-	4/9/9/9	-
4	NAD	A	508	-	-	11/30/62/62	0/5/5/5
4	NAD	F	507	-	-	11/30/62/62	0/5/5/5
4	NAD	E	508	-	-	11/30/62/62	0/5/5/5
3	AKG	A	506	-	-	4/9/9/9	-
3	AKG	F	506	-	-	4/9/9/9	-
4	NAD	A	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	D	507[A]	-	-	9/30/62/62	0/5/5/5
3	AKG	E	506	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	A	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	D	507[B]	-	-	10/30/62/62	0/5/5/5
4	NAD	B	507[A]	-	-	9/30/62/62	0/5/5/5
4	NAD	B	507[B]	-	-	10/30/62/62	0/5/5/5

All (299) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[A]	NAD	PN-O3	8.78	1.69	1.59
4	A	507[A]	NAD	PN-O3	8.75	1.68	1.59
4	D	507[A]	NAD	PN-O3	8.74	1.68	1.59
4	F	508[A]	NAD	PN-O3	8.73	1.68	1.59
4	E	507[A]	NAD	PN-O3	8.71	1.68	1.59
4	B	507[A]	NAD	PN-O3	8.70	1.68	1.59
4	E	507[B]	NAD	PN-O3	7.41	1.67	1.59
4	A	507[B]	NAD	PN-O3	7.39	1.67	1.59
4	C	507[B]	NAD	PN-O3	7.37	1.67	1.59
4	F	508[B]	NAD	PN-O3	7.36	1.67	1.59
4	B	507[B]	NAD	PN-O3	7.32	1.67	1.59
4	D	507[B]	NAD	PN-O3	7.31	1.67	1.59
4	E	507[B]	NAD	C7N-N7N	7.27	1.46	1.33
4	B	507[B]	NAD	C7N-N7N	7.24	1.46	1.33
4	A	507[B]	NAD	C7N-N7N	7.23	1.46	1.33
4	F	508[B]	NAD	C7N-N7N	7.23	1.46	1.33
4	C	507[B]	NAD	C7N-N7N	7.23	1.46	1.33
4	D	507[B]	NAD	C7N-N7N	7.22	1.46	1.33
4	E	508	NAD	PA-O3	-6.55	1.52	1.59
4	C	508	NAD	PA-O3	-6.53	1.52	1.59
4	A	508	NAD	PA-O3	-6.51	1.52	1.59
4	B	508	NAD	PA-O3	-6.50	1.52	1.59
4	F	507	NAD	PA-O3	-6.49	1.52	1.59
4	E	507[A]	NAD	PA-O1A	6.48	1.73	1.50
4	B	507[A]	NAD	PA-O1A	6.48	1.73	1.50
4	C	507[A]	NAD	PA-O1A	6.48	1.73	1.50
4	F	508[A]	NAD	PA-O1A	6.47	1.73	1.50
4	A	507[A]	NAD	PA-O1A	6.47	1.73	1.50
4	D	507[A]	NAD	PA-O1A	6.45	1.73	1.50
4	D	508	NAD	PA-O3	-6.45	1.52	1.59
4	D	507[B]	NAD	PA-O1A	6.34	1.72	1.50
4	A	507[B]	NAD	PA-O1A	6.34	1.72	1.50
4	E	507[B]	NAD	PA-O1A	6.33	1.72	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	508[B]	NAD	PA-O1A	6.33	1.72	1.50
4	B	507[B]	NAD	PA-O1A	6.33	1.72	1.50
4	C	507[B]	NAD	PA-O1A	6.32	1.72	1.50
4	C	508	NAD	PN-O3	6.24	1.66	1.59
4	E	508	NAD	PN-O3	6.21	1.66	1.59
4	B	508	NAD	PN-O3	6.21	1.66	1.59
4	A	508	NAD	PN-O3	6.18	1.66	1.59
4	F	507	NAD	PN-O3	6.17	1.66	1.59
4	D	508	NAD	PN-O3	6.14	1.66	1.59
4	F	507	NAD	C2N-N1N	5.70	1.41	1.35
4	E	508	NAD	C2N-N1N	5.66	1.41	1.35
4	D	508	NAD	C2N-N1N	5.65	1.41	1.35
4	C	508	NAD	C2N-N1N	5.65	1.41	1.35
4	A	508	NAD	C2N-N1N	5.61	1.41	1.35
4	B	508	NAD	C2N-N1N	5.58	1.41	1.35
4	C	507[A]	NAD	C7N-N7N	5.56	1.43	1.33
4	A	507[A]	NAD	C7N-N7N	5.54	1.43	1.33
4	F	508[A]	NAD	C7N-N7N	5.51	1.43	1.33
4	D	507[A]	NAD	C7N-N7N	5.51	1.43	1.33
4	E	507[A]	NAD	C7N-N7N	5.50	1.43	1.33
4	B	507[A]	NAD	C7N-N7N	5.50	1.43	1.33
4	D	507[B]	NAD	C3N-C7N	5.47	1.58	1.50
4	F	508[B]	NAD	C3N-C7N	5.44	1.58	1.50
4	C	507[B]	NAD	C3N-C7N	5.44	1.58	1.50
4	E	507[B]	NAD	C3N-C7N	5.43	1.58	1.50
4	B	507[B]	NAD	C3N-C7N	5.43	1.58	1.50
4	F	507	NAD	PA-O1A	5.42	1.69	1.50
4	E	508	NAD	PA-O1A	5.42	1.69	1.50
4	B	508	NAD	PA-O1A	5.40	1.69	1.50
4	A	508	NAD	PA-O1A	5.40	1.69	1.50
4	C	508	NAD	PA-O1A	5.40	1.69	1.50
4	A	507[B]	NAD	C3N-C7N	5.39	1.58	1.50
4	D	508	NAD	PA-O1A	5.38	1.69	1.50
4	D	508	NAD	C4A-N3A	5.10	1.43	1.34
4	F	507	NAD	C4A-N3A	5.09	1.43	1.34
4	E	508	NAD	C4A-N3A	5.06	1.43	1.34
4	A	508	NAD	C4A-N3A	5.06	1.43	1.34
4	B	508	NAD	C4A-N3A	5.03	1.43	1.34
4	C	508	NAD	C4A-N3A	5.02	1.43	1.34
4	A	507[A]	NAD	C3N-C7N	4.82	1.57	1.50
4	D	507[A]	NAD	C3N-C7N	4.79	1.57	1.50
4	F	508[A]	NAD	C3N-C7N	4.78	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	507[B]	NAD	PA-O3	-4.78	1.54	1.59
4	C	507[A]	NAD	C3N-C7N	4.76	1.57	1.50
4	B	507[A]	NAD	C3N-C7N	4.76	1.57	1.50
4	E	507[A]	NAD	C3N-C7N	4.74	1.57	1.50
4	A	507[B]	NAD	PA-O3	-4.73	1.54	1.59
4	C	507[B]	NAD	PA-O3	-4.71	1.54	1.59
4	F	508[B]	NAD	PA-O3	-4.71	1.54	1.59
4	D	507[B]	NAD	PA-O3	-4.69	1.54	1.59
4	B	507[B]	NAD	PA-O3	-4.67	1.54	1.59
4	E	507[B]	NAD	C4A-N3A	4.25	1.42	1.34
4	D	507[B]	NAD	C4A-N3A	4.22	1.42	1.34
4	A	507[B]	NAD	C4A-N3A	4.19	1.42	1.34
4	F	508[B]	NAD	C4A-N3A	4.18	1.42	1.34
4	C	507[B]	NAD	C4A-N3A	4.17	1.42	1.34
4	A	507[B]	NAD	C2N-C3N	-4.17	1.32	1.39
4	B	507[B]	NAD	C2N-C3N	-4.16	1.32	1.39
4	B	507[B]	NAD	C4A-N3A	4.15	1.42	1.34
4	B	507[B]	NAD	C2A-N3A	4.14	1.41	1.33
4	E	507[B]	NAD	C2N-C3N	-4.14	1.32	1.39
4	F	508[B]	NAD	C2N-C3N	-4.14	1.32	1.39
4	C	507[B]	NAD	C2N-C3N	-4.12	1.32	1.39
4	F	508[B]	NAD	C2A-N3A	4.11	1.41	1.33
4	D	507[B]	NAD	C2N-C3N	-4.10	1.32	1.39
4	C	507[B]	NAD	C2A-N3A	4.10	1.41	1.33
4	E	507[B]	NAD	C2A-N3A	4.09	1.41	1.33
4	D	507[B]	NAD	C2A-N3A	4.08	1.41	1.33
4	A	507[B]	NAD	C2A-N3A	4.05	1.41	1.33
4	E	507[A]	NAD	C4A-N3A	3.90	1.41	1.34
4	C	507[A]	NAD	C4A-N3A	3.88	1.41	1.34
4	F	508[A]	NAD	C4A-N3A	3.88	1.41	1.34
4	B	507[A]	NAD	C4A-N3A	3.88	1.41	1.34
4	A	507[A]	NAD	C4A-N3A	3.87	1.41	1.34
3	C	506	AKG	C2-C1	3.87	1.59	1.53
3	D	506	AKG	C2-C1	3.86	1.59	1.53
4	D	507[A]	NAD	C4A-N3A	3.85	1.41	1.34
3	B	506	AKG	C2-C1	3.84	1.59	1.53
3	A	506	AKG	C2-C1	3.84	1.59	1.53
3	F	506	AKG	C2-C1	3.84	1.59	1.53
3	E	506	AKG	C2-C1	3.83	1.59	1.53
4	A	507[A]	NAD	C2A-N3A	3.73	1.40	1.33
4	F	508[A]	NAD	C2A-N3A	3.72	1.40	1.33
4	B	507[A]	NAD	C2A-N3A	3.72	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[A]	NAD	C2A-N3A	3.70	1.40	1.33
4	D	507[A]	NAD	C2A-N3A	3.69	1.40	1.33
4	E	507[A]	NAD	C2A-N3A	3.69	1.40	1.33
4	E	508	NAD	C2N-C3N	-3.55	1.33	1.39
4	D	508	NAD	C2N-C3N	-3.55	1.33	1.39
4	C	508	NAD	C2N-C3N	-3.53	1.33	1.39
4	F	507	NAD	C2N-C3N	-3.53	1.33	1.39
4	A	508	NAD	C2N-C3N	-3.53	1.33	1.39
4	B	508	NAD	C2N-C3N	-3.50	1.33	1.39
2	C	504	PO4	P-O4	3.48	1.64	1.54
2	E	505	PO4	P-O4	3.47	1.64	1.54
2	B	504	PO4	P-O4	3.46	1.64	1.54
4	E	507[A]	NAD	PA-O5B	-3.46	1.45	1.59
4	D	507[A]	NAD	PA-O5B	-3.46	1.45	1.59
2	A	505	PO4	P-O4	3.46	1.64	1.54
2	F	505	PO4	P-O4	3.46	1.64	1.54
4	A	507[A]	NAD	PA-O5B	-3.45	1.45	1.59
4	F	508[A]	NAD	PA-O5B	-3.45	1.45	1.59
2	D	505	PO4	P-O4	3.45	1.64	1.54
4	C	507[A]	NAD	PA-O5B	-3.45	1.45	1.59
4	B	507[A]	NAD	PA-O5B	-3.44	1.45	1.59
4	D	508	NAD	C7N-N7N	3.40	1.39	1.33
4	E	508	NAD	C7N-N7N	3.39	1.39	1.33
4	F	507	NAD	C7N-N7N	3.38	1.39	1.33
4	A	508	NAD	C7N-N7N	3.37	1.39	1.33
4	C	508	NAD	C7N-N7N	3.36	1.39	1.33
4	C	508	NAD	C6N-N1N	3.36	1.43	1.35
4	D	508	NAD	C6N-N1N	3.35	1.43	1.35
4	B	508	NAD	C7N-N7N	3.35	1.39	1.33
4	A	508	NAD	C6N-N1N	3.34	1.42	1.35
4	A	507[A]	NAD	C2N-C3N	-3.34	1.33	1.39
4	F	508[A]	NAD	C2N-C3N	-3.34	1.33	1.39
4	B	508	NAD	C6N-N1N	3.33	1.42	1.35
4	C	507[A]	NAD	C2N-C3N	-3.33	1.33	1.39
4	E	507[A]	NAD	C2N-C3N	-3.33	1.33	1.39
4	B	507[A]	NAD	C2N-C3N	-3.32	1.33	1.39
4	E	508	NAD	C6N-N1N	3.31	1.42	1.35
4	F	507	NAD	C6N-N1N	3.31	1.42	1.35
4	D	507[A]	NAD	C2N-C3N	-3.30	1.33	1.39
4	E	508	NAD	C3N-C7N	3.29	1.55	1.50
4	D	508	NAD	C3N-C7N	3.27	1.55	1.50
4	D	507[B]	NAD	PA-O5B	-3.27	1.46	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	508[B]	NAD	PA-O5B	-3.27	1.46	1.59
4	B	507[B]	NAD	PA-O5B	-3.26	1.46	1.59
4	E	507[B]	NAD	PA-O5B	-3.26	1.46	1.59
4	C	507[B]	NAD	PA-O5B	-3.26	1.46	1.59
4	A	508	NAD	C3N-C7N	3.25	1.55	1.50
4	A	507[B]	NAD	PA-O5B	-3.25	1.46	1.59
4	F	507	NAD	C3N-C7N	3.25	1.55	1.50
4	A	507[B]	NAD	C5N-C4N	3.22	1.44	1.38
4	C	508	NAD	C3N-C7N	3.21	1.55	1.50
4	E	507[B]	NAD	C5N-C4N	3.21	1.44	1.38
4	B	508	NAD	C3N-C7N	3.21	1.55	1.50
4	E	507[A]	NAD	PN-O1N	-3.20	1.39	1.50
4	D	507[A]	NAD	PA-O3	-3.20	1.56	1.59
4	D	507[B]	NAD	C5N-C4N	3.19	1.44	1.38
4	C	507[A]	NAD	PN-O1N	-3.19	1.39	1.50
4	A	507[A]	NAD	PN-O1N	-3.19	1.39	1.50
4	F	508[A]	NAD	PN-O1N	-3.19	1.39	1.50
4	F	508[B]	NAD	C5N-C4N	3.19	1.44	1.38
4	B	507[A]	NAD	PN-O1N	-3.18	1.39	1.50
4	B	507[B]	NAD	C5N-C4N	3.18	1.44	1.38
4	D	507[A]	NAD	PN-O1N	-3.17	1.39	1.50
4	C	507[A]	NAD	PA-O3	-3.17	1.56	1.59
4	C	507[B]	NAD	C5N-C4N	3.17	1.44	1.38
4	B	507[A]	NAD	PA-O3	-3.15	1.56	1.59
4	A	507[A]	NAD	PA-O3	-3.15	1.56	1.59
4	F	508[A]	NAD	PA-O3	-3.14	1.56	1.59
4	E	507[A]	NAD	PA-O3	-3.09	1.56	1.59
4	D	508	NAD	PA-O5B	-3.07	1.47	1.59
4	C	508	NAD	PA-O5B	-3.07	1.47	1.59
4	B	508	NAD	PA-O5B	-3.05	1.47	1.59
4	A	508	NAD	PA-O5B	-3.05	1.47	1.59
4	F	507	NAD	PA-O5B	-3.05	1.47	1.59
4	E	508	NAD	PA-O5B	-3.04	1.47	1.59
4	E	508	NAD	O4B-C1B	2.94	1.48	1.42
4	C	508	NAD	O4B-C1B	2.93	1.48	1.42
4	D	508	NAD	O4B-C1B	2.92	1.48	1.42
4	A	508	NAD	O4B-C1B	2.91	1.48	1.42
4	F	507	NAD	O4B-C1B	2.91	1.48	1.42
4	B	508	NAD	O4B-C1B	2.90	1.48	1.42
4	B	508	NAD	C5N-C4N	2.77	1.43	1.38
4	D	508	NAD	C5N-C4N	2.75	1.43	1.38
4	A	508	NAD	C5N-C4N	2.75	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	508	NAD	C5N-C4N	2.74	1.43	1.38
4	C	508	NAD	C5N-C4N	2.73	1.43	1.38
4	F	507	NAD	C5N-C4N	2.72	1.43	1.38
4	D	507[A]	NAD	C5A-C6A	2.63	1.48	1.41
4	A	507[A]	NAD	C5A-C6A	2.62	1.48	1.41
4	F	508[A]	NAD	C5A-C6A	2.60	1.48	1.41
4	E	507[A]	NAD	C5A-C6A	2.60	1.48	1.41
4	C	507[A]	NAD	C5A-C6A	2.60	1.48	1.41
4	B	507[A]	NAD	C5A-C6A	2.60	1.48	1.41
4	E	507[B]	NAD	C5A-C6A	2.55	1.48	1.41
4	F	508[B]	NAD	C5A-C6A	2.53	1.48	1.41
4	A	507[B]	NAD	C5A-C6A	2.53	1.48	1.41
4	B	507[B]	NAD	C5A-C6A	2.52	1.48	1.41
4	D	507[B]	NAD	C5A-C6A	2.51	1.48	1.41
4	C	507[B]	NAD	C5A-C6A	2.51	1.48	1.41
4	A	507[B]	NAD	C6N-N1N	2.50	1.41	1.35
4	F	508[B]	NAD	C6N-N1N	2.49	1.41	1.35
3	E	506	AKG	C3-C2	2.49	1.53	1.51
4	E	507[A]	NAD	C6N-N1N	2.49	1.41	1.35
4	D	507[B]	NAD	C6N-N1N	2.49	1.41	1.35
4	B	507[B]	NAD	C6N-N1N	2.48	1.41	1.35
4	B	507[A]	NAD	C6N-N1N	2.48	1.41	1.35
4	C	507[A]	NAD	C6N-N1N	2.48	1.41	1.35
4	F	508[A]	NAD	C6N-N1N	2.48	1.41	1.35
4	E	507[B]	NAD	PN-O1N	-2.48	1.42	1.50
4	D	507[B]	NAD	PN-O1N	-2.47	1.42	1.50
4	D	507[A]	NAD	C6N-N1N	2.47	1.41	1.35
4	F	508[B]	NAD	PN-O1N	-2.47	1.42	1.50
3	F	506	AKG	C3-C2	2.47	1.53	1.51
4	C	507[B]	NAD	PN-O1N	-2.47	1.42	1.50
4	A	507[B]	NAD	PN-O1N	-2.46	1.42	1.50
4	A	507[A]	NAD	C6N-N1N	2.46	1.40	1.35
4	E	507[B]	NAD	C6N-N1N	2.46	1.40	1.35
4	C	507[B]	NAD	C6N-N1N	2.45	1.40	1.35
4	B	507[B]	NAD	PN-O1N	-2.44	1.42	1.50
3	C	506	AKG	C3-C2	2.44	1.53	1.51
3	A	506	AKG	C3-C2	2.43	1.53	1.51
3	B	506	AKG	C3-C2	2.39	1.53	1.51
3	D	506	AKG	C3-C2	2.38	1.53	1.51
4	A	507[A]	NAD	O2D-C2D	2.36	1.48	1.43
4	F	508[A]	NAD	O2D-C2D	2.35	1.48	1.43
4	E	507[A]	NAD	O2D-C2D	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[A]	NAD	O2D-C2D	2.35	1.48	1.43
4	D	507[A]	NAD	O2D-C2D	2.33	1.48	1.43
4	B	507[A]	NAD	O2D-C2D	2.32	1.48	1.43
2	F	504	PO4	P-O4	2.29	1.61	1.54
2	E	503	PO4	P-O4	2.29	1.61	1.54
2	B	503	PO4	P-O4	2.28	1.61	1.54
2	F	502	PO4	P-O4	2.28	1.61	1.54
2	A	502	PO4	P-O4	2.28	1.61	1.54
2	E	504	PO4	P-O4	2.28	1.61	1.54
2	C	505	PO4	P-O4	2.27	1.61	1.54
4	F	507	NAD	C3B-C4B	2.27	1.58	1.53
2	A	504	PO4	P-O4	2.27	1.61	1.54
2	D	502	PO4	P-O4	2.27	1.61	1.54
2	D	504	PO4	P-O4	2.27	1.61	1.54
2	C	503	PO4	P-O4	2.27	1.61	1.54
4	D	508	NAD	C3B-C4B	2.27	1.58	1.53
2	C	502	PO4	P-O4	2.27	1.61	1.54
4	E	508	NAD	C3B-C4B	2.27	1.58	1.53
4	A	508	NAD	C3B-C4B	2.27	1.58	1.53
2	B	502	PO4	P-O4	2.26	1.61	1.54
2	B	505	PO4	P-O4	2.26	1.61	1.54
2	A	503	PO4	P-O4	2.26	1.61	1.54
2	D	503	PO4	P-O4	2.26	1.61	1.54
2	F	503	PO4	P-O4	2.26	1.61	1.54
2	E	502	PO4	P-O4	2.25	1.61	1.54
4	C	508	NAD	C3B-C4B	2.25	1.58	1.53
4	B	508	NAD	C3B-C4B	2.24	1.58	1.53
4	A	507[A]	NAD	C6A-N6A	-2.20	1.28	1.34
4	E	507[A]	NAD	C6A-N6A	-2.19	1.28	1.34
4	E	508	NAD	C3D-C4D	-2.19	1.47	1.53
4	D	508	NAD	C3D-C4D	-2.19	1.47	1.53
4	F	507	NAD	C3D-C4D	-2.19	1.47	1.53
4	D	507[A]	NAD	C6A-N6A	-2.18	1.28	1.34
4	F	508[A]	NAD	C6A-N6A	-2.18	1.28	1.34
4	A	508	NAD	C3D-C4D	-2.18	1.47	1.53
4	C	508	NAD	C3D-C4D	-2.18	1.47	1.53
4	B	507[A]	NAD	C6A-N6A	-2.18	1.28	1.34
4	C	507[A]	NAD	C6A-N6A	-2.17	1.28	1.34
4	B	508	NAD	C3D-C4D	-2.17	1.47	1.53
4	D	507[B]	NAD	O4D-C1D	2.14	1.43	1.40
4	A	507[B]	NAD	O7N-C7N	2.12	1.28	1.24
4	E	507[B]	NAD	O7N-C7N	2.11	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[B]	NAD	O7N-C7N	2.11	1.28	1.24
4	F	508[B]	NAD	O7N-C7N	2.11	1.28	1.24
4	A	507[B]	NAD	O4D-C1D	2.09	1.43	1.40
4	B	507[B]	NAD	O7N-C7N	2.09	1.28	1.24
4	B	507[B]	NAD	O4D-C1D	2.09	1.43	1.40
4	E	507[B]	NAD	O4D-C1D	2.08	1.43	1.40
4	F	508[B]	NAD	O4D-C1D	2.08	1.43	1.40
4	D	507[B]	NAD	O7N-C7N	2.07	1.28	1.24
4	C	507[B]	NAD	O4D-C1D	2.06	1.43	1.40
4	B	508	NAD	C2A-N3A	2.05	1.37	1.33
4	F	507	NAD	C2A-N3A	2.04	1.37	1.33
4	E	508	NAD	C2A-N3A	2.03	1.37	1.33
4	C	508	NAD	C2A-N3A	2.03	1.37	1.33
4	A	508	NAD	C2A-N3A	2.01	1.37	1.33

All (337) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	506	AKG	O1-C1-C2	-6.87	113.27	121.81
3	B	506	AKG	O1-C1-C2	-6.87	113.27	121.81
3	F	506	AKG	O1-C1-C2	-6.85	113.29	121.81
3	A	506	AKG	O1-C1-C2	-6.84	113.30	121.81
3	C	506	AKG	O1-C1-C2	-6.84	113.31	121.81
3	E	506	AKG	O1-C1-C2	-6.80	113.35	121.81
4	D	508	NAD	C2A-N1A-C6A	6.53	129.46	118.73
4	E	508	NAD	C2A-N1A-C6A	6.52	129.44	118.73
4	A	508	NAD	C2A-N1A-C6A	6.51	129.43	118.73
4	C	508	NAD	C2A-N1A-C6A	6.51	129.42	118.73
4	B	508	NAD	C2A-N1A-C6A	6.51	129.42	118.73
4	F	507	NAD	C2A-N1A-C6A	6.50	129.40	118.73
4	F	507	NAD	N3A-C2A-N1A	-5.54	120.20	128.58
4	D	508	NAD	N3A-C2A-N1A	-5.53	120.20	128.58
4	C	508	NAD	N3A-C2A-N1A	-5.53	120.21	128.58
4	A	508	NAD	N3A-C2A-N1A	-5.53	120.21	128.58
4	B	508	NAD	N3A-C2A-N1A	-5.53	120.22	128.58
4	E	508	NAD	N3A-C2A-N1A	-5.52	120.22	128.58
4	C	508	NAD	C5N-C6N-N1N	-5.50	112.88	120.38
4	E	508	NAD	C5N-C6N-N1N	-5.49	112.90	120.38
4	A	508	NAD	C5N-C6N-N1N	-5.48	112.90	120.38
4	F	507	NAD	C5N-C6N-N1N	-5.48	112.91	120.38
4	D	508	NAD	C5N-C6N-N1N	-5.48	112.91	120.38
4	B	508	NAD	C5N-C6N-N1N	-5.46	112.93	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	507[B]	NAD	C5N-C4N-C3N	-5.38	115.08	120.36
4	A	507[B]	NAD	C5N-C4N-C3N	-5.37	115.09	120.36
4	A	507[B]	NAD	C5N-C6N-N1N	-5.35	113.09	120.38
4	F	508[B]	NAD	C5N-C6N-N1N	-5.34	113.10	120.38
4	F	508[B]	NAD	C5N-C4N-C3N	-5.34	115.12	120.36
4	C	507[B]	NAD	C5N-C6N-N1N	-5.33	113.11	120.38
4	C	507[B]	NAD	C5N-C4N-C3N	-5.33	115.13	120.36
4	E	507[B]	NAD	C5N-C6N-N1N	-5.32	113.12	120.38
4	B	507[B]	NAD	C5N-C4N-C3N	-5.32	115.13	120.36
4	D	507[B]	NAD	C5N-C6N-N1N	-5.31	113.14	120.38
4	B	507[B]	NAD	C5N-C6N-N1N	-5.30	113.15	120.38
4	E	507[B]	NAD	C5N-C4N-C3N	-5.30	115.15	120.36
4	B	507[A]	NAD	C2A-N1A-C6A	5.25	127.35	118.73
4	A	507[A]	NAD	C5N-C4N-C3N	-5.24	115.22	120.36
4	E	507[A]	NAD	C2A-N1A-C6A	5.24	127.33	118.73
4	C	507[A]	NAD	C2A-N1A-C6A	5.24	127.33	118.73
4	C	507[A]	NAD	C5N-C4N-C3N	-5.23	115.22	120.36
4	F	508[A]	NAD	C2A-N1A-C6A	5.22	127.31	118.73
4	A	507[A]	NAD	C2A-N1A-C6A	5.22	127.31	118.73
4	F	508[A]	NAD	C5N-C4N-C3N	-5.22	115.23	120.36
4	D	507[A]	NAD	C2A-N1A-C6A	5.22	127.30	118.73
4	D	507[A]	NAD	C5N-C4N-C3N	-5.20	115.25	120.36
4	B	507[A]	NAD	C5N-C4N-C3N	-5.18	115.27	120.36
4	E	507[A]	NAD	C5N-C4N-C3N	-5.17	115.28	120.36
4	C	507[A]	NAD	C5N-C6N-N1N	-5.17	113.34	120.38
4	E	507[A]	NAD	C5N-C6N-N1N	-5.16	113.35	120.38
4	A	507[A]	NAD	C5N-C6N-N1N	-5.15	113.35	120.38
4	F	508[A]	NAD	C5N-C6N-N1N	-5.14	113.37	120.38
4	D	507[A]	NAD	C5N-C6N-N1N	-5.11	113.41	120.38
4	B	507[A]	NAD	C5N-C6N-N1N	-5.10	113.42	120.38
4	B	507[B]	NAD	C2A-N1A-C6A	5.08	127.07	118.73
4	E	507[B]	NAD	C2A-N1A-C6A	5.05	127.03	118.73
4	F	508[B]	NAD	C2A-N1A-C6A	5.05	127.03	118.73
4	C	507[B]	NAD	C2A-N1A-C6A	5.05	127.03	118.73
4	A	507[B]	NAD	C2A-N1A-C6A	5.05	127.02	118.73
4	D	507[B]	NAD	C2A-N1A-C6A	5.03	127.00	118.73
3	C	506	AKG	O2-C1-O1	5.00	135.80	123.90
3	B	506	AKG	O2-C1-O1	4.99	135.78	123.90
3	A	506	AKG	O2-C1-O1	4.98	135.75	123.90
3	D	506	AKG	O2-C1-O1	4.98	135.75	123.90
3	F	506	AKG	O2-C1-O1	4.98	135.75	123.90
3	E	506	AKG	O2-C1-O1	4.97	135.74	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507[A]	NAD	N3A-C2A-N1A	-4.92	121.13	128.58
4	C	507[A]	NAD	N3A-C2A-N1A	-4.91	121.15	128.58
4	F	508[A]	NAD	N3A-C2A-N1A	-4.88	121.19	128.58
4	D	507[A]	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
4	E	507[A]	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
4	A	507[A]	NAD	N3A-C2A-N1A	-4.86	121.22	128.58
4	C	507[A]	NAD	C6N-N1N-C2N	4.86	126.01	121.88
4	A	507[A]	NAD	C6N-N1N-C2N	4.85	126.00	121.88
4	D	508	NAD	O4B-C1B-N9A	-4.81	98.86	108.09
4	F	508[A]	NAD	C6N-N1N-C2N	4.80	125.96	121.88
4	E	508	NAD	O4B-C1B-N9A	-4.79	98.88	108.09
4	D	507[A]	NAD	C6N-N1N-C2N	4.79	125.95	121.88
4	C	508	NAD	O4B-C1B-N9A	-4.78	98.91	108.09
4	A	508	NAD	O4B-C1B-N9A	-4.77	98.92	108.09
4	B	508	NAD	O4B-C1B-N9A	-4.77	98.92	108.09
4	E	507[A]	NAD	C6N-N1N-C2N	4.77	125.94	121.88
4	F	507	NAD	O4B-C1B-N9A	-4.77	98.93	108.09
4	B	507[A]	NAD	C6N-N1N-C2N	4.76	125.92	121.88
4	D	507[A]	NAD	C2N-C3N-C4N	4.62	123.63	118.26
4	A	507[A]	NAD	C2N-C3N-C4N	4.62	123.63	118.26
4	C	507[A]	NAD	C2N-C3N-C4N	4.60	123.61	118.26
4	E	508	NAD	C5N-C4N-C3N	-4.60	115.84	120.36
4	F	508[A]	NAD	C2N-C3N-C4N	4.59	123.60	118.26
4	B	507[A]	NAD	C2N-C3N-C4N	4.58	123.58	118.26
4	A	508	NAD	C5N-C4N-C3N	-4.57	115.87	120.36
4	E	507[A]	NAD	C2N-C3N-C4N	4.55	123.56	118.26
4	B	508	NAD	C5N-C4N-C3N	-4.55	115.89	120.36
4	F	507	NAD	C5N-C4N-C3N	-4.54	115.90	120.36
4	D	508	NAD	C5N-C4N-C3N	-4.54	115.90	120.36
4	C	508	NAD	C5N-C4N-C3N	-4.52	115.92	120.36
4	C	507[B]	NAD	C6N-N1N-C2N	4.51	125.71	121.88
4	E	507[B]	NAD	C6N-N1N-C2N	4.49	125.69	121.88
4	F	508[B]	NAD	C6N-N1N-C2N	4.47	125.68	121.88
4	A	507[B]	NAD	C6N-N1N-C2N	4.47	125.68	121.88
4	C	507[B]	NAD	N3A-C2A-N1A	-4.45	121.85	128.58
4	B	507[B]	NAD	N3A-C2A-N1A	-4.45	121.85	128.58
4	F	508[B]	NAD	N3A-C2A-N1A	-4.44	121.86	128.58
4	A	507[B]	NAD	N3A-C2A-N1A	-4.44	121.86	128.58
4	E	507[B]	NAD	N3A-C2A-N1A	-4.43	121.87	128.58
4	D	507[B]	NAD	C6N-N1N-C2N	4.43	125.64	121.88
4	B	507[B]	NAD	C6N-N1N-C2N	4.43	125.64	121.88
4	D	507[B]	NAD	N3A-C2A-N1A	-4.42	121.89	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	508[A]	NAD	O4B-C1B-N9A	-4.31	99.81	108.09
4	D	507[A]	NAD	O4B-C1B-N9A	-4.31	99.82	108.09
4	C	507[A]	NAD	O4B-C1B-N9A	-4.30	99.83	108.09
4	E	507[A]	NAD	O4B-C1B-N9A	-4.30	99.83	108.09
4	A	507[A]	NAD	O4B-C1B-N9A	-4.30	99.84	108.09
4	B	507[A]	NAD	O4B-C1B-N9A	-4.30	99.84	108.09
3	D	506	AKG	O5-C2-C1	-4.23	113.62	119.67
4	C	507[A]	NAD	C3B-C2B-C1B	-4.20	93.51	101.46
4	E	507[A]	NAD	C3B-C2B-C1B	-4.20	93.52	101.46
3	B	506	AKG	O5-C2-C1	-4.20	113.67	119.67
4	B	507[A]	NAD	C3B-C2B-C1B	-4.20	93.52	101.46
4	D	507[A]	NAD	C3B-C2B-C1B	-4.20	93.52	101.46
3	F	506	AKG	O5-C2-C1	-4.20	113.67	119.67
3	A	506	AKG	O5-C2-C1	-4.19	113.68	119.67
4	F	508[A]	NAD	C3B-C2B-C1B	-4.19	93.53	101.46
4	A	507[A]	NAD	C3B-C2B-C1B	-4.18	93.55	101.46
3	C	506	AKG	O5-C2-C1	-4.17	113.72	119.67
3	E	506	AKG	O5-C2-C1	-4.16	113.72	119.67
4	E	508	NAD	C2N-C3N-C4N	4.02	122.94	118.26
4	D	508	NAD	C2N-C3N-C4N	4.01	122.92	118.26
4	F	507	NAD	C2N-C3N-C4N	4.01	122.92	118.26
4	E	508	NAD	C6N-C5N-C4N	4.00	125.22	119.45
4	C	508	NAD	C6N-C5N-C4N	4.00	125.22	119.45
4	A	508	NAD	C6N-C5N-C4N	3.99	125.20	119.45
4	A	508	NAD	C2N-C3N-C4N	3.98	122.89	118.26
4	F	507	NAD	C6N-C5N-C4N	3.97	125.18	119.45
4	B	508	NAD	C6N-C5N-C4N	3.97	125.17	119.45
4	D	508	NAD	C6N-C5N-C4N	3.97	125.16	119.45
4	B	508	NAD	C2N-C3N-C4N	3.96	122.87	118.26
4	C	508	NAD	C2N-C3N-C4N	3.95	122.85	118.26
4	E	507[B]	NAD	C2N-C3N-C4N	3.88	122.77	118.26
4	D	507[B]	NAD	C2N-C3N-C4N	3.88	122.77	118.26
4	F	508[B]	NAD	C2N-C3N-C4N	3.87	122.76	118.26
4	C	507[B]	NAD	C2N-C3N-C4N	3.87	122.76	118.26
4	A	507[B]	NAD	C2N-C3N-C4N	3.87	122.76	118.26
4	B	507[B]	NAD	C2N-C3N-C4N	3.85	122.74	118.26
3	D	506	AKG	O5-C2-C3	3.68	129.06	121.17
3	F	506	AKG	O5-C2-C3	3.66	129.03	121.17
3	A	506	AKG	O5-C2-C3	3.65	129.01	121.17
3	E	506	AKG	O5-C2-C3	3.65	129.01	121.17
4	A	507[A]	NAD	C3N-C7N-N7N	-3.65	113.24	117.74
3	B	506	AKG	O5-C2-C3	3.65	129.00	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	506	AKG	O5-C2-C3	3.64	128.98	121.17
4	F	508[A]	NAD	C3N-C7N-N7N	-3.62	113.28	117.74
4	B	507[A]	NAD	C3N-C7N-N7N	-3.61	113.28	117.74
4	C	507[A]	NAD	C3N-C7N-N7N	-3.61	113.29	117.74
4	D	507[A]	NAD	C3N-C7N-N7N	-3.61	113.29	117.74
4	E	507[A]	NAD	C3N-C7N-N7N	-3.58	113.33	117.74
4	E	507[B]	NAD	O4B-C1B-N9A	-3.57	101.24	108.09
4	C	507[B]	NAD	O4B-C1B-N9A	-3.56	101.25	108.09
4	F	508[B]	NAD	O4B-C1B-N9A	-3.55	101.27	108.09
4	D	507[B]	NAD	O4B-C1B-N9A	-3.55	101.27	108.09
4	A	507[B]	NAD	O4B-C1B-N9A	-3.54	101.28	108.09
4	B	507[B]	NAD	O4B-C1B-N9A	-3.53	101.30	108.09
4	A	507[A]	NAD	C2B-C1B-N9A	3.53	122.08	113.30
4	D	507[A]	NAD	C2B-C1B-N9A	3.53	122.06	113.30
4	F	508[A]	NAD	C2B-C1B-N9A	3.53	122.06	113.30
4	B	507[A]	NAD	C2B-C1B-N9A	3.53	122.06	113.30
4	E	507[A]	NAD	C2B-C1B-N9A	3.52	122.05	113.30
4	C	507[A]	NAD	C2B-C1B-N9A	3.52	122.04	113.30
4	D	507[A]	NAD	C2D-C3D-C4D	3.47	109.32	102.61
4	B	507[A]	NAD	C2D-C3D-C4D	3.47	109.31	102.61
4	F	508[A]	NAD	C2D-C3D-C4D	3.46	109.30	102.61
4	E	507[A]	NAD	C2D-C3D-C4D	3.46	109.29	102.61
4	C	507[A]	NAD	C2D-C3D-C4D	3.45	109.28	102.61
4	A	507[A]	NAD	C2D-C3D-C4D	3.45	109.27	102.61
4	D	507[B]	NAD	C6N-C5N-C4N	3.41	124.36	119.45
4	A	507[B]	NAD	C6N-C5N-C4N	3.41	124.36	119.45
4	F	508[B]	NAD	C6N-C5N-C4N	3.39	124.34	119.45
4	C	507[B]	NAD	C6N-C5N-C4N	3.39	124.33	119.45
4	B	507[B]	NAD	C6N-C5N-C4N	3.37	124.31	119.45
4	E	507[B]	NAD	C6N-C5N-C4N	3.35	124.28	119.45
4	A	507[A]	NAD	C6N-C5N-C4N	3.30	124.20	119.45
4	E	507[A]	NAD	C6N-C5N-C4N	3.30	124.20	119.45
4	C	507[A]	NAD	C6N-C5N-C4N	3.29	124.20	119.45
4	F	508[A]	NAD	C6N-C5N-C4N	3.29	124.19	119.45
4	B	507[A]	NAD	C6N-C5N-C4N	3.27	124.17	119.45
3	C	506	AKG	C4-C3-C2	3.27	119.05	112.91
4	D	507[A]	NAD	C6N-C5N-C4N	3.26	124.15	119.45
3	E	506	AKG	C4-C3-C2	3.26	119.03	112.91
3	F	506	AKG	C4-C3-C2	3.26	119.03	112.91
3	A	506	AKG	C4-C3-C2	3.25	119.01	112.91
3	B	506	AKG	C4-C3-C2	3.24	118.99	112.91
3	D	506	AKG	C4-C3-C2	3.24	118.99	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	508	NAD	C6N-N1N-C2N	3.18	124.58	121.88
4	F	507	NAD	C6N-N1N-C2N	3.16	124.57	121.88
4	B	508	NAD	C6N-N1N-C2N	3.15	124.56	121.88
4	A	508	NAD	C6N-N1N-C2N	3.14	124.55	121.88
4	C	508	NAD	C6N-N1N-C2N	3.13	124.54	121.88
4	D	508	NAD	C6N-N1N-C2N	3.13	124.54	121.88
4	B	508	NAD	C6N-N1N-C1D	-3.10	113.64	119.73
4	C	508	NAD	C6N-N1N-C1D	-3.09	113.65	119.73
4	D	508	NAD	C6N-N1N-C1D	-3.09	113.65	119.73
4	A	508	NAD	C6N-N1N-C1D	-3.09	113.66	119.73
4	E	508	NAD	C6N-N1N-C1D	-3.09	113.66	119.73
4	F	507	NAD	C6N-N1N-C1D	-3.08	113.68	119.73
4	D	507[B]	NAD	C3N-C7N-N7N	-3.03	114.01	117.74
4	B	507[B]	NAD	C3N-C7N-N7N	-3.03	114.01	117.74
4	C	507[B]	NAD	C3N-C7N-N7N	-3.01	114.03	117.74
4	F	508[B]	NAD	C3N-C7N-N7N	-3.00	114.04	117.74
4	A	507[B]	NAD	C3N-C7N-N7N	-3.00	114.05	117.74
4	E	507[B]	NAD	C3N-C7N-N7N	-3.00	114.05	117.74
4	A	507[A]	NAD	O7N-C7N-N7N	2.91	126.82	122.62
4	B	507[A]	NAD	O7N-C7N-N7N	2.89	126.80	122.62
4	D	507[A]	NAD	O7N-C7N-N7N	2.89	126.79	122.62
4	F	508[A]	NAD	O7N-C7N-N7N	2.89	126.79	122.62
4	E	507[A]	NAD	O7N-C7N-N7N	2.88	126.78	122.62
4	C	507[A]	NAD	O7N-C7N-N7N	2.85	126.74	122.62
4	F	507	NAD	C4D-O4D-C1D	-2.67	107.48	109.92
4	C	508	NAD	C4D-O4D-C1D	-2.65	107.49	109.92
4	D	508	NAD	C4D-O4D-C1D	-2.63	107.52	109.92
4	A	508	NAD	C4D-O4D-C1D	-2.63	107.52	109.92
4	B	507[B]	NAD	O2N-PN-O1N	2.62	124.62	112.44
4	B	508	NAD	C4D-O4D-C1D	-2.61	107.53	109.92
4	E	508	NAD	C4D-O4D-C1D	-2.61	107.53	109.92
4	E	507[B]	NAD	O2N-PN-O1N	2.61	124.59	112.44
4	A	507[B]	NAD	O2N-PN-O1N	2.61	124.58	112.44
4	F	508[B]	NAD	O2N-PN-O1N	2.61	124.58	112.44
4	D	507[B]	NAD	O2N-PN-O1N	2.61	124.57	112.44
4	C	507[B]	NAD	O2N-PN-O1N	2.61	124.56	112.44
4	D	508	NAD	C3B-C2B-C1B	-2.60	96.55	101.46
4	C	508	NAD	C3B-C2B-C1B	-2.58	96.58	101.46
4	A	508	NAD	C3B-C2B-C1B	-2.58	96.59	101.46
4	B	508	NAD	C3B-C2B-C1B	-2.57	96.60	101.46
4	F	507	NAD	C3B-C2B-C1B	-2.57	96.60	101.46
4	E	508	NAD	C3B-C2B-C1B	-2.56	96.61	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	507[B]	NAD	C2B-C3B-C4B	2.49	107.42	102.61
4	A	507[B]	NAD	C2B-C3B-C4B	2.48	107.40	102.61
4	E	507[B]	NAD	C2B-C3B-C4B	2.48	107.39	102.61
4	B	507[B]	NAD	C2B-C3B-C4B	2.48	107.39	102.61
4	F	508[B]	NAD	C2B-C3B-C4B	2.48	107.39	102.61
4	C	507[B]	NAD	C2B-C3B-C4B	2.47	107.38	102.61
4	E	508	NAD	N6A-C6A-N1A	2.40	123.72	118.38
4	D	508	NAD	N6A-C6A-N1A	2.39	123.71	118.38
4	B	508	NAD	N6A-C6A-N1A	2.39	123.69	118.38
4	A	508	NAD	N6A-C6A-N1A	2.38	123.68	118.38
4	C	508	NAD	N6A-C6A-N1A	2.37	123.66	118.38
4	D	508	NAD	O2N-PN-O1N	2.37	123.47	112.44
4	F	507	NAD	O2N-PN-O1N	2.37	123.46	112.44
4	A	508	NAD	O2N-PN-O1N	2.37	123.46	112.44
4	C	508	NAD	O2N-PN-O1N	2.37	123.45	112.44
4	E	508	NAD	O2N-PN-O1N	2.36	123.44	112.44
4	B	508	NAD	O2N-PN-O1N	2.36	123.44	112.44
4	F	507	NAD	N6A-C6A-N1A	2.36	123.62	118.38
4	E	507[A]	NAD	C1B-N9A-C8A	2.30	132.20	127.09
4	B	507[A]	NAD	C1B-N9A-C8A	2.30	132.20	127.09
4	F	508[A]	NAD	C1B-N9A-C8A	2.30	132.20	127.09
4	C	507[A]	NAD	C1B-N9A-C8A	2.29	132.19	127.09
4	A	507[A]	NAD	C1B-N9A-C8A	2.29	132.19	127.09
4	B	507[B]	NAD	C2D-C3D-C4D	2.29	107.04	102.61
4	A	507[B]	NAD	C2D-C3D-C4D	2.29	107.03	102.61
4	D	507[A]	NAD	C1B-N9A-C8A	2.29	132.17	127.09
4	D	507[A]	NAD	O5B-C5B-C4B	2.28	116.76	108.99
4	C	507[A]	NAD	C4B-O4B-C1B	-2.28	104.43	109.47
4	E	507[B]	NAD	C2D-C3D-C4D	2.28	107.01	102.61
4	F	508[B]	NAD	C2D-C3D-C4D	2.28	107.00	102.61
4	E	507[A]	NAD	O5B-C5B-C4B	2.27	116.74	108.99
4	D	507[B]	NAD	C2D-C3D-C4D	2.27	107.00	102.61
4	B	507[A]	NAD	O5B-C5B-C4B	2.27	116.73	108.99
4	F	508[A]	NAD	C4B-O4B-C1B	-2.27	104.46	109.47
4	F	508[A]	NAD	O5B-C5B-C4B	2.27	116.71	108.99
4	D	507[A]	NAD	C4B-O4B-C1B	-2.27	104.46	109.47
4	C	507[B]	NAD	C2D-C3D-C4D	2.27	106.99	102.61
4	B	507[A]	NAD	C4B-O4B-C1B	-2.26	104.47	109.47
4	A	507[A]	NAD	O5B-C5B-C4B	2.26	116.70	108.99
4	E	507[A]	NAD	C4B-O4B-C1B	-2.26	104.48	109.47
4	C	507[A]	NAD	O5B-C5B-C4B	2.26	116.68	108.99
4	A	507[A]	NAD	C4B-O4B-C1B	-2.25	104.50	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	508	NAD	O7N-C7N-C3N	-2.21	116.89	119.60
4	B	508	NAD	O7N-C7N-C3N	-2.19	116.92	119.60
4	A	507[A]	NAD	O4B-C4B-C5B	2.19	116.35	109.33
4	A	508	NAD	O7N-C7N-C3N	-2.18	116.93	119.60
4	C	507[A]	NAD	O4B-C4B-C5B	2.18	116.33	109.33
4	F	508[A]	NAD	O4B-C4B-C5B	2.18	116.32	109.33
4	D	508	NAD	O7N-C7N-C3N	-2.18	116.93	119.60
4	B	507[A]	NAD	O4B-C4B-C5B	2.18	116.31	109.33
4	D	507[A]	NAD	O4B-C4B-C5B	2.18	116.31	109.33
4	E	507[A]	NAD	O4B-C4B-C5B	2.18	116.30	109.33
4	F	507	NAD	O7N-C7N-C3N	-2.17	116.95	119.60
4	E	508	NAD	O7N-C7N-C3N	-2.16	116.95	119.60
4	A	507[B]	NAD	O2B-C2B-C3B	2.14	118.69	111.82
4	D	508	NAD	O7N-C7N-N7N	2.14	125.70	122.62
4	C	507[B]	NAD	O2B-C2B-C3B	2.13	118.65	111.82
4	D	507[B]	NAD	O7N-C7N-N7N	2.13	125.69	122.62
4	C	508	NAD	O7N-C7N-N7N	2.13	125.69	122.62
4	E	508	NAD	O7N-C7N-N7N	2.13	125.69	122.62
4	F	508[B]	NAD	O2B-C2B-C3B	2.13	118.63	111.82
4	F	507	NAD	O7N-C7N-N7N	2.12	125.69	122.62
4	D	507[B]	NAD	O2B-C2B-C3B	2.12	118.62	111.82
4	E	507[B]	NAD	C3B-C2B-C1B	-2.12	97.45	101.46
4	E	507[B]	NAD	O2B-C2B-C3B	2.12	118.61	111.82
4	A	508	NAD	O7N-C7N-N7N	2.12	125.68	122.62
4	B	507[B]	NAD	O2B-C2B-C3B	2.11	118.59	111.82
4	B	507[B]	NAD	O7N-C7N-N7N	2.11	125.67	122.62
4	B	507[B]	NAD	C3B-C2B-C1B	-2.11	97.48	101.46
4	B	508	NAD	O7N-C7N-N7N	2.10	125.66	122.62
4	A	507[B]	NAD	C3B-C2B-C1B	-2.10	97.49	101.46
4	F	508[B]	NAD	C3B-C2B-C1B	-2.10	97.49	101.46
4	C	507[B]	NAD	C3B-C2B-C1B	-2.10	97.50	101.46
4	D	507[B]	NAD	C3B-C2B-C1B	-2.09	97.51	101.46
4	F	508[B]	NAD	O7N-C7N-N7N	2.09	125.64	122.62
4	A	507[A]	NAD	O2N-PN-O1N	2.08	122.12	112.44
4	E	507[A]	NAD	O2N-PN-O1N	2.08	122.12	112.44
4	C	507[B]	NAD	O7N-C7N-N7N	2.08	125.62	122.62
4	C	507[A]	NAD	O2N-PN-O1N	2.08	122.10	112.44
4	E	507[B]	NAD	O7N-C7N-N7N	2.07	125.61	122.62
4	F	508[A]	NAD	O2N-PN-O1N	2.07	122.09	112.44
4	B	507[A]	NAD	O2N-PN-O1N	2.07	122.09	112.44
4	D	507[A]	NAD	O2N-PN-O1N	2.07	122.06	112.44
4	A	507[B]	NAD	O7N-C7N-N7N	2.07	125.60	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	507[B]	NAD	PN-O5D-C5D	-2.07	109.52	121.35
4	B	508	NAD	O2A-PA-O1A	2.06	122.05	112.44
4	B	507[B]	NAD	PN-O5D-C5D	-2.06	109.52	121.35
4	E	508	NAD	O2A-PA-O1A	2.06	122.05	112.44
4	C	507[B]	NAD	PN-O5D-C5D	-2.06	109.53	121.35
4	F	508[B]	NAD	PN-O5D-C5D	-2.06	109.53	121.35
4	A	507[B]	NAD	PN-O5D-C5D	-2.06	109.54	121.35
4	E	507[B]	NAD	PN-O5D-C5D	-2.06	109.56	121.35
4	F	507	NAD	O2A-PA-O1A	2.06	122.01	112.44
4	A	508	NAD	O2A-PA-O1A	2.06	122.01	112.44
4	D	508	NAD	O2A-PA-O1A	2.06	122.01	112.44
4	C	508	NAD	O2A-PA-O1A	2.05	121.99	112.44
4	E	507[B]	NAD	O4B-C1B-C2B	2.05	111.00	106.62
4	A	507[B]	NAD	O4B-C1B-C2B	2.04	110.99	106.62
4	C	507[B]	NAD	O4B-C1B-C2B	2.03	110.97	106.62
4	B	507[B]	NAD	O4B-C1B-C2B	2.03	110.96	106.62
4	F	508[B]	NAD	O4B-C1B-C2B	2.03	110.96	106.62
4	D	507[B]	NAD	O4B-C1B-C2B	2.01	110.92	106.62
4	B	507[B]	NAD	N6A-C6A-N1A	2.01	122.84	118.38

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	AKG	C1-C2-C3-C4
3	B	506	AKG	C1-C2-C3-C4
3	C	506	AKG	C1-C2-C3-C4
3	D	506	AKG	C1-C2-C3-C4
3	E	506	AKG	C1-C2-C3-C4
3	F	506	AKG	C1-C2-C3-C4
4	A	507[A]	NAD	O4B-C4B-C5B-O5B
4	A	507[A]	NAD	C3B-C4B-C5B-O5B
4	A	507[A]	NAD	O4D-C4D-C5D-O5D
4	A	507[A]	NAD	C3D-C4D-C5D-O5D
4	A	507[B]	NAD	O4D-C4D-C5D-O5D
4	A	507[B]	NAD	C3D-C4D-C5D-O5D
4	A	508	NAD	O4B-C4B-C5B-O5B
4	A	508	NAD	C3B-C4B-C5B-O5B
4	A	508	NAD	C5D-O5D-PN-O1N
4	A	508	NAD	O4D-C4D-C5D-O5D
4	A	508	NAD	C3D-C4D-C5D-O5D
4	B	507[A]	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	B	507[A]	NAD	C3B-C4B-C5B-O5B
4	B	507[A]	NAD	O4D-C4D-C5D-O5D
4	B	507[A]	NAD	C3D-C4D-C5D-O5D
4	B	507[B]	NAD	O4D-C4D-C5D-O5D
4	B	507[B]	NAD	C3D-C4D-C5D-O5D
4	B	508	NAD	O4B-C4B-C5B-O5B
4	B	508	NAD	C3B-C4B-C5B-O5B
4	B	508	NAD	C5D-O5D-PN-O1N
4	B	508	NAD	O4D-C4D-C5D-O5D
4	B	508	NAD	C3D-C4D-C5D-O5D
4	C	507[A]	NAD	O4B-C4B-C5B-O5B
4	C	507[A]	NAD	C3B-C4B-C5B-O5B
4	C	507[A]	NAD	O4D-C4D-C5D-O5D
4	C	507[A]	NAD	C3D-C4D-C5D-O5D
4	C	507[B]	NAD	O4D-C4D-C5D-O5D
4	C	507[B]	NAD	C3D-C4D-C5D-O5D
4	C	508	NAD	O4B-C4B-C5B-O5B
4	C	508	NAD	C3B-C4B-C5B-O5B
4	C	508	NAD	C5D-O5D-PN-O1N
4	C	508	NAD	O4D-C4D-C5D-O5D
4	C	508	NAD	C3D-C4D-C5D-O5D
4	D	507[A]	NAD	O4B-C4B-C5B-O5B
4	D	507[A]	NAD	C3B-C4B-C5B-O5B
4	D	507[A]	NAD	O4D-C4D-C5D-O5D
4	D	507[A]	NAD	C3D-C4D-C5D-O5D
4	D	507[B]	NAD	O4D-C4D-C5D-O5D
4	D	507[B]	NAD	C3D-C4D-C5D-O5D
4	D	508	NAD	O4B-C4B-C5B-O5B
4	D	508	NAD	C3B-C4B-C5B-O5B
4	D	508	NAD	C5D-O5D-PN-O1N
4	D	508	NAD	O4D-C4D-C5D-O5D
4	D	508	NAD	C3D-C4D-C5D-O5D
4	E	507[A]	NAD	O4B-C4B-C5B-O5B
4	E	507[A]	NAD	C3B-C4B-C5B-O5B
4	E	507[A]	NAD	O4D-C4D-C5D-O5D
4	E	507[A]	NAD	C3D-C4D-C5D-O5D
4	E	507[B]	NAD	O4D-C4D-C5D-O5D
4	E	507[B]	NAD	C3D-C4D-C5D-O5D
4	E	508	NAD	O4B-C4B-C5B-O5B
4	E	508	NAD	C3B-C4B-C5B-O5B
4	E	508	NAD	C5D-O5D-PN-O1N
4	E	508	NAD	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
4	E	508	NAD	C3D-C4D-C5D-O5D
4	F	507	NAD	O4B-C4B-C5B-O5B
4	F	507	NAD	C3B-C4B-C5B-O5B
4	F	507	NAD	C5D-O5D-PN-O1N
4	F	507	NAD	O4D-C4D-C5D-O5D
4	F	507	NAD	C3D-C4D-C5D-O5D
4	F	508[A]	NAD	O4B-C4B-C5B-O5B
4	F	508[A]	NAD	C3B-C4B-C5B-O5B
4	F	508[A]	NAD	O4D-C4D-C5D-O5D
4	F	508[A]	NAD	C3D-C4D-C5D-O5D
4	F	508[B]	NAD	O4D-C4D-C5D-O5D
4	F	508[B]	NAD	C3D-C4D-C5D-O5D
4	A	507[B]	NAD	C3B-C4B-C5B-O5B
4	B	507[B]	NAD	C3B-C4B-C5B-O5B
4	C	507[B]	NAD	C3B-C4B-C5B-O5B
4	D	507[B]	NAD	C3B-C4B-C5B-O5B
4	E	507[B]	NAD	C3B-C4B-C5B-O5B
4	F	508[B]	NAD	C3B-C4B-C5B-O5B
4	A	507[B]	NAD	O4B-C4B-C5B-O5B
4	B	507[B]	NAD	O4B-C4B-C5B-O5B
4	C	507[B]	NAD	O4B-C4B-C5B-O5B
4	D	507[B]	NAD	O4B-C4B-C5B-O5B
4	E	507[B]	NAD	O4B-C4B-C5B-O5B
4	F	508[B]	NAD	O4B-C4B-C5B-O5B
4	B	507[A]	NAD	PN-O3-PA-O1A
4	D	507[A]	NAD	PN-O3-PA-O1A
4	E	507[A]	NAD	PN-O3-PA-O1A
4	F	508[A]	NAD	PN-O3-PA-O1A
4	A	507[A]	NAD	C4D-C5D-O5D-PN
4	B	507[A]	NAD	C4D-C5D-O5D-PN
4	C	507[A]	NAD	C4D-C5D-O5D-PN
4	D	507[A]	NAD	C4D-C5D-O5D-PN
4	E	507[A]	NAD	C4D-C5D-O5D-PN
4	F	508[A]	NAD	C4D-C5D-O5D-PN
4	A	507[A]	NAD	PN-O3-PA-O5B
4	A	507[B]	NAD	PN-O3-PA-O5B
4	B	507[A]	NAD	PN-O3-PA-O5B
4	B	507[B]	NAD	PN-O3-PA-O5B
4	C	507[A]	NAD	PN-O3-PA-O5B
4	C	507[B]	NAD	PN-O3-PA-O5B
4	D	507[A]	NAD	PN-O3-PA-O5B
4	D	507[B]	NAD	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
4	E	507[A]	NAD	PN-O3-PA-O5B
4	E	507[B]	NAD	PN-O3-PA-O5B
4	F	508[A]	NAD	PN-O3-PA-O5B
4	F	508[B]	NAD	PN-O3-PA-O5B
4	A	507[B]	NAD	C2B-C1B-N9A-C8A
4	B	507[B]	NAD	C2B-C1B-N9A-C8A
4	C	507[B]	NAD	C2B-C1B-N9A-C8A
4	D	507[B]	NAD	C2B-C1B-N9A-C8A
4	E	507[B]	NAD	C2B-C1B-N9A-C8A
4	F	508[B]	NAD	C2B-C1B-N9A-C8A
4	A	507[A]	NAD	PN-O3-PA-O1A
4	A	507[A]	NAD	PA-O3-PN-O1N
4	A	507[B]	NAD	PA-O3-PN-O1N
4	A	508	NAD	PA-O3-PN-O1N
4	B	507[A]	NAD	PA-O3-PN-O1N
4	B	507[B]	NAD	PA-O3-PN-O1N
4	B	508	NAD	PA-O3-PN-O1N
4	C	507[A]	NAD	PN-O3-PA-O1A
4	C	507[A]	NAD	PA-O3-PN-O1N
4	C	507[B]	NAD	PA-O3-PN-O1N
4	C	508	NAD	PA-O3-PN-O1N
4	D	507[A]	NAD	PA-O3-PN-O1N
4	D	507[B]	NAD	PA-O3-PN-O1N
4	D	508	NAD	PA-O3-PN-O1N
4	E	507[A]	NAD	PA-O3-PN-O1N
4	E	507[B]	NAD	PA-O3-PN-O1N
4	E	508	NAD	PA-O3-PN-O1N
4	F	507	NAD	PA-O3-PN-O1N
4	F	508[A]	NAD	PA-O3-PN-O1N
4	F	508[B]	NAD	PA-O3-PN-O1N
3	A	506	AKG	O5-C2-C3-C4
3	B	506	AKG	O5-C2-C3-C4
3	C	506	AKG	O5-C2-C3-C4
3	D	506	AKG	O5-C2-C3-C4
3	E	506	AKG	O5-C2-C3-C4
3	F	506	AKG	O5-C2-C3-C4
4	A	508	NAD	C5B-O5B-PA-O1A
4	A	508	NAD	C5D-O5D-PN-O3
4	A	508	NAD	C5D-O5D-PN-O2N
4	B	508	NAD	C5B-O5B-PA-O1A
4	B	508	NAD	C5D-O5D-PN-O3
4	B	508	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
4	C	508	NAD	C5B-O5B-PA-O1A
4	C	508	NAD	C5D-O5D-PN-O3
4	C	508	NAD	C5D-O5D-PN-O2N
4	D	508	NAD	C5B-O5B-PA-O1A
4	D	508	NAD	C5D-O5D-PN-O3
4	D	508	NAD	C5D-O5D-PN-O2N
4	E	508	NAD	C5B-O5B-PA-O1A
4	E	508	NAD	C5D-O5D-PN-O3
4	E	508	NAD	C5D-O5D-PN-O2N
4	F	507	NAD	C5B-O5B-PA-O1A
4	F	507	NAD	C5D-O5D-PN-O3
4	F	507	NAD	C5D-O5D-PN-O2N
4	A	508	NAD	C4B-C5B-O5B-PA
4	B	508	NAD	C4B-C5B-O5B-PA
4	C	508	NAD	C4B-C5B-O5B-PA
4	D	508	NAD	C4B-C5B-O5B-PA
4	E	508	NAD	C4B-C5B-O5B-PA
4	F	507	NAD	C4B-C5B-O5B-PA
3	A	506	AKG	C3-C4-C5-O4
3	B	506	AKG	C3-C4-C5-O4
3	C	506	AKG	C3-C4-C5-O4
3	D	506	AKG	C3-C4-C5-O4
3	E	506	AKG	C3-C4-C5-O4
3	F	506	AKG	C3-C4-C5-O4
3	B	506	AKG	C3-C4-C5-O3
3	C	506	AKG	C3-C4-C5-O3
4	A	507[B]	NAD	O4B-C1B-N9A-C8A
4	B	507[B]	NAD	O4B-C1B-N9A-C8A
4	C	507[B]	NAD	O4B-C1B-N9A-C8A
4	D	507[B]	NAD	O4B-C1B-N9A-C8A
4	E	507[B]	NAD	O4B-C1B-N9A-C8A
4	F	508[B]	NAD	O4B-C1B-N9A-C8A
3	A	506	AKG	C3-C4-C5-O3
3	D	506	AKG	C3-C4-C5-O3
3	E	506	AKG	C3-C4-C5-O3
3	F	506	AKG	C3-C4-C5-O3
4	A	507[A]	NAD	PA-O3-PN-O2N
4	A	507[B]	NAD	PN-O3-PA-O2A
4	B	507[A]	NAD	PA-O3-PN-O2N
4	B	507[B]	NAD	PN-O3-PA-O2A
4	C	507[A]	NAD	PA-O3-PN-O2N
4	C	507[B]	NAD	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	D	507[A]	NAD	PA-O3-PN-O2N
4	D	507[B]	NAD	PN-O3-PA-O2A
4	E	507[A]	NAD	PA-O3-PN-O2N
4	E	507[B]	NAD	PN-O3-PA-O2A
4	F	508[A]	NAD	PA-O3-PN-O2N
4	F	508[B]	NAD	PN-O3-PA-O2A
4	A	507[B]	NAD	PA-O3-PN-O2N
4	A	508	NAD	PA-O3-PN-O2N
4	B	507[B]	NAD	PA-O3-PN-O2N
4	B	508	NAD	PA-O3-PN-O2N
4	C	507[B]	NAD	PA-O3-PN-O2N
4	C	508	NAD	PA-O3-PN-O2N
4	D	507[B]	NAD	PA-O3-PN-O2N
4	D	508	NAD	PA-O3-PN-O2N
4	E	507[B]	NAD	PA-O3-PN-O2N
4	E	508	NAD	PA-O3-PN-O2N
4	F	507	NAD	PA-O3-PN-O2N
4	F	508[B]	NAD	PA-O3-PN-O2N

There are no ring outliers.

48 monomers are involved in 262 short contacts:

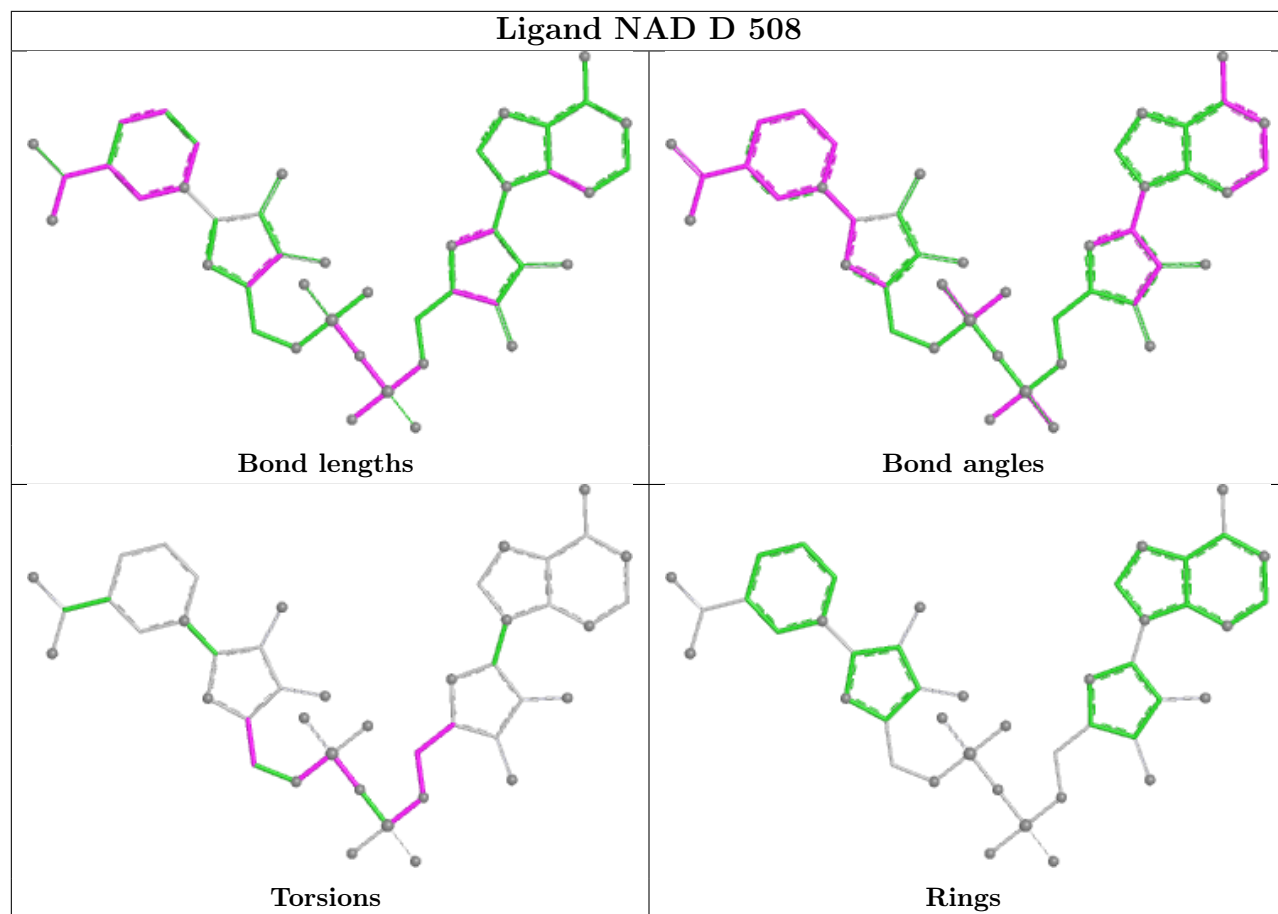
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	503	PO4	1	0
2	B	505	PO4	2	0
2	D	503	PO4	2	0
4	D	508	NAD	12	0
2	A	502	PO4	2	0
2	C	503	PO4	2	0
3	C	506	AKG	7	0
4	C	508	NAD	13	0
4	E	507[A]	NAD	12	0
4	B	508	NAD	12	0
3	B	506	AKG	7	0
4	E	507[B]	NAD	7	0
2	B	504	PO4	1	0
4	C	507[A]	NAD	19	0
2	A	504	PO4	2	0
2	E	502	PO4	1	0
2	E	505	PO4	1	0
4	C	507[B]	NAD	7	0
4	F	508[A]	NAD	14	0

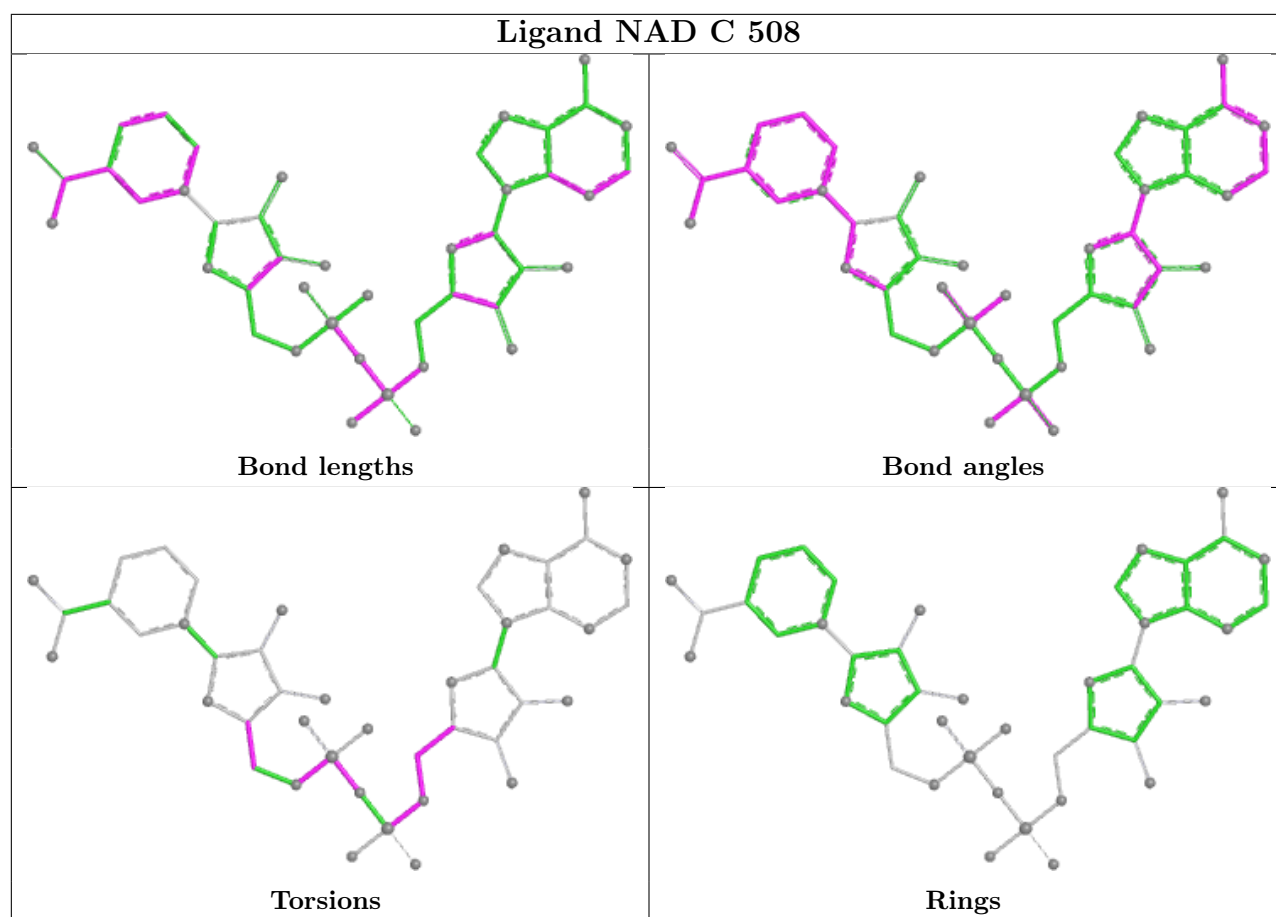
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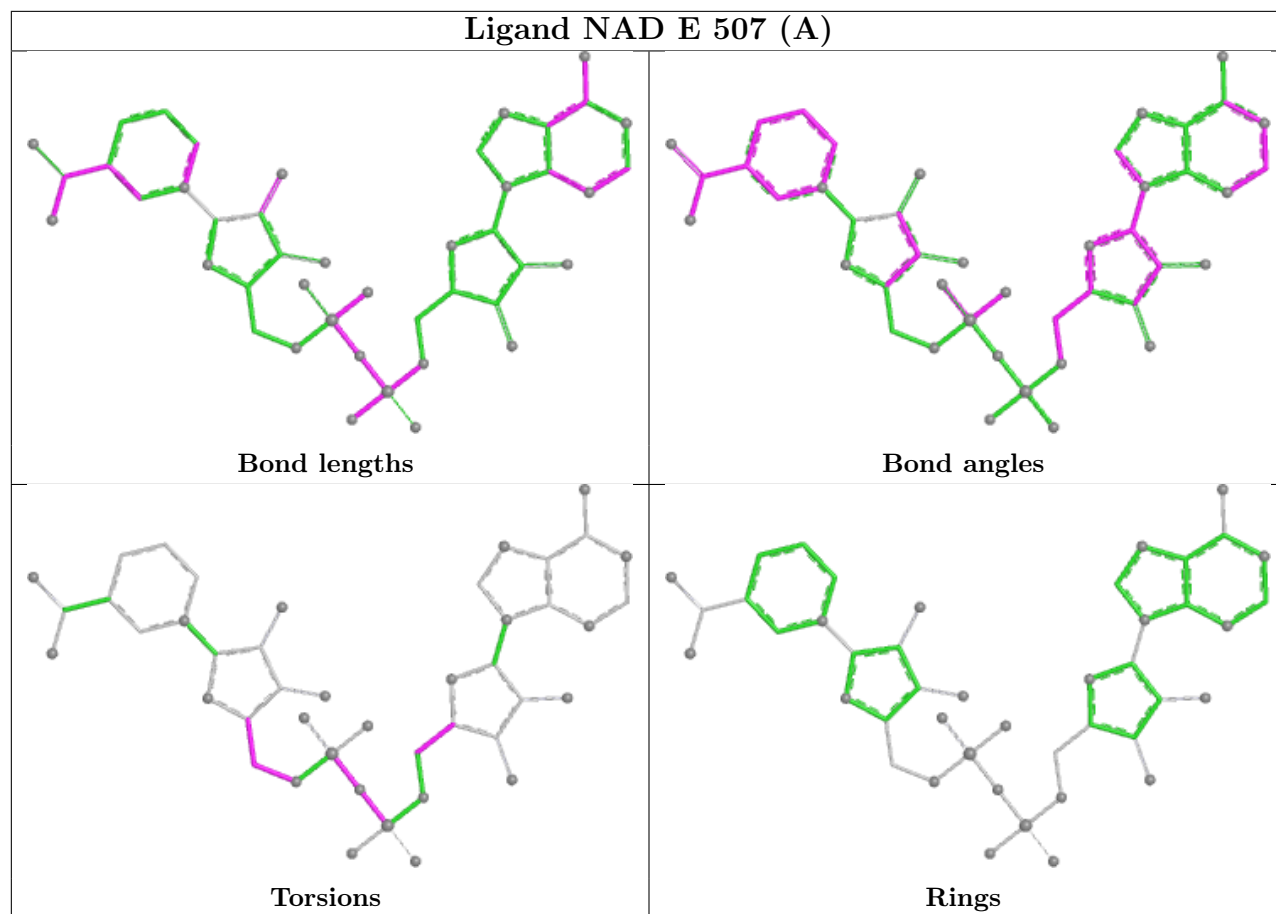
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	508[B]	NAD	7	0
3	D	506	AKG	7	0
2	C	502	PO4	1	0
2	B	502	PO4	1	0
2	A	503	PO4	1	0
4	A	508	NAD	11	0
2	C	504	PO4	1	0
2	D	505	PO4	1	0
4	F	507	NAD	13	0
2	D	504	PO4	2	0
2	F	505	PO4	1	0
2	C	505	PO4	2	0
2	F	504	PO4	2	0
2	E	504	PO4	2	0
4	E	508	NAD	12	0
3	A	506	AKG	6	0
3	F	506	AKG	7	0
2	B	503	PO4	2	0
2	E	503	PO4	2	0
4	A	507[A]	NAD	16	0
2	D	502	PO4	1	0
2	F	502	PO4	2	0
4	D	507[A]	NAD	16	0
3	E	506	AKG	6	0
4	A	507[B]	NAD	6	0
4	D	507[B]	NAD	7	0
2	A	505	PO4	1	0
4	B	507[A]	NAD	17	0
4	B	507[B]	NAD	7	0

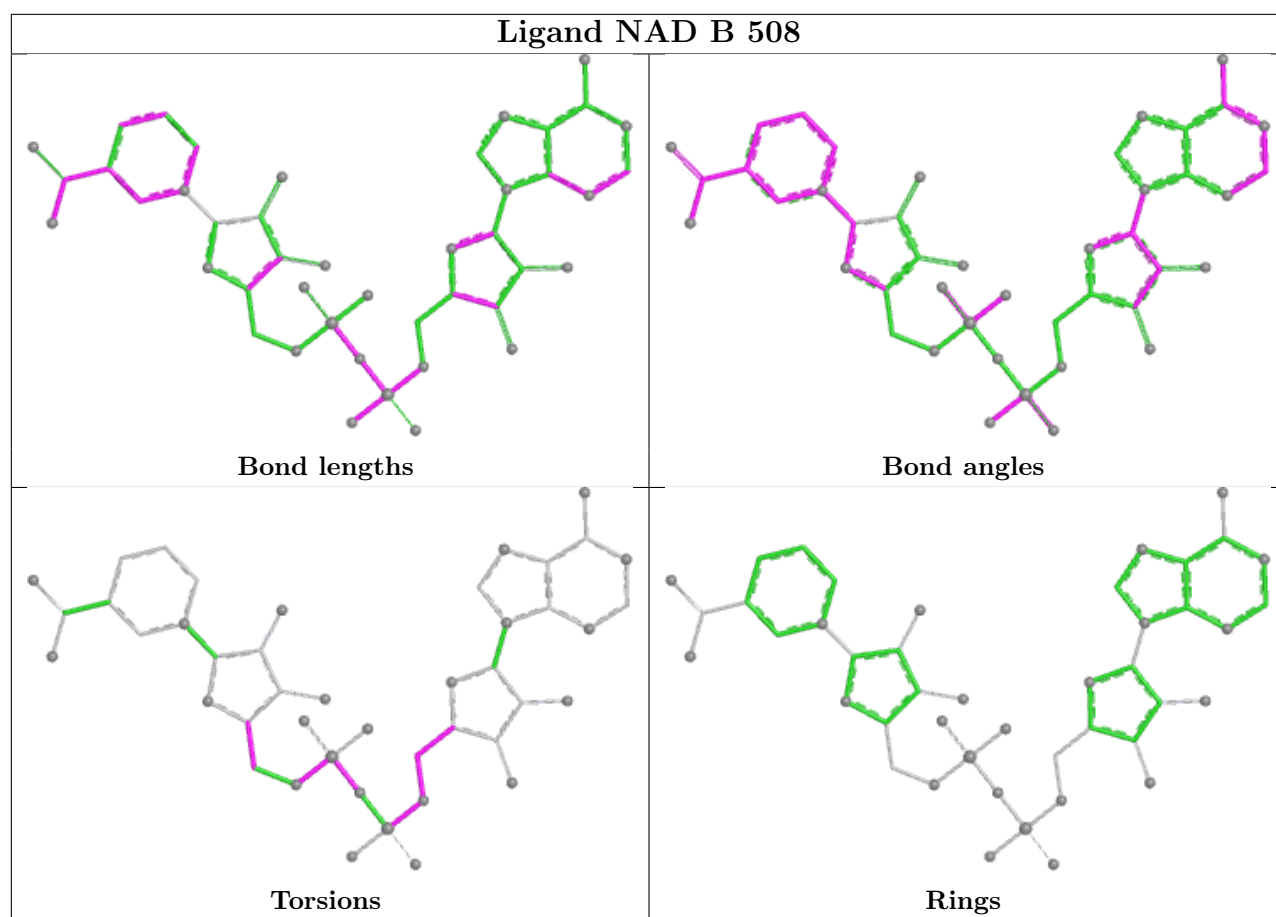
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



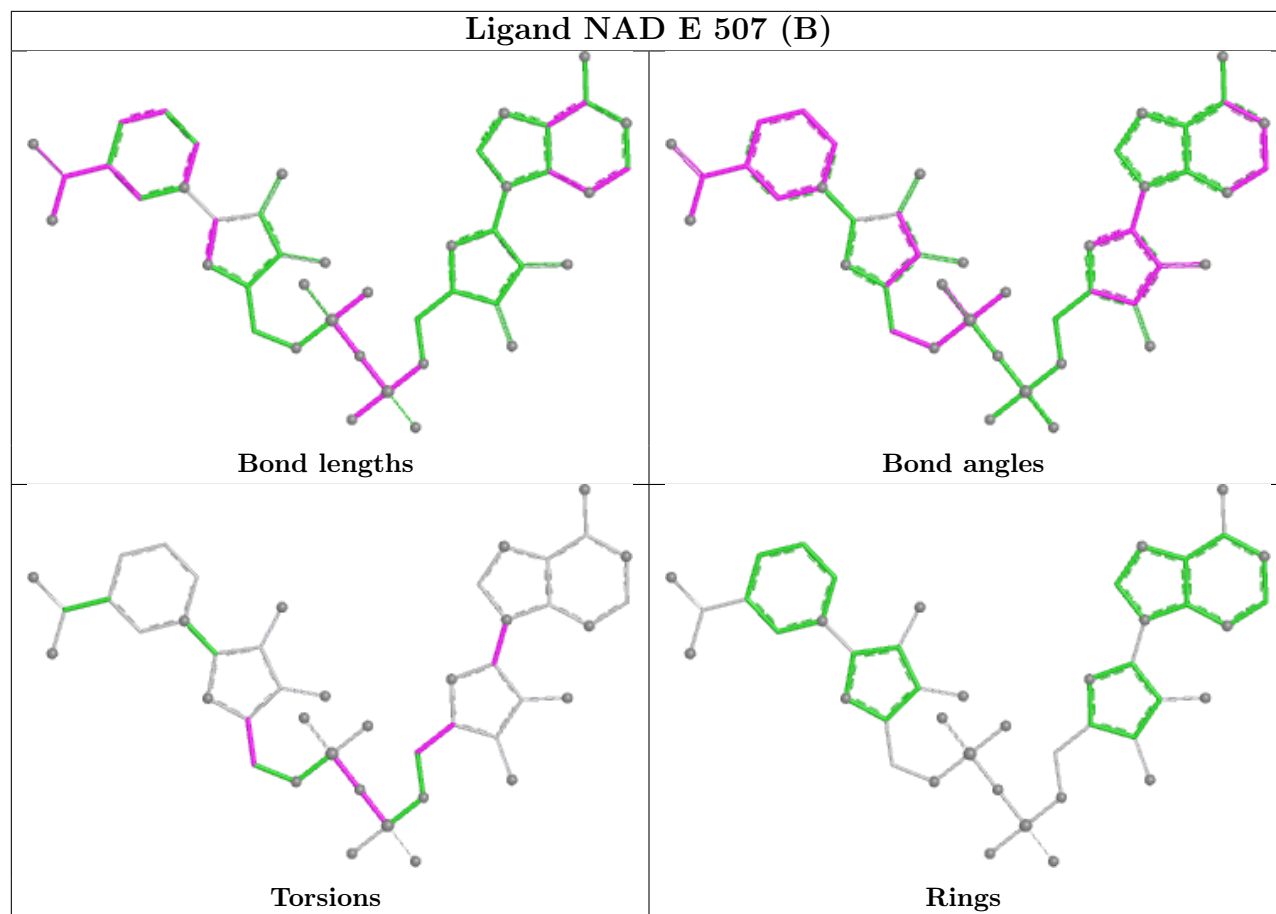


Ligand NAD E 507 (A)

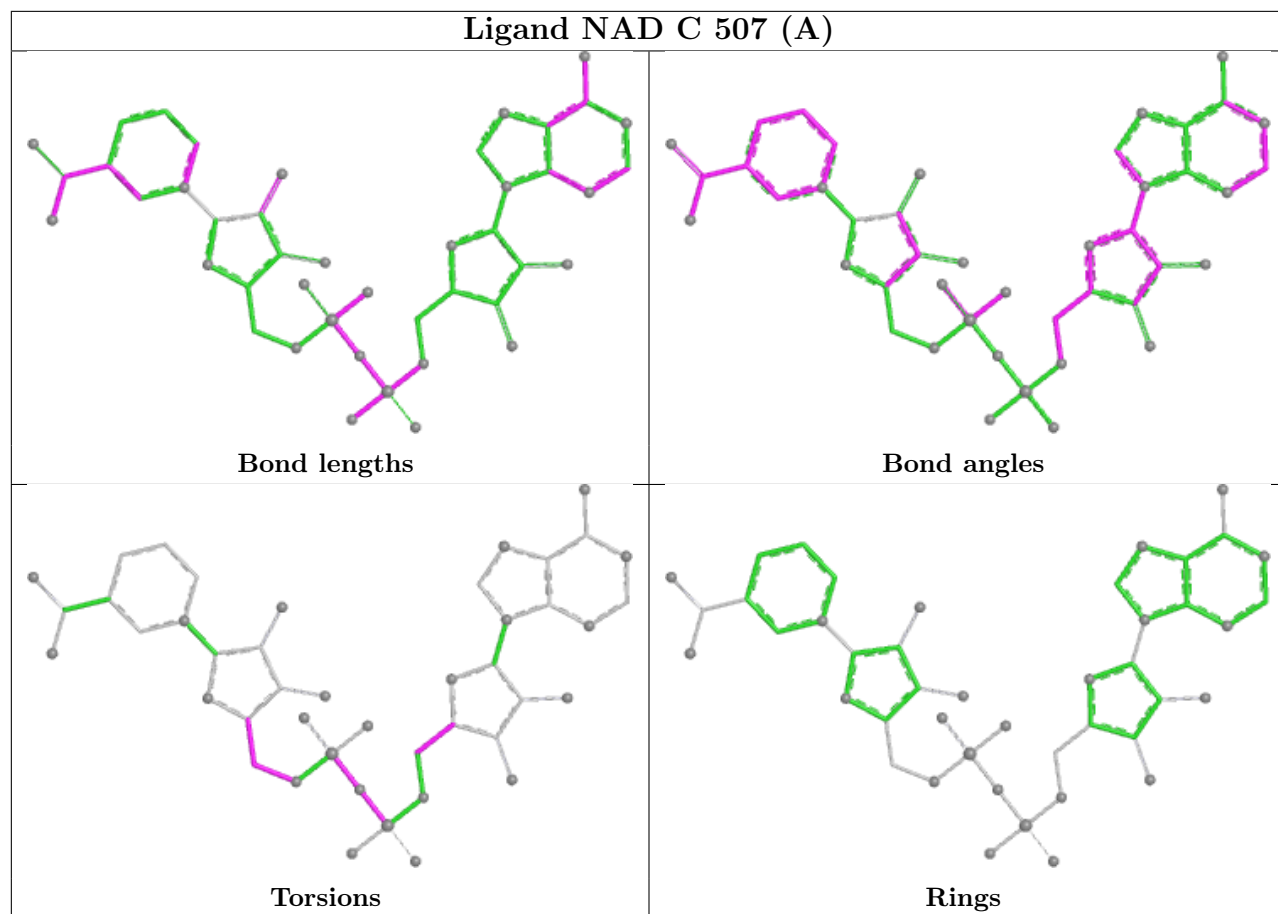




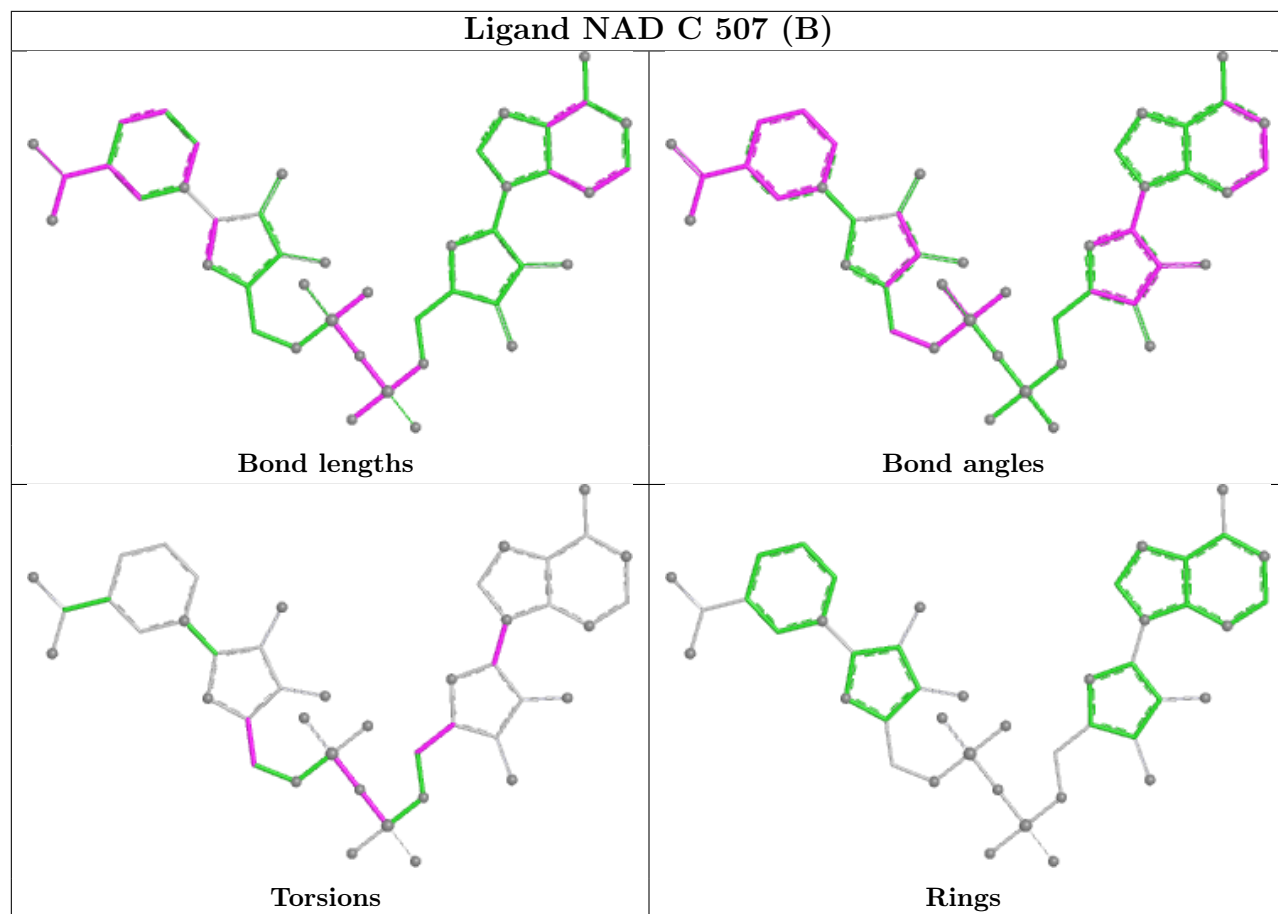
Ligand NAD E 507 (B)



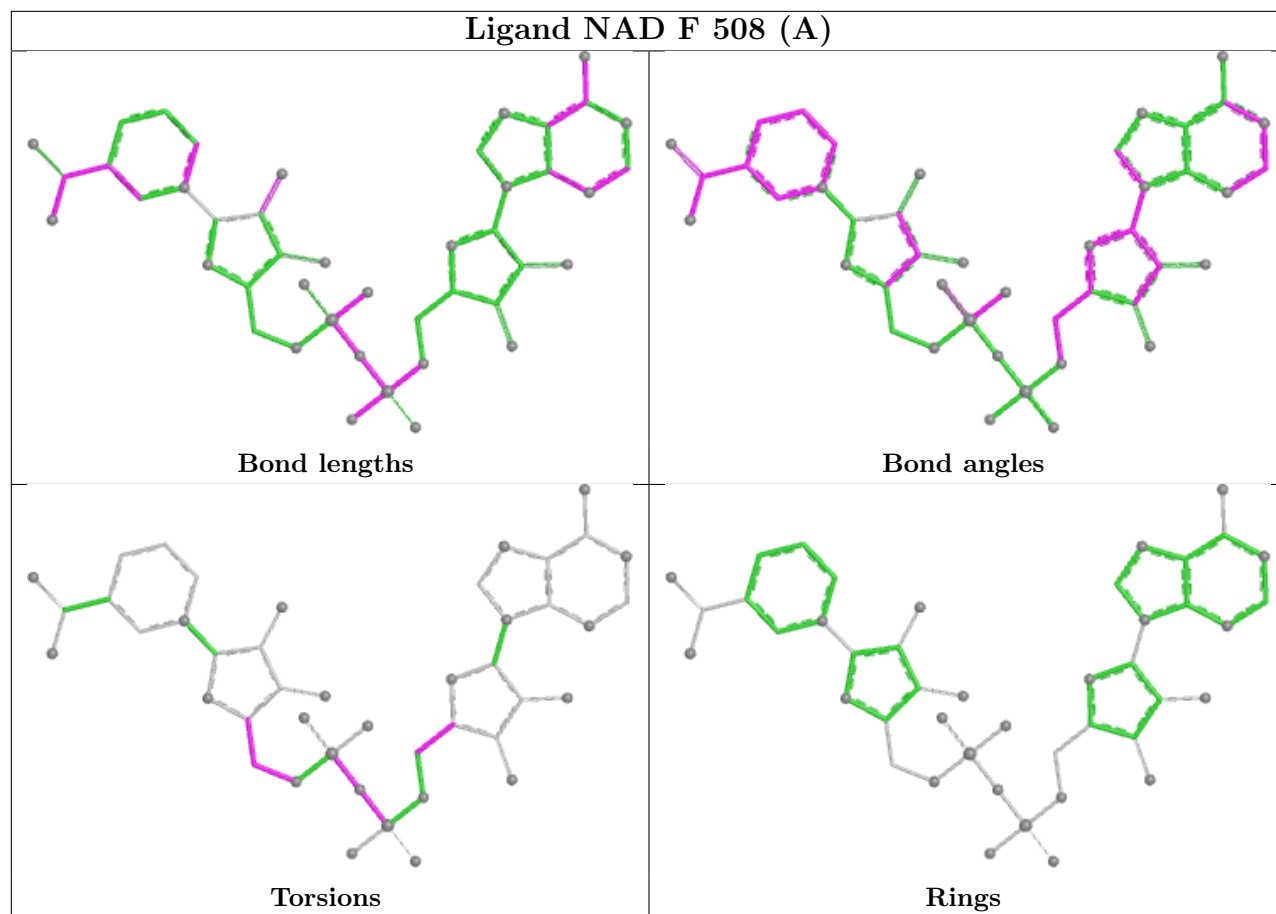
Ligand NAD C 507 (A)



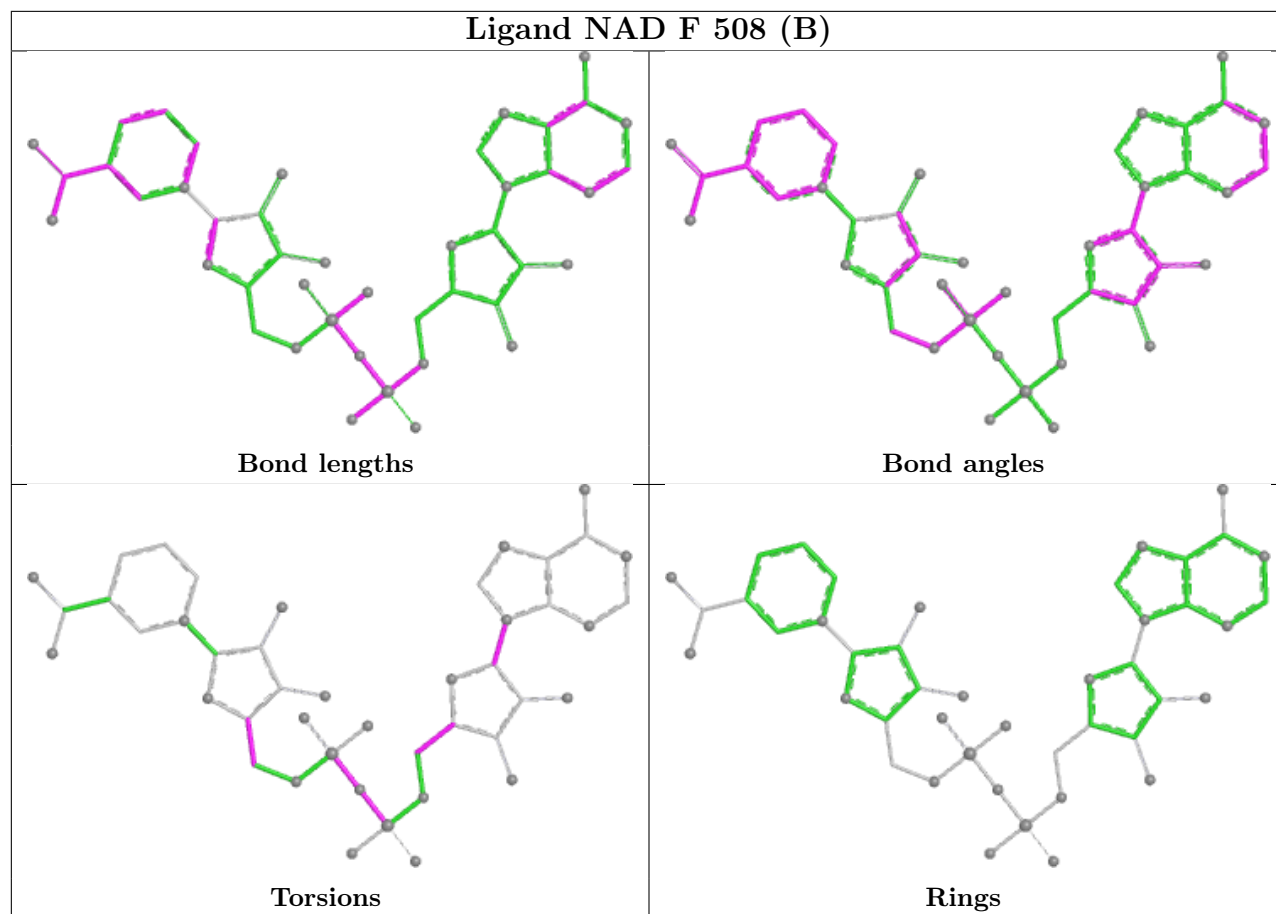
Ligand NAD C 507 (B)

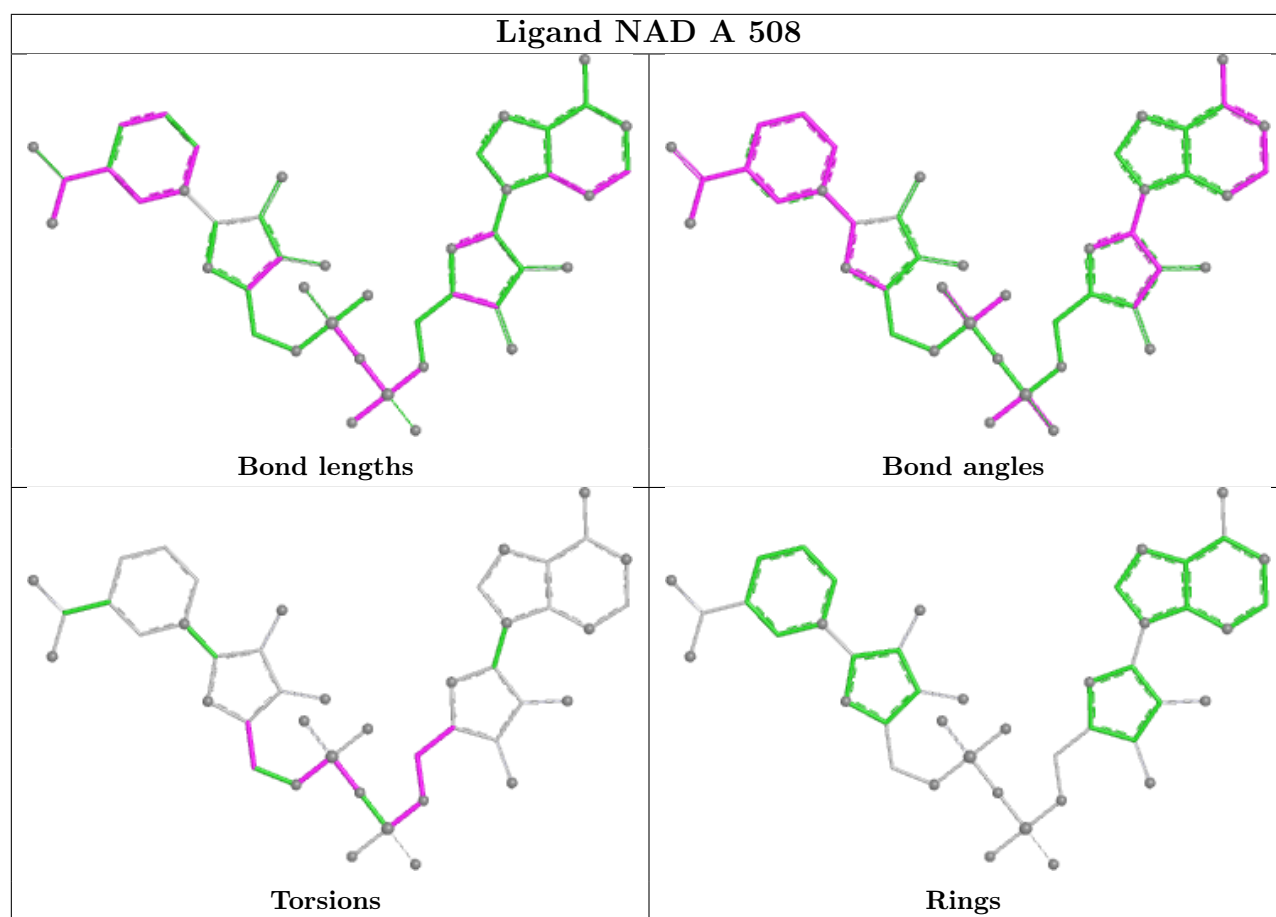


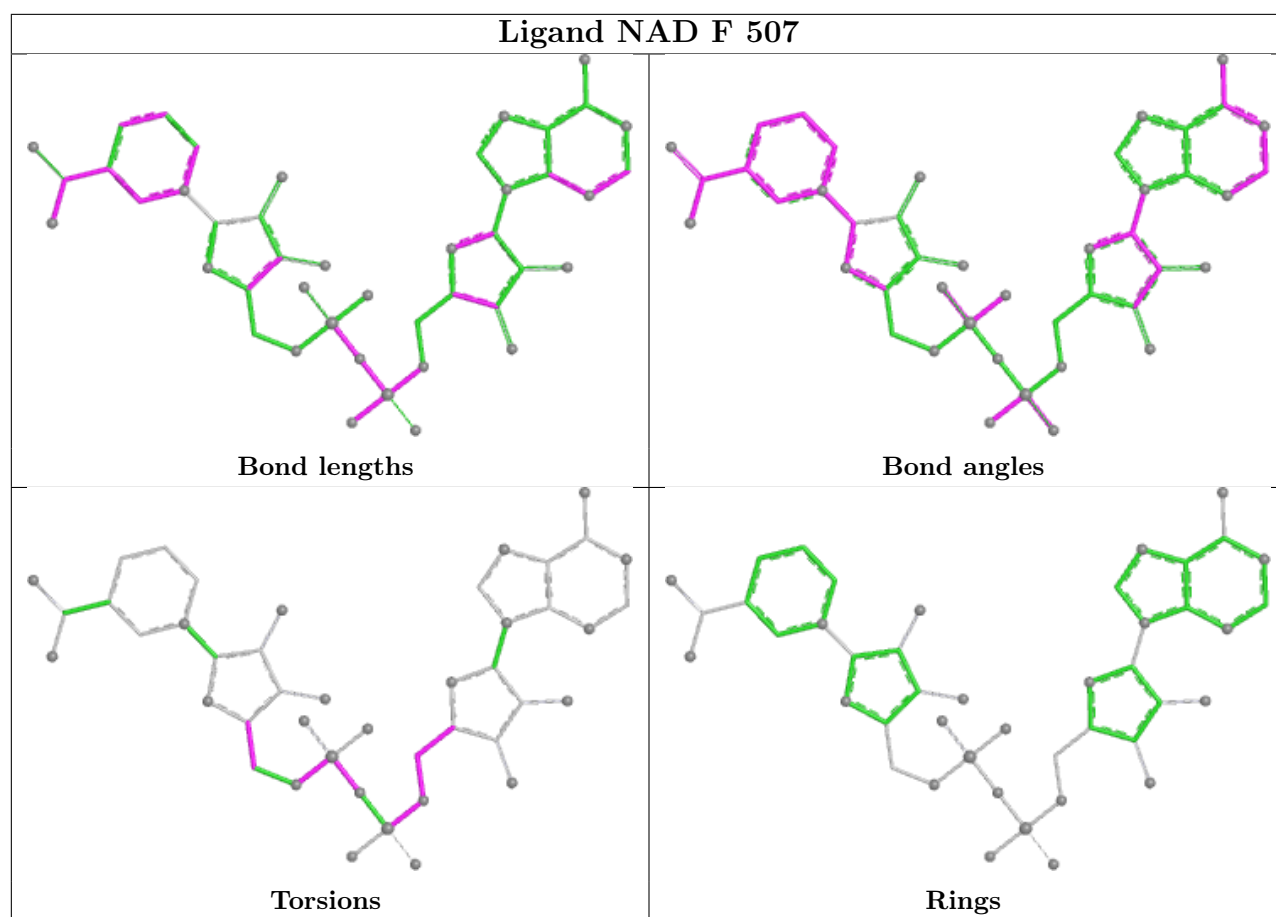
Ligand NAD F 508 (A)

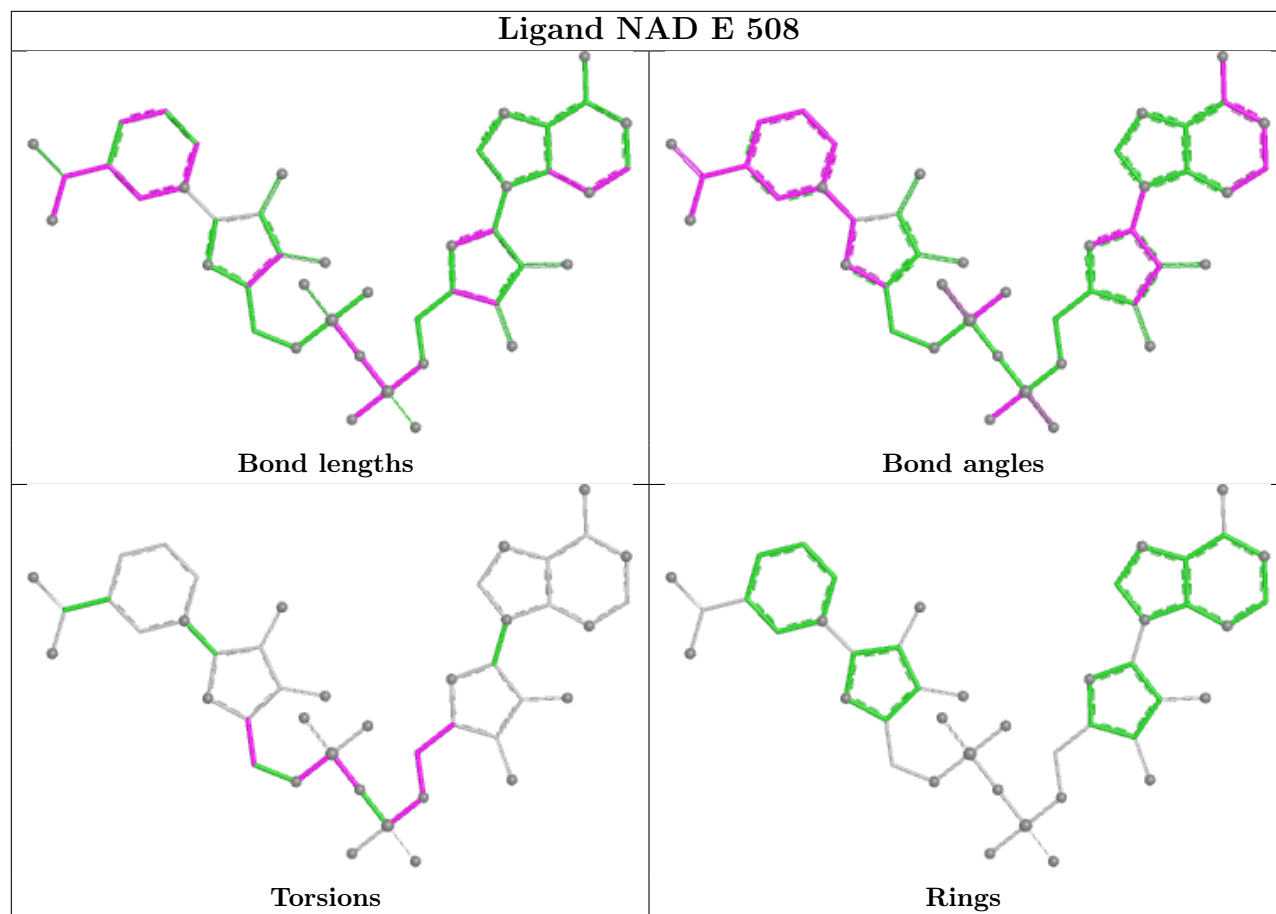


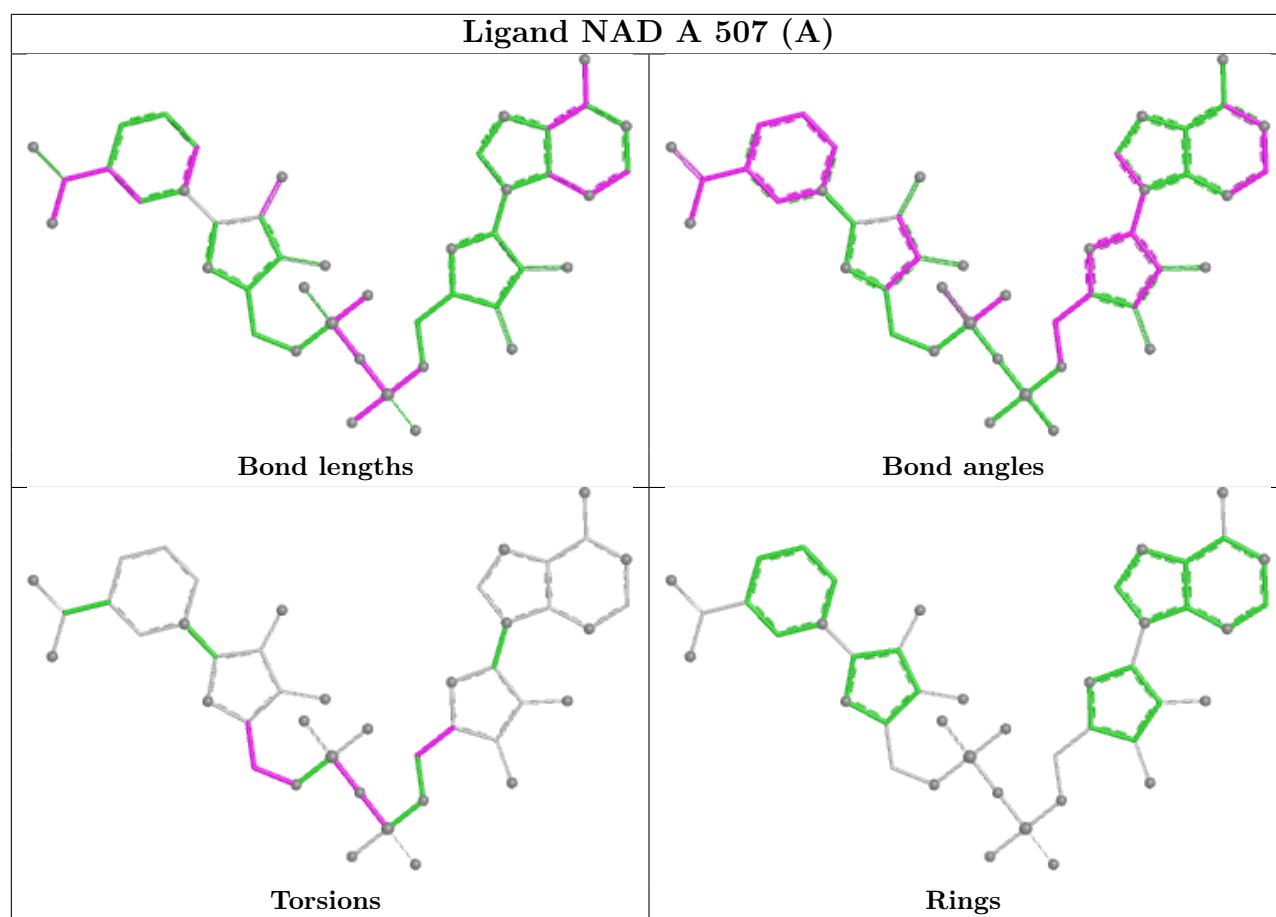
Ligand NAD F 508 (B)

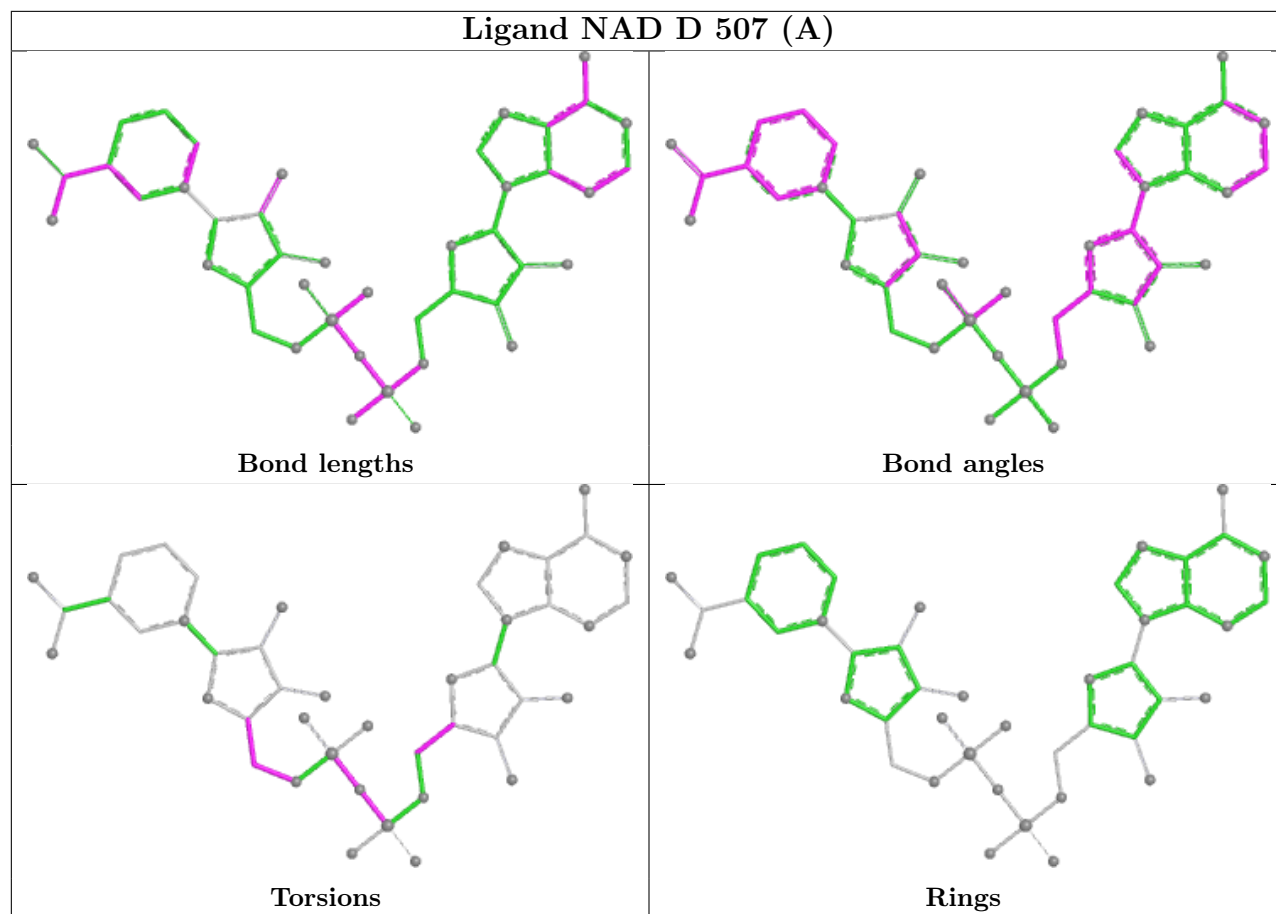




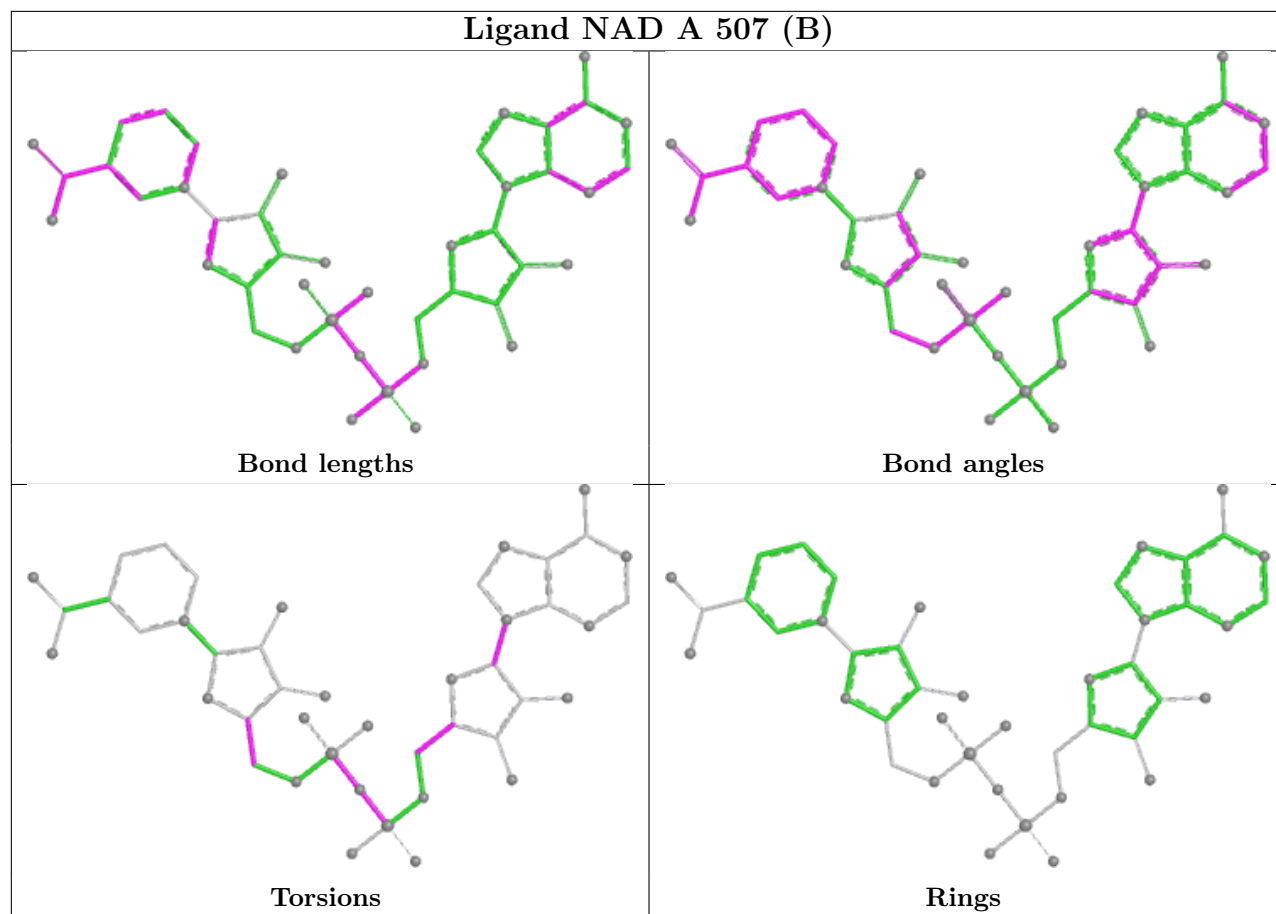




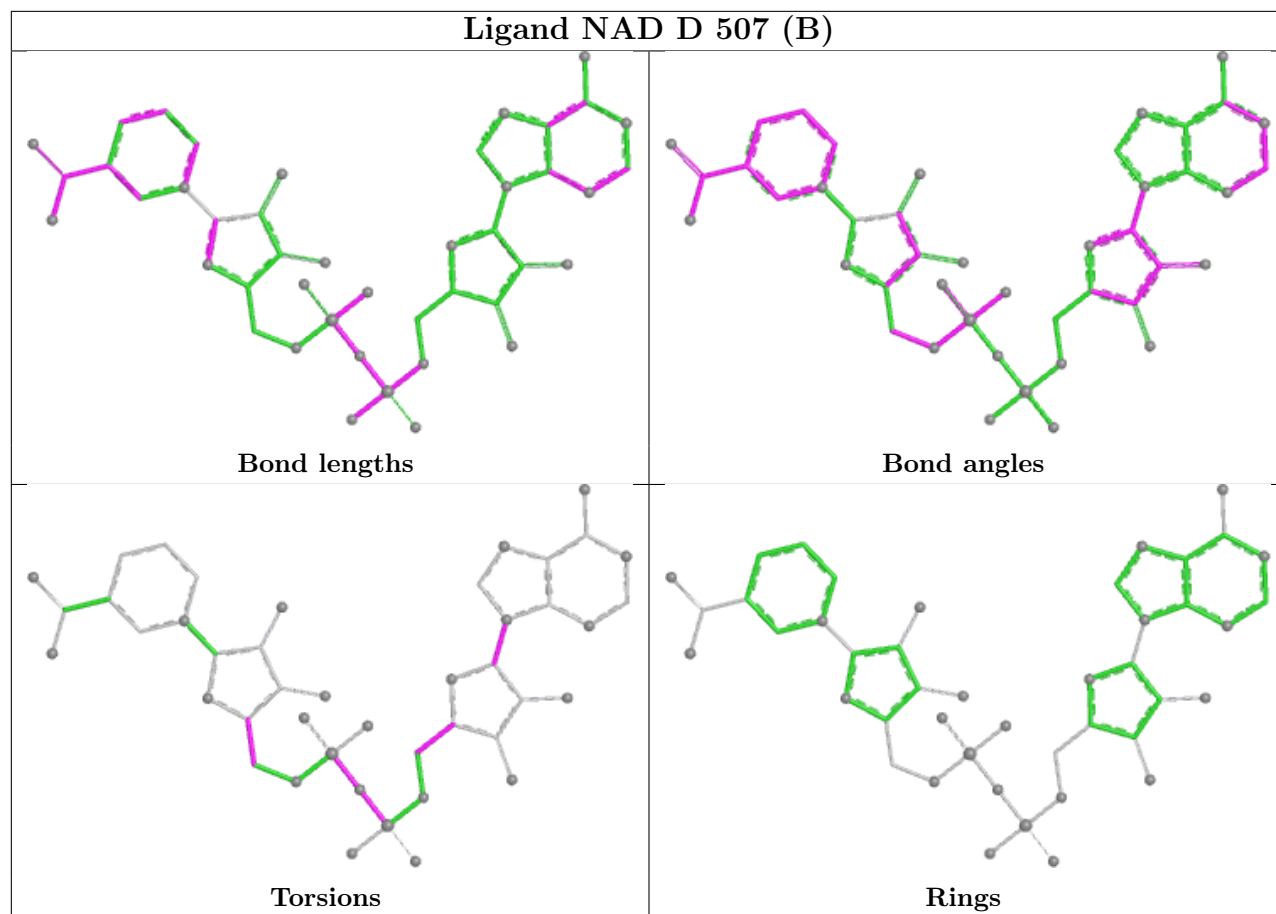




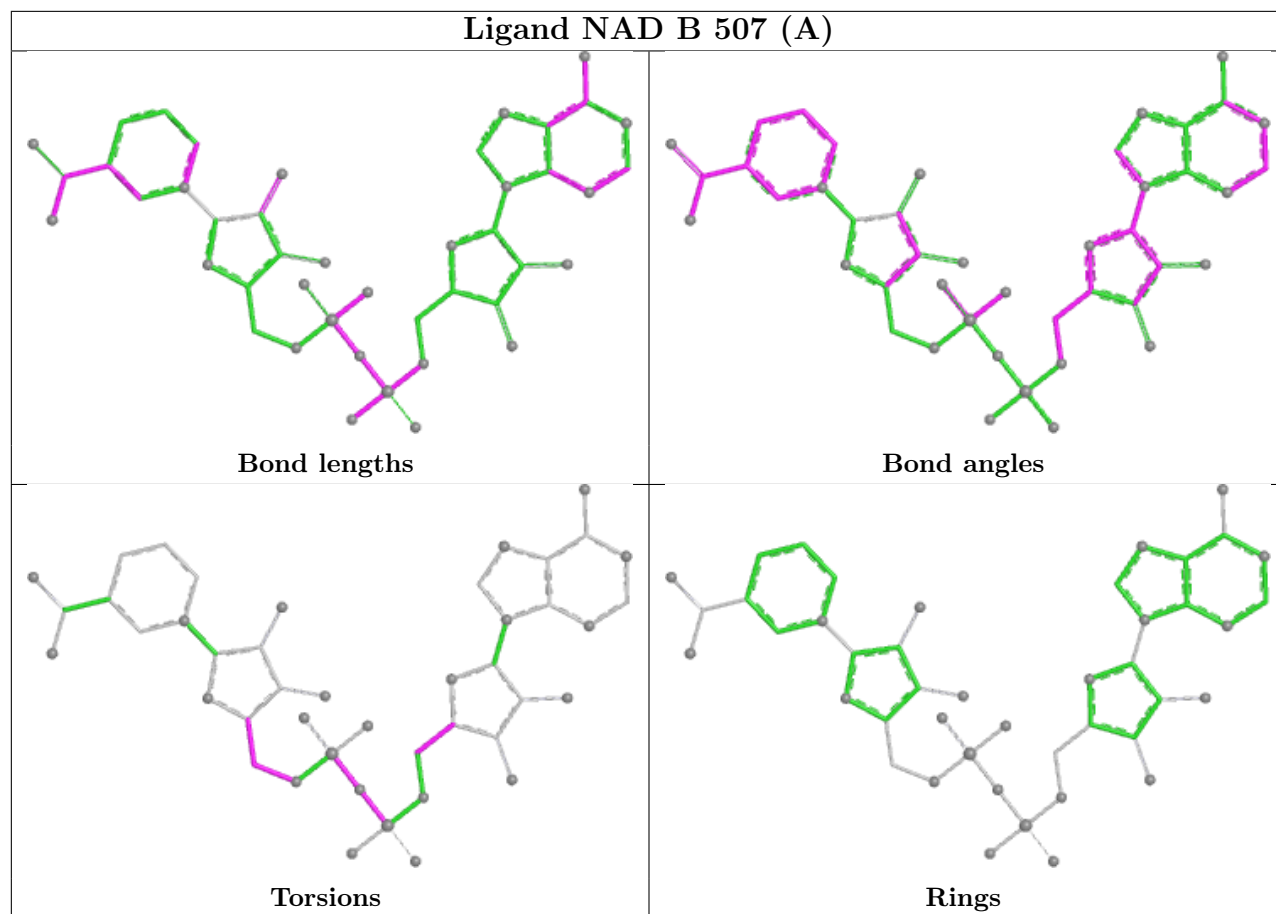
Ligand NAD A 507 (B)

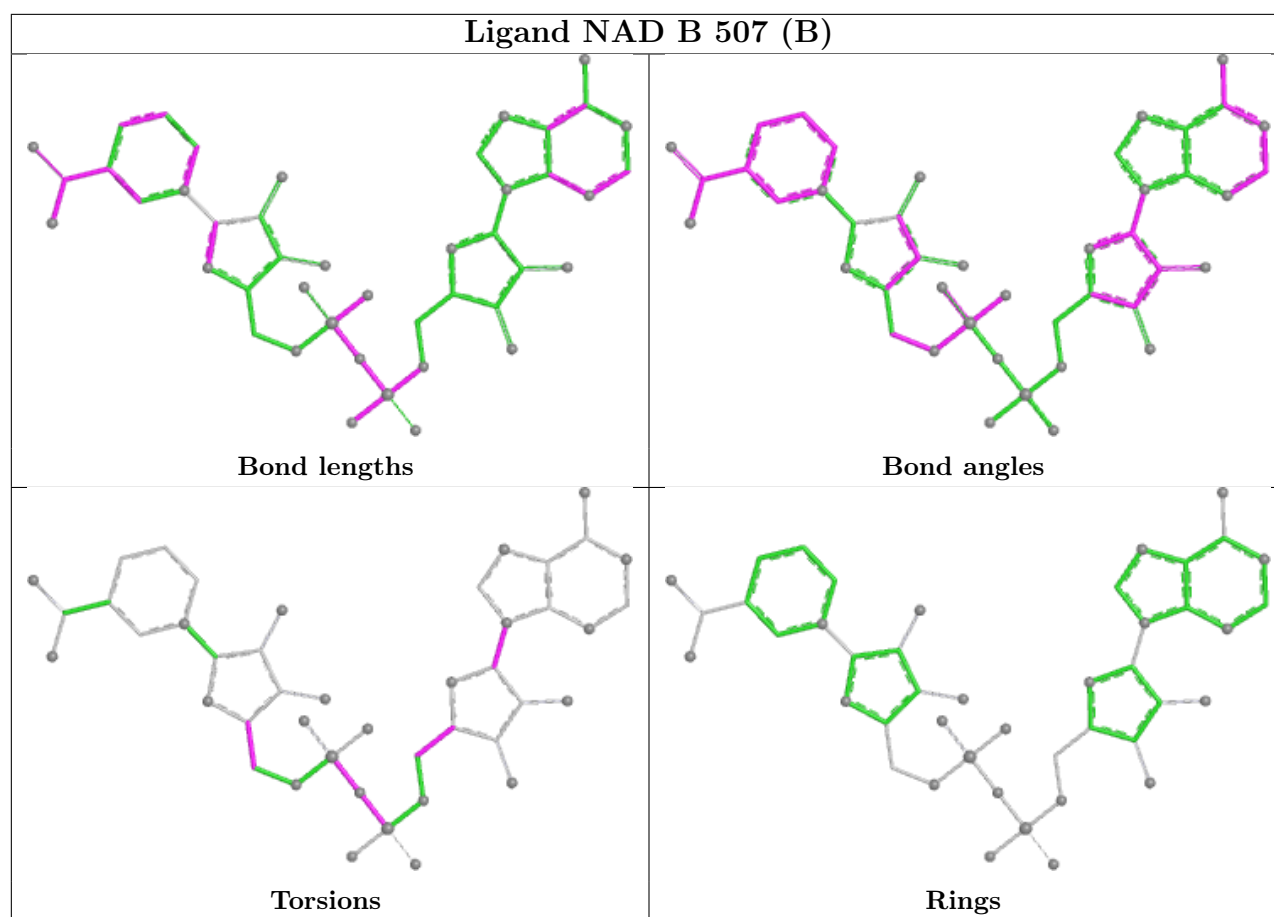


Ligand NAD D 507 (B)



Ligand NAD B 507 (A)





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.