



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:51 am GMT

PDB ID : 1HWY
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

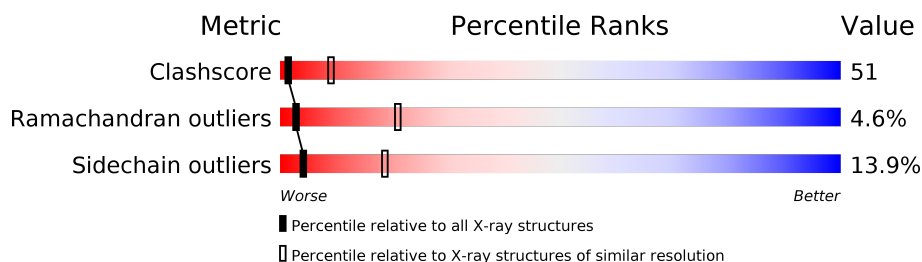
1 Overall quality at a glance

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	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	501	
1	B	501	
1	C	501	
1	D	501	
1	E	501	
1	F	501	

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:

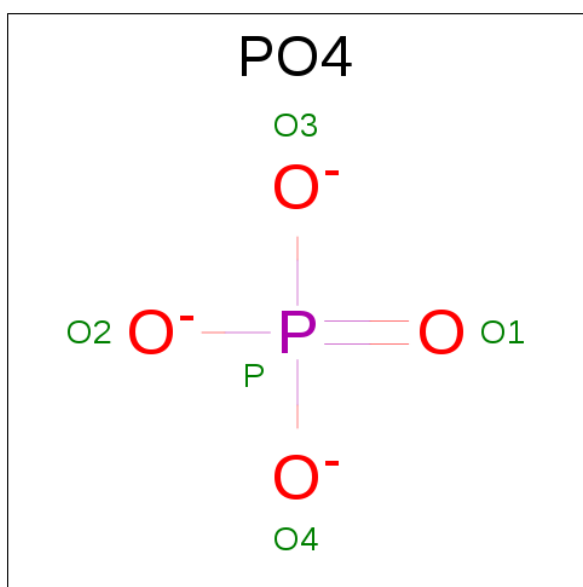
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO	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 (three-letter code: PO4) (formula: O_4P).



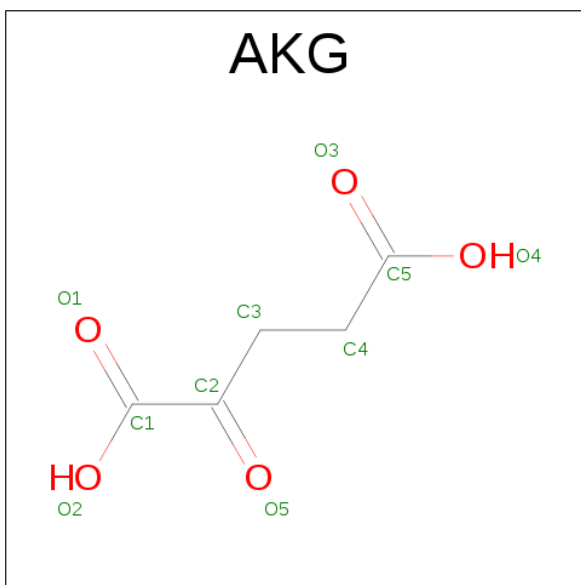
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

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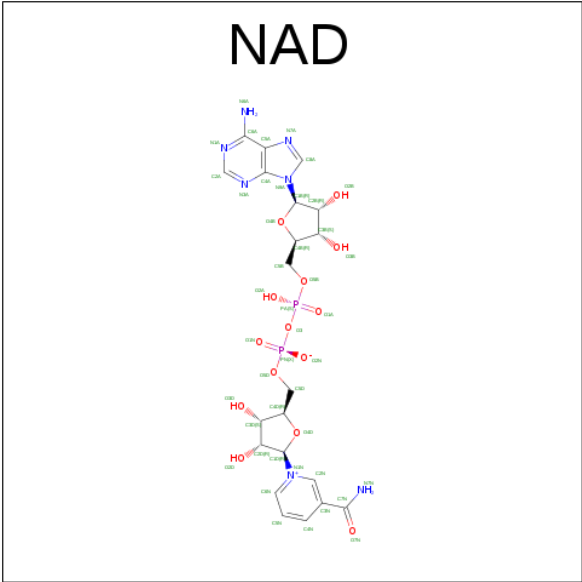
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



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

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



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

- Molecule 5 is water.

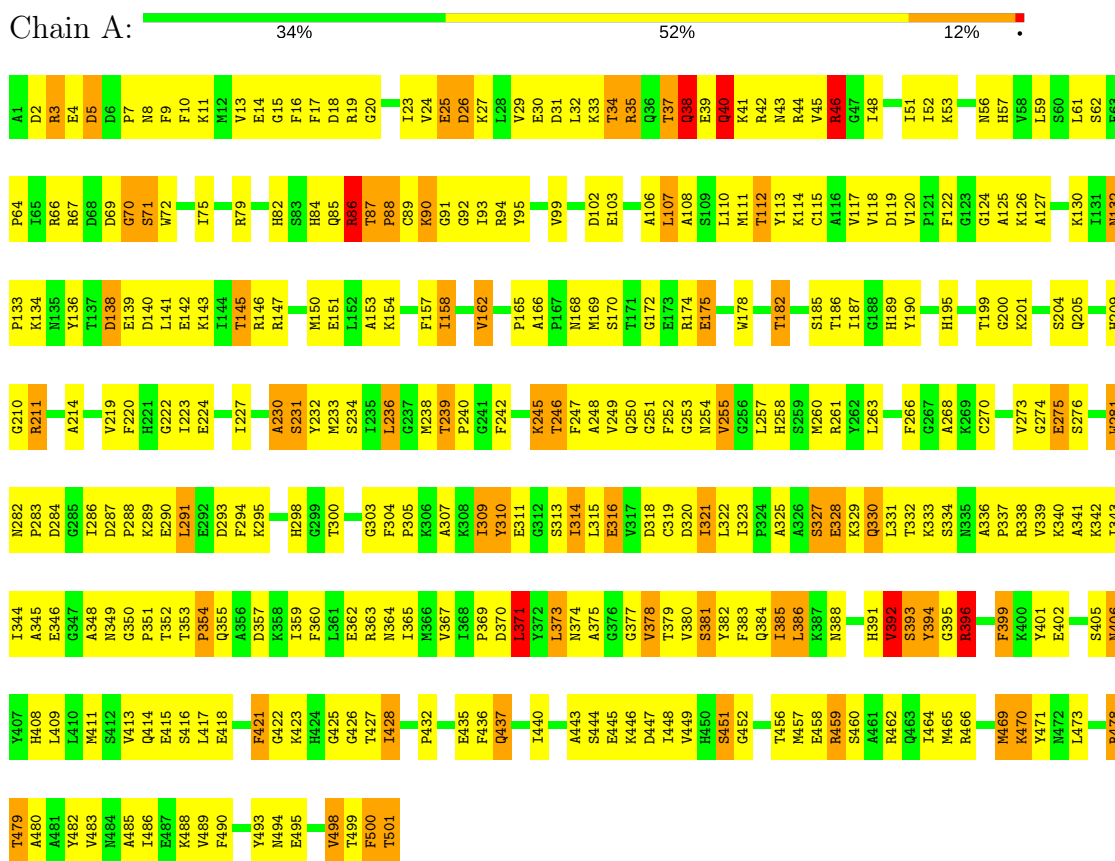
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0
5	C	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0

3 Residue-property plots

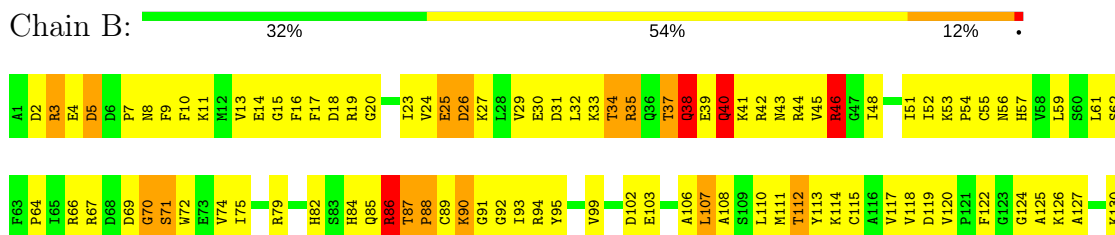
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

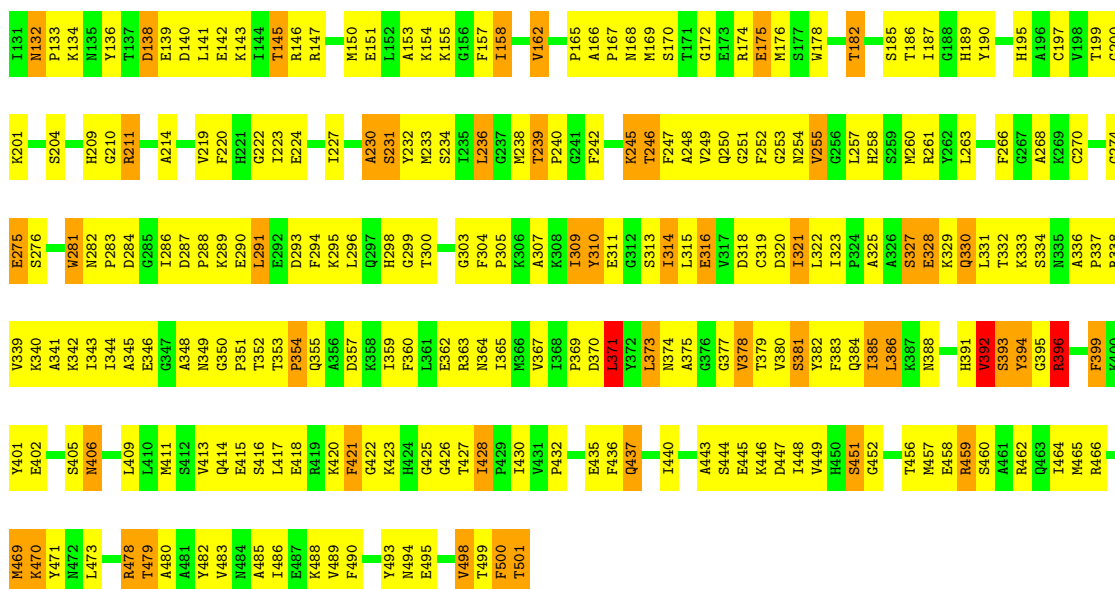
Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE



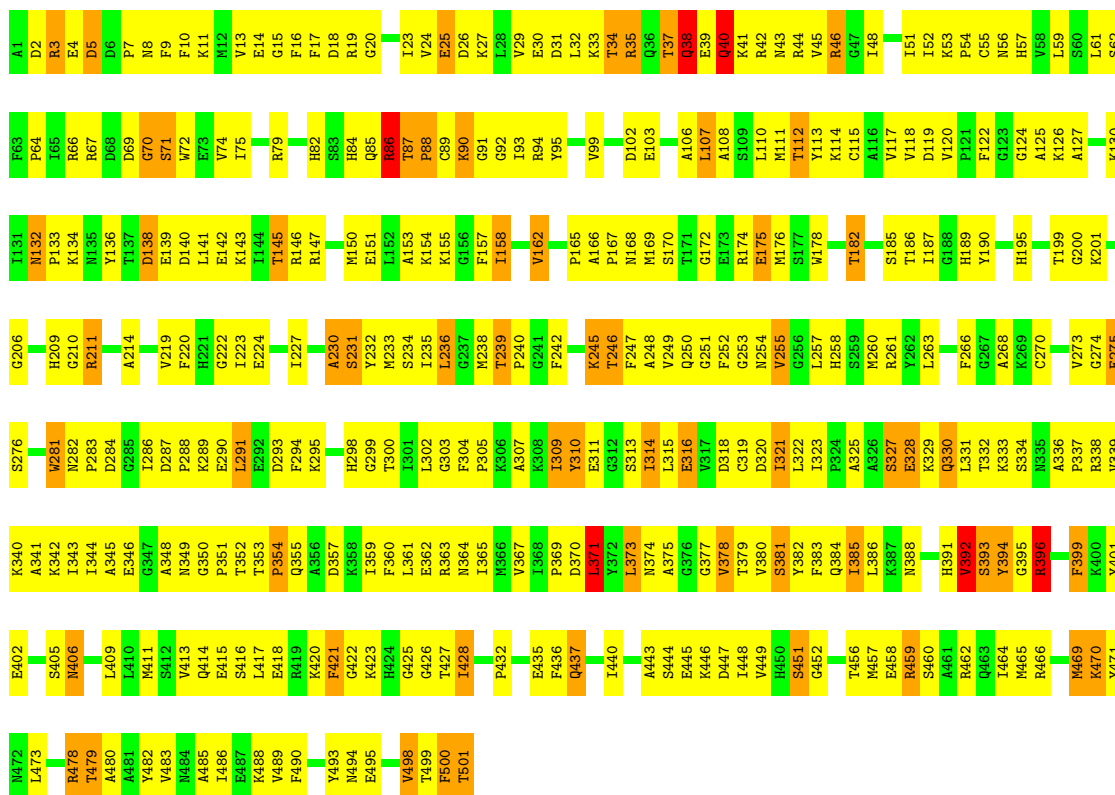
• Molecule 1: GLUTAMATE DEHYDROGENASE





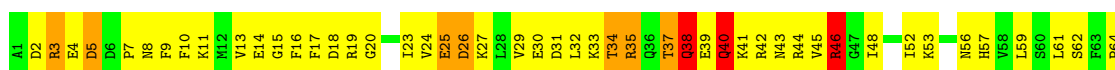
• Molecule 1: GLUTAMATE DEHYDROGENASE

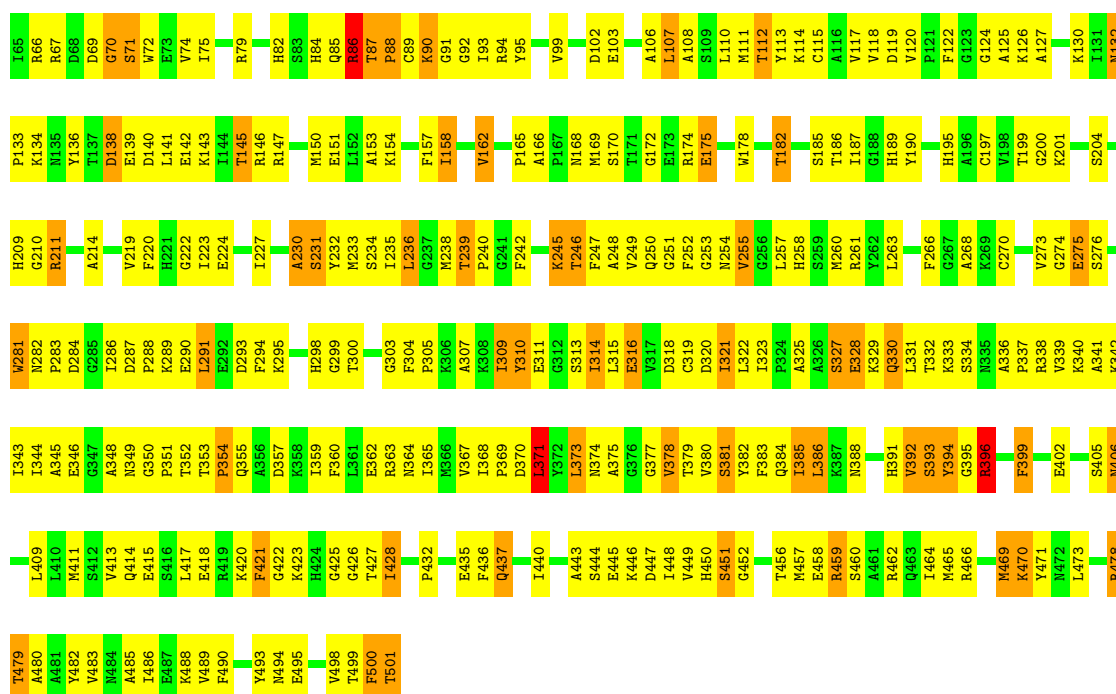
Chain C: 32% 55% 12%



• Molecule 1: GLUTAMATE DEHYDROGENASE

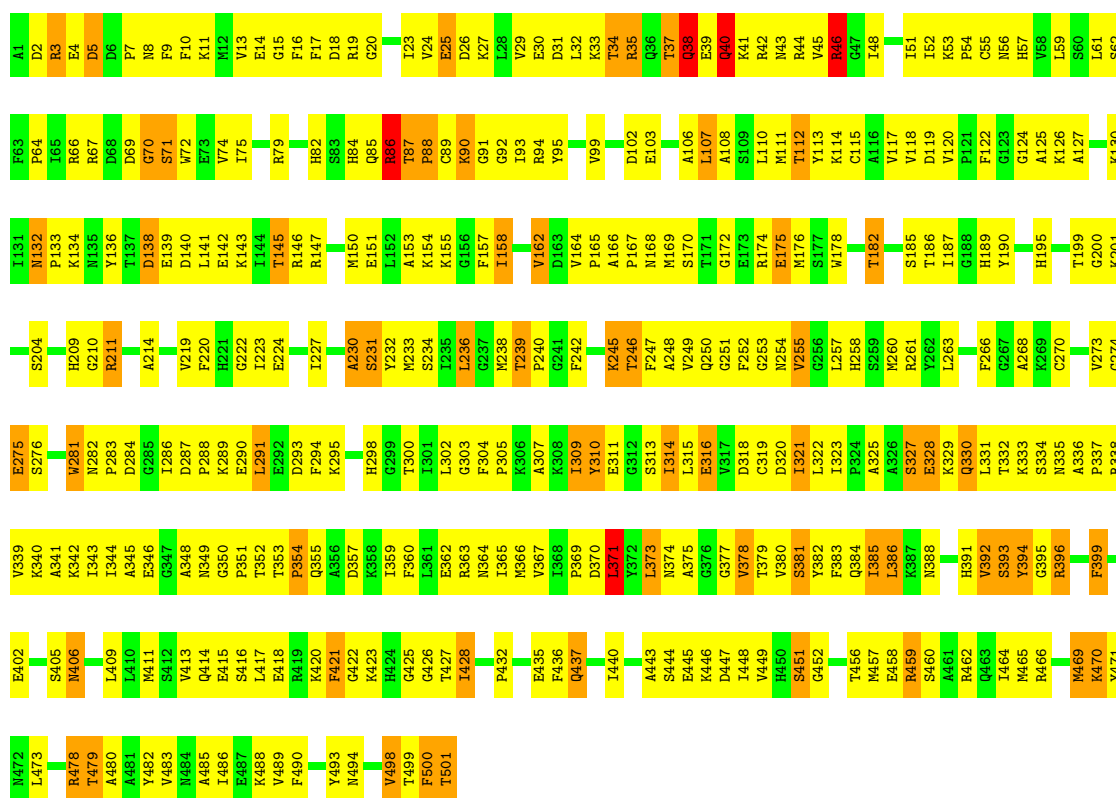
Chain D: 33% 53% 12%





• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain E: 32% 54% 13%



• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 32% 54% 12%

M469	Y401	V339	E275	S204	I131	F63	A1
K470	E402	K340	S276	Q205	M132	P64	R2
N471	A341	A341	S276		P133	I65	D3
N472	S405	K342	W281	H209	K134	R66	E4
L473	N406	T343	P283	G210	N135	R67	D5
		T344	P283	R211	Y136	D68	D6
	L409	A345	D284		T137	D69	P7
T479	L410	E346	G285	A214	D138	G70	N8
A480	M411	G347	I286		E139	S71	F10
A481	S412	A348	D287	V219	D140	W72	F11
Y482	N349	P348	P288	F220	L141	E73	K11
M483	Q414	G350	K289	H221	E142	V74	M12
N484	E415	P351	E290	G222	K143	I75	V13
A485	S416	T352	L291	I223	T144	R79	E14
L486	L417	T353	E292	E224	T145		G15
E487	E418	P354	D293		R146		F16
K488	R419	G355	F294	I227	R147	H82	F17
V489	K420	K356	K295			S83	D18
F490	F421	P357		A230	M150	H84	R19
	G422	K358	H298	S231	E151	Q85	G20
Y493	K423	F360	G299	M233	L152	R86	I23
N494	H424	K360	T300	M233	A153	T87	V24
E495	G425	L361	I301	S234	K154	P88	E25
	G426	E362	L302	I235	K155	C89	D26
V498	T427	R363	G303	L236	G156	K90	E26
T499	L428	N364	F304	G237	F157	G91	K27
F500	P429	I365	P305	M238	I158	G92	L28
	L430	K366	K306	T239		I93	V29
V481	V367	K367	A307	P240	V162	R94	E30
P432	L368	K308	K308	G241		Y95	D31
				P242	P165		
E435	P369	D370	I309		A166	V99	K32
F436	L371	R371	E311	K245	P167		K33
Q437	Y372	Y372	G312	T246	N168	D102	T34
	L373	L373	S313	F247	M169	E103	R35
I440	K374	K374	I314	A248	S170	A106	Q36
	A375	A375	L315	V249	T171	A106	T37
A443	G376	G376	E316	Q250	G172	L107	Q38
S444	G377	G377	V317	G251	E173	A108	E39
E445	V378	V378	D318	F252	R174	S109	R40
K446	T379	T379	C319	G253	E175	L110	K41
D447	V380	V380	D320	N254	M176	M111	R42
L448	S381	S381	I321	V255	S177	T112	M43
V449	Y382	Y382	L322	G256	H178	Y113	R44
H450	F383	F383	I323	L257	K114	C115	V45
S451	Q384	Q384	P324	H258	T182	G115	R46
G452	L385	L385	A325	S259		A116	R47
	L386	L386	A326	N260	S185	V117	I48
T456	K387	K387	S327	R261	T186	V118	I51
M457	N388	N388	E328	Y262	I187	D119	I52
E458			K329	L263	G188	V120	K53
R459	H391	H391	Q330	F266	H189	P121	P54
S460	V392	V392	L331	G267	Y190	F122	C55
A461	S393	S393	T332	K267		G123	N56
R462	Y394	Y394	K333	A268	H195	G124	H57
Q463	G395	G395	S334	K269	T199	A125	V58
L464	R396	R396	N335	C270	G200	K126	L59
M465	F399	F399	A336	V273	K201	A127	S60
R466	K400	K400	P337	G274			S62

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, AKG, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/3991	0.84	10/5384 (0.2%)
1	B	0.62	0/3991	0.84	10/5384 (0.2%)
1	C	0.62	0/3991	0.84	9/5384 (0.2%)
1	D	0.62	0/3991	0.84	10/5384 (0.2%)
1	E	0.62	0/3991	0.84	10/5384 (0.2%)
1	F	0.62	0/3991	0.84	10/5384 (0.2%)
All	All	0.62	0/23946	0.84	59/32304 (0.2%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	478	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	478	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	E	478	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	C	478	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	F	478	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	D	86	ARG	N-CA-C	-6.13	94.44	111.00
1	B	86	ARG	N-CA-C	-6.13	94.46	111.00
1	E	86	ARG	N-CA-C	-6.13	94.46	111.00
1	F	86	ARG	N-CA-C	-6.13	94.46	111.00
1	A	86	ARG	N-CA-C	-6.12	94.47	111.00
1	C	86	ARG	N-CA-C	-6.11	94.50	111.00
1	C	459	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	E	459	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	459	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	459	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	F	459	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	459	ARG	NE-CZ-NH2	-5.99	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	281	TRP	N-CA-C	5.37	125.50	111.00
1	F	281	TRP	N-CA-C	5.37	125.49	111.00
1	A	281	TRP	N-CA-C	5.36	125.46	111.00
1	C	281	TRP	N-CA-C	5.36	125.47	111.00
1	B	281	TRP	N-CA-C	5.35	125.45	111.00
1	D	281	TRP	N-CA-C	5.35	125.44	111.00
1	A	371	LEU	CA-CB-CG	5.29	127.47	115.30
1	F	371	LEU	CA-CB-CG	5.29	127.46	115.30
1	E	371	LEU	CA-CB-CG	5.29	127.46	115.30
1	D	371	LEU	CA-CB-CG	5.29	127.45	115.30
1	C	371	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	371	LEU	CA-CB-CG	5.27	127.43	115.30
1	E	46	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	392	VAL	CB-CA-C	-5.16	101.59	111.40
1	A	392	VAL	CB-CA-C	-5.16	101.59	111.40
1	F	392	VAL	CB-CA-C	-5.16	101.59	111.40
1	E	392	VAL	CB-CA-C	-5.16	101.60	111.40
1	C	392	VAL	CB-CA-C	-5.14	101.62	111.40
1	C	87	THR	N-CA-C	5.14	124.88	111.00
1	D	87	THR	N-CA-C	5.14	124.88	111.00
1	D	392	VAL	CB-CA-C	-5.14	101.64	111.40
1	F	46	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	87	THR	N-CA-C	5.13	124.87	111.00
1	A	87	THR	N-CA-C	5.13	124.86	111.00
1	F	87	THR	N-CA-C	5.13	124.85	111.00
1	E	87	THR	N-CA-C	5.13	124.85	111.00
1	B	119	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	119	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	119	ASP	CB-CG-OD2	5.09	122.89	118.30
1	E	119	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	46	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	119	ASP	CB-CG-OD2	5.08	122.88	118.30
1	F	119	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	46	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	40	GLN	N-CA-C	-5.05	97.36	111.00
1	D	40	GLN	N-CA-C	-5.05	97.38	111.00
1	D	46	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	F	40	GLN	N-CA-C	-5.04	97.38	111.00
1	C	40	GLN	N-CA-C	-5.04	97.39	111.00
1	A	40	GLN	N-CA-C	-5.04	97.40	111.00
1	B	40	GLN	N-CA-C	-5.04	97.40	111.00

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	431	1
1	B	3910	0	3888	453	2
1	C	3910	0	3888	431	2
1	D	3910	0	3888	419	0
1	E	3910	0	3888	437	1
1	F	3910	0	3888	444	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
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	7	0
3	F	10	0	4	7	0
4	A	132	0	78	32	0
4	B	132	0	78	35	0
4	C	132	0	78	38	0
4	D	132	0	77	34	0
4	E	132	0	77	30	0
4	F	132	0	77	33	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	2472	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 51.

All (2472) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:VAL:HG12	3:F:506:AKG:O4	1.65	0.94
1:C:391:HIS:CA	4:C:507[A]:NAD:HO3N	1.64	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:505:PO4:O3	5:B:510:HOH:O	1.91	0.88
1:B:391:HIS:CA	4:B:507[A]:NAD:HO3N	1.61	0.88
1:B:195:HIS:HE1	1:F:87:THR:CG2	1.86	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: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
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: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:209:HIS:CD2	2:E:503:PO4:O3	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HG3	1:A:46:ARG:HH11	1.44	0.83
1:B:46:ARG:HG3	1:B:46:ARG:HH11	1.44	0.83
1:D:118:VAL:HG21	1:D:375:ALA:HB1	1.59	0.83
1:D:46:ARG:HG3	1:D:46:ARG:HH11	1.44	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:141:LEU:O	1:C:145:THR:HG23	1.77	0.83
1:C:118:VAL:HG21	1:C:375:ALA:CB	2.09	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
1:D:391:HIS:HD2	4:D:507[A]:NAD:HO2N	1.26	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:HH11	1:C:46:ARG:HG3	1.44	0.82
1:D:118:VAL:HG21	1:D:375:ALA:CB	2.09	0.82
1:D:87:THR:H	4:E:507[A]:NAD:H72N	1.27	0.82
1:E:118:VAL:HG21	1:E:375:ALA:CB	2.09	0.82
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.44	0.82
1:E:9:PHE:HE1	1:E:107:LEU:HD13	1.43	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
4:C:507[A]:NAD:H72N	1:E:87:THR:H	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:THR:H	4:D:507[A]:NAD:H72N	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
3:C:506:AKG:O2	4:C:508:NAD:C5N	2.29	0.81
1:F:242:PHE:HB3	1:F:268:ALA:HB2	1.62	0.80
1:F:46:ARG:HH11	1:F:46:ARG:HG3	1.44	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
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: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:E:275:GLU:OE1	4:E:508:NAD:H1B	1.83	0.79
1:D:275:GLU:OE1	4:D:508:NAD:H1B	1.83	0.79
1:A:87:THR:H	4:F:508[A]:NAD:H72N	1.27	0.79
1:C:275:GLU:OE1	4:C:508:NAD:H1B	1.83	0.79
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.69	0.75
1:F:457:MET:HA	1:F:457:MET:HE2	1.68	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: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:B:457:MET:HA	1:B:457:MET:HE2	1.67	0.74
1:C:2:ASP:HB3	1:C:5:ASP:O	1.88	0.74
1:C:457:MET:HA	1:C:457:MET:HE2	1.69	0.74
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.69	0.74
1:C:195:HIS:HE1	1:E:87:THR:HG23	1.52	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: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:313:SER:HB3	1:E:316:GLU:HB2	1.68	0.73
1:E:2:ASP:HB3	1:E:5:ASP:O	1.87	0.73
1:C:313:SER:HB3	1:C:316:GLU:HB2	1.68	0.73
1:B:2:ASP:HB3	1:B:5:ASP:O	1.88	0.73
1:A:499:THR:HG21	1:D:64:PRO:HG2	1.70	0.73
1:F:282:ASN:ND2	1:F:284:ASP:H	1.84	0.73
1:A:195:HIS:HE1	1:B:87:THR:CG2	2.01	0.73
1:C:391:HIS:HA	4:C:507[A]:NAD:C3D	2.16	0.73
1:A:457:MET:HA	1:A:457:MET:HE2	1.71	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:E:20:GLY:O	1:E:24:VAL:HG22	1.89	0.73
1:D:20:GLY:O	1:D:24:VAL:HG22	1.89	0.72
1:B:195:HIS:CE1	1:F:87:THR:HG23	2.24	0.72
1:B:20:GLY:O	1:B:24:VAL:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:MET:HE2	1:D:457:MET:HA	1.71	0.72
1:D:87:THR:CG2	1:E:195:HIS:HE1	2.02	0.72
1:C:195:HIS:CE1	1:E:87:THR:HG23	2.24	0.72
1:B:195:HIS:HE1	1:F:87:THR:HG23	1.51	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: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:A:66:ARG:H	1:D:501:THR:HG22	1.55	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: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:C:303:GLY:H	1:C:309:ILE:HD11	1.55	0.71
1:B:195:HIS:HE1	1:F:87:THR:HG21	1.54	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: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:421:PHE:HE1	1:F:421:PHE:HE1	1.38	0.71
1:B:418:GLU:OE2	1:B:427:THR:HA	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:417:LEU:CD2	1:F:417:LEU:CD1	2.69	0.70
1:B:310:TYR:HD1	1:B:311:GLU:N	1.88	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:C:417:LEU:HD21	1:E:417:LEU:CD1	2.20	0.70
1:F:239:THR:HG22	1:F:245:LYS:HE3	1.72	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:25:GLU:O	1:D:29:VAL:HG23	1.92	0.69
1:B:409:LEU:HD11	1:F:409:LEU:HD22	1.73	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:N	1:D:428:ILE:HD13	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:460:SER:O	1:E:464:ILE:HG13	1.92	0.69
1:E:17:PHE:HA	1:E:482:TYR:CD2	2.28	0.69
1:A:72:TRP:CZ3	1:D:499:THR:HG22	2.28	0.69
1:B:25:GLU:O	1:B:29:VAL:HG23	1.92	0.69
1:B:17:PHE:HA	1:B:482:TYR:CD2	2.28	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:B:428:ILE:HD13	1:B:428:ILE:N	2.07	0.69
1:B:62:SER:HA	1:B:75:ILE:O	1.93	0.69
1:E:391:HIS:HD2	4:E:507[A]:NAD:HO2N	1.39	0.69
1:A:132:ASN:HD21	1:A:134:LYS:HG3	1.56	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: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:C:31:ASP:O	1:C:33:LYS:HG2	1.93	0.69
1:B:499:THR:HG22	1:E:72:TRP:CZ3	2.26	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:F:17:PHE:HA	1:F:482:TYR:CD2	2.28	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:N	1:C:428:ILE:HD13	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:29:VAL:HG21	1:A:42:ARG:HG2	1.76	0.68
1:C:460:SER:O	1:C:464:ILE:HG13	1.92	0.68
1:C:62:SER:HA	1:C:75:ILE:O	1.93	0.68
1:E:62:SER:HA	1:E:75:ILE:O	1.93	0.68
1:A:460:SER:O	1:A:464:ILE:HG13	1.92	0.68
1:A:87:THR:HG23	1:F:195:HIS:HE1	1.57	0.68
1:D:17:PHE:HA	1:D:482:TYR:CD2	2.28	0.68
1:C:499:THR:HG22	1:F:72:TRP:HZ3	1.57	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:444:SER:OG	1:C:446:LYS:HG2	1.93	0.68
1:C:87:THR:OG1	1:C:88:PRO:HD3	1.92	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: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: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:E:32:LEU:HD11	1:E:34:THR:OG1	1.94	0.68
1:C:142:GLU:O	1:C:146:ARG:HG3	1.94	0.67
1:F:391:HIS:HD2	4:F:508[A]:NAD:HO2N	1.40	0.67
1:B:195:HIS:CE1	1:F:87:THR:CG2	2.74	0.67
1:A:499:THR:HG22	1:D:72:TRP:HZ3	1.60	0.67
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.07	0.67
1:A:142:GLU:O	1:A:146:ARG:HG3	1.94	0.67
1:A:32:LEU:HD11	1:A:34:THR:OG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:CG1	3:A:506:AKG:O4	2.39	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: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:D:417:LEU:CD1	1:E:417:LEU:HD21	2.25	0.67
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.24	0.67
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.59	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:C:499:THR:HG21	1:F:64:PRO:HG2	1.75	0.66
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: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:495:GLU:OE1	1:F:204:SER:OG	2.08	0.65
1:C:72:TRP:HZ3	1:F:499:THR:HG22	1.59	0.65
1:B:66:ARG:H	1:E:501:THR:HG22	1.61	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:411:MET:CE	1:D:415:GLU:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:THR:HG23	1:D:354:PRO:HD2	1.79	0.65
1:C:411:MET:CE	1:C: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: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:A:204:SER:OG	1:B:495:GLU:OE1	2.07	0.65
1:E:339:VAL:HG22	1:E:363:ARG:NH2	2.12	0.65
1:E:79:ARG:HG2	1:E:157:PHE:HB3	1.79	0.65
1:A:353:THR:HG23	1:A:354:PRO:HD2	1.79	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:B:499:THR:OG1	1:E:147:ARG:NH1	2.29	0.65
1:E:457:MET:HA	1:E:457:MET:HE2	1.79	0.65
1:F:132:ASN:ND2	1:F:134:LYS:HG3	2.12	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
1:D:40:GLN:NE2	1:D:40:GLN:HA	2.12	0.64
1:A:501:THR:HG22	1:D:66:ARG:H	1.61	0.64
1:F:281:TRP:HB2	1:F:310:TYR:CD2	2.28	0.64
1:F:40:GLN:HA	1:F:40:GLN:NE2	2.12	0.64
1:C:501:THR:HG22	1:F:66:ARG:H	1.62	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:411:MET:CE	1:B:415:GLU:HG3	2.26	0.64
1:B:391:HIS:N	4:B:507[A]:NAD:O3D	2.29	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:HA	1:A:40:GLN:NE2	2.12	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:A:417:LEU:HD21	1:B:417:LEU:HD12	1.80	0.64
1:E:40:GLN:NE2	1:E:40:GLN:HA	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:411:MET:HE2	1:F:415:GLU:HG3	1.79	0.63
1:A:107:LEU:HG	1:A:126:LYS:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:THR:HG23	1:B:354:PRO:HD2	1.79	0.63
1:C:40:GLN:HA	1:C:40:GLN:NE2	2.13	0.63
1:F:378:VAL:HG13	3:F:506:AKG:H31	1.81	0.63
1:B:46:ARG:NH1	1:B:46:ARG:HG3	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:A:500:PHE:HE2	1:F:185:SER:HB2	1.63	0.63
1:B:107:LEU:HG	1:B:126:LYS:HE2	1.80	0.63
1:C:353:THR:HG23	1:C:354:PRO:HD2	1.79	0.63
1:C:5:ASP:OD2	1:C:332:THR:HB	1.99	0.63
1:F:79:ARG:HG2	1:F:157:PHE:HB3	1.79	0.63
1:B:40:GLN:NE2	1:B:40:GLN:HA	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:B:5:ASP:OD2	1:B:332:THR:HB	1.99	0.63
1:E:107:LEU:HG	1:E:126:LYS:HE2	1.80	0.63
1:C:391:HIS:C	4:C:507[A]:NAD:O3D	2.35	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:B:281:TRP:CB	1:B:310:TYR:HD2	2.11	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:D:378:VAL:HG13	3:D:506:AKG:H31	1.81	0.62
1:F:107:LEU:HG	1:F:126:LYS:HE2	1.80	0.62
1:F:5:ASP:OD2	1:F:332:THR:HB	1.99	0.62
1:A:391:HIS:HD2	4:A:507[A]:NAD:HO2N	1.41	0.62
1:C:142:GLU:CG	1:C:146:ARG:HD2	2.29	0.62
1:D:391:HIS:C	4:D:507[A]:NAD:O3D	2.36	0.62
1:E:27:LYS:HA	1:E:30:GLU:HB3	1.81	0.62
1:E:5:ASP:OD2	1:E:332:THR:HB	1.99	0.62
1:A:378:VAL:HG13	3:A:506:AKG:H31	1.81	0.62
1:B:391:HIS:C	4:B:507[A]:NAD:O3D	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:391:HIS:HA	4:C:507[A]:NAD:HO3N	0.79	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:D:428:ILE:HG23	1:E:420:LYS:HZ2	1.65	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: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
1:B:452:GLY:O	1:B:456:THR:HG23	2.00	0.61
1:B:51:ILE:HA	1:E:74:VAL:CG2	2.31	0.61
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.36	0.61
4:C:507[B]:NAD:H2B	4:C:507[B]:NAD:O1N	2.01	0.61
4:D:507[B]:NAD:H2B	4:D:507[B]:NAD:O1N	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:281:TRP:O	1:B:281:TRP:CG	2.54	0.61
1:B:32:LEU:HG	1:B:41:LYS:HG2	1.82	0.61
4:B:507[B]:NAD:O1N	4:B:507[B]:NAD:H2B	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:360:PHE:HD2	1:A:365:ILE:HD12	1.66	0.61
1:A:411:MET:HE2	1:A:415:GLU:HG3	1.81	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:O	1:F:281:TRP:CG	2.54	0.61
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:281:TRP:O	2.54	0.60
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.36	0.60
1:C:281:TRP:O	1:C:281:TRP:CG	2.54	0.60
1:C:360:PHE:HD2	1:C:365:ILE:HD12	1.66	0.60
1:D:94:ARG:HH21	1:D:168:ASN:HD21	1.49	0.60
1:D:33:LYS:HA	1:D:41:LYS:NZ	2.16	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
1:C:420:LYS:HZ2	1:E:428:ILE:HG23	1.66	0.60
4:F:508[B]:NAD:H2B	4:F:508[B]:NAD:O1N	2.01	0.60
1:A:142:GLU:CG	1:A:146:ARG:HD2	2.29	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
1:B:69:ASP:O	1:B:71:SER:N	2.35	0.60
1:C:391:HIS:HD2	4:C:507[A]:NAD:HO2N	1.47	0.60
1:D:281:TRP:O	1:D:281:TRP:CG	2.54	0.60
1:E:452:GLY:O	1:E:456:THR:HG23	2.00	0.60
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.36	0.60
1:F:391:HIS:C	4:F:508[A]:NAD:O3D	2.36	0.60
1:F:94:ARG:HH21	1:F:168:ASN:HD21	1.50	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:O	1:E:281:TRP:CG	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:94:ARG:HH21	1:E:168:ASN:HD21	1.49	0.60
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.31	0.60
1:A:136:TYR:HB3	1:A:140:ASP:CB	2.32	0.60
1:A:391:HIS:C	4:A:507[A]:NAD:O3D	2.38	0.60
1:A:94:ARG:HH21	1:A:168:ASN:HD21	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:411:MET:HE2	1:C:415:GLU:HG3	1.84	0.59
1:E:33:LYS:HA	1:E:41:LYS:NZ	2.16	0.59
1:F:153:ALA:HB1	1:F:187:ILE:CD1	2.25	0.59
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.59
1:C:136:TYR:HB3	1:C:140:ASP:CB	2.32	0.59
1:E:393:SER:HB3	4:E:507[A]:NAD:PA	2.42	0.59
1:E:69:ASP:O	1:E:71:SER:N	2.35	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:E:360:PHE:HD2	1:E:365:ILE:HD12	1.66	0.59
1:C:421:PHE:N	1:C:421:PHE:CD2	2.70	0.59
1:C:276:SER:N	4:C:508:NAD:N3A	2.51	0.59
1:B:411:MET:HE2	1:B:415:GLU:HG3	1.84	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
1:C:195:HIS:CE1	1:E:87:THR:HG21	2.35	0.59
1:F:33:LYS:HA	1:F:41:LYS:NZ	2.16	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:N	1:F:421:PHE:CD2	2.70	0.59
1:A:459:ARG:NH2	4:F:508[B]:NAD:H6N	2.18	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: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:258:HIS:HD2	1:B:261:ARG:NH1	2.00	0.59
1:D:411:MET:HE2	1:D:415:GLU:HG3	1.83	0.59
1:D:421:PHE:N	1:D:421:PHE:CD2	2.70	0.59
1:D:276:SER:N	4:D:508:NAD:N3A	2.51	0.59
1:B:74:VAL:CG2	1:E:51:ILE:HA	2.32	0.59
1:A:238:MET:SD	1:A:342:LYS:CB	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.38	0.58
1:B:391:HIS:HD2	4:B:507[A]:NAD:HO2N	1.46	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:D:142:GLU:CG	1:D:146:ARG:HD2	2.29	0.58
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.68	0.58
1:C:185:SER:HB2	1:E:500:PHE:HE2	1.68	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:B:260:MET:HE2	1:B:288:PRO:HG3	1.85	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: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
1:E:136:TYR:HB3	1:E:140:ASP:CB	2.32	0.58
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.69	0.58
1:F:136:TYR:HB3	1:F:140:ASP:CB	2.32	0.58
1:B:185:SER:HB2	1:F:500:PHE:HE2	1.69	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: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:51:ILE:HD11	1:E:72:TRP:HB3	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:MET:HE3	1:E:320:ASP:HB3	1.86	0.58
1:E:91:GLY:HA3	1:E:125:ALA:O	2.04	0.58
1:F:258:HIS:CD2	1:F:261:ARG:NH1	2.72	0.58
1:F:260:MET:HE2	1:F:288:PRO:HG3	1.86	0.58
4:B:507[B]:NAD:H6N	1:F:459:ARG:NH2	2.18	0.58
1:F:92:GLY:HA2	1:F:166:ALA:O	2.04	0.58
1:D:178:TRP:O	1:D:182:THR:HG23	2.03	0.58
1:D:66:ARG:HG2	1:D:70:GLY:O	2.04	0.58
1:B:238:MET:SD	1:B:342:LYS:CB	2.91	0.58
1:B:54:PRO:HG3	1:E:74:VAL:HG11	1.84	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:C:91:GLY:HA3	1:C:125:ALA:O	2.04	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
1:E:233:MET:HA	1:E:236:LEU:HB2	1.86	0.57
1:A:260:MET:HE2	1:A:288:PRO:HG3	1.84	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:250:GLN:O	1:B:325:ALA:HB3	2.05	0.57
1:B:219:VAL:HG22	1:B:373:LEU:CD1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:238:MET:HE3	1:D:320:ASP:HB3	1.87	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:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.57
1:C:37:THR:HG21	1:C:41:LYS:HE3	1.87	0.57
1:A:421:PHE:CD2	1:A:421:PHE:N	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:91:GLY:HA3	1:F:125:ALA:O	2.04	0.56
1:F:33:LYS:HD3	1:F:41:LYS:HZ3	1.69	0.56
1:B:139:GLU:OE2	1:B:143:LYS:HE3	2.05	0.56
1:B:41:LYS:O	1:B:45:VAL:HG23	2.05	0.56
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:250:GLN:O	1:E:325:ALA:HB3	2.05	0.56
1:E:37:THR:HG21	1:E:41:LYS:HE3	1.87	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:C:153:ALA:HB1	1:C:187:ILE:CD1	2.25	0.56
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.87	0.56
1:C:409:LEU:HD11	1:E:409:LEU:HD22	1.87	0.56
1:F:254:ASN:HB3	4:F:507:NAD:O2N	2.06	0.56
1:A:260:MET:HG2	1:A: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:VAL:O	1:C:118:VAL:HG12	2.06	0.56
1:C:29:VAL:HG13	1:C:41:LYS:HB3	1.87	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:411:MET:HE2	1:E:415:GLU:HG3	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:254:ASN:HB3	4:C:508:NAD:O2N	2.06	0.56
1:D:118:VAL:HG12	1:D:118:VAL:O	2.06	0.56
1:E:260:MET:HE2	1:E:288:PRO:HG3	1.88	0.56
1:A:142:GLU:HG2	1:A:146:ARG:CD	2.33	0.56
1:A:29:VAL:HG13	1:A:41:LYS:HB3	1.87	0.56
1:A:250:GLN:O	1:A:325:ALA:HB3	2.05	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: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: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: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:A:421:PHE:HD2	1:A:421:PHE:N	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:337:PRO:HD3	1:A:359:ILE:HD13	1.88	0.55
1:A:39:GLU:O	1:A:42:ARG:HB2	2.06	0.55
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.87	0.55
1:E:117:VAL:HG21	1:E:371:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:118:VAL:HG12	1:B:118:VAL:O	2.06	0.55
1:C:238:MET:HE3	1:C:320:ASP:HB3	1.88	0.55
1:E:118:VAL:HG12	1:E:118:VAL:O	2.06	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:B:420:LYS:HZ2	1:F:428:ILE:HG23	1.72	0.55
1:A:118:VAL:HG12	1:A:118:VAL:O	2.06	0.55
1:A:35:ARG:O	1:A:37:THR:HG22	2.07	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:HE3	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:112:THR:HG22	1:D:124:GLY:CA	2.32	0.55
1:D:29:VAL:HG13	1:D:41:LYS:HB3	1.88	0.55
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.41	0.55
1:A:46:ARG:CG	1:A:46:ARG:HH11	2.18	0.55
1:F:369:PRO:HG2	1:F:478:ARG:HA	1.89	0.55
1:A:436:PHE:CZ	1:F:409:LEU:HD12	2.42	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:D:33:LYS:HD3	1:D:41:LYS:HZ3	1.71	0.55
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.41	0.55
1:B:425:GLY:O	1:B:427:THR:N	2.40	0.55
1:B:39:GLU:O	1:B:42:ARG:HB2	2.06	0.55
1:B:46:ARG:CG	1:B:46:ARG:HH11	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:CG2	1:F:51:ILE:HA	2.37	0.55
1:E:236:LEU:HD13	1:E:342:LYS:HB3	1.88	0.55
1:E:39:GLU:O	1:E:42:ARG:HB2	2.06	0.55
1:E:425:GLY:O	1:E:427:THR:N	2.40	0.55
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.89	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: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:D:260:MET:HE2	1:D:288:PRO:HG3	1.89	0.54
1:F:24:VAL:HG11	1:F:483:VAL:HG13	1.89	0.54
1:F:337:PRO:HD3	1:F:359:ILE:HD13	1.88	0.54
1:F:35:ARG:O	1:F:37:THR:HG22	2.07	0.54
1:C:51:ILE:HD11	1:F:72:TRP:HB3	1.88	0.54
1:F:95:TYR:OH	1:F:145:THR:HG22	2.07	0.54
1:B:421:PHE:N	1:B:421:PHE:HD2	2.04	0.54
1:C:425:GLY:O	1:C:427:THR:N	2.40	0.54
1:C:19:ARG:HD2	1:C:479:THR:HG21	1.89	0.54
1:D:95:TYR:OH	1:D:145:THR:HG22	2.07	0.54
1:D:236:LEU:HD13	1:D:342:LYS:HB3	1.88	0.54
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.42	0.54
1:D:250:GLN:OE1	1:D:315:LEU:HD21	2.07	0.54
1:D:46:ARG:CG	1:D:46:ARG:HH11	2.18	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:H6N	4:B:507[A]:NAD:O5D	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: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:A:33:LYS:HD3	1:A:41:LYS:HZ3	1.71	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:260:MET:HE1	1:C:288:PRO:HA	1.89	0.54
1:C:35:ARG:O	1:C:37:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:GLN:OE1	1:F:315:LEU:HD21	2.07	0.54
1:F:29:VAL:HA	1:F:45:VAL:HG21	1.90	0.54
1:B:498:VAL:HB	1:E:72:TRP:CZ2	2.43	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:D:87:THR:O	1:D:89:CYS: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: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: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:310:TYR:CD1	1:C:311:GLU:N	2.75	0.54
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.05	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:B:55:CYS:O	1:E:62:SER:HB3	2.07	0.54
1:F:112:THR:HG22	1:F:124:GLY:CA	2.32	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
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:C:459:ARG:NH2	4:D:507[B]:NAD:C6N	2.71	0.54
1:F:34:THR:HG21	1:F:44:ARG:NH1	2.23	0.54
4:F:508[A]:NAD:O5D	4:F:508[A]:NAD:H6N	2.08	0.54
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.89	0.54
1:A:425:GLY:O	1:A:427:THR:N	2.40	0.54
1:A:34:THR:HG21	1:A:44:ARG:NH1	2.23	0.54
1:A:29:VAL:HA	1:A:45:VAL:HG21	1.90	0.54
4:A:507[B]:NAD:C6N	1:B:459:ARG:NH2	2.71	0.54
4:A:507[A]:NAD:O5D	4:A:507[A]:NAD:H6N	2.08	0.54
1:B:189:HIS:CD2	1:C:154:LYS:HD2	2.43	0.54
1:E:142:GLU:HG2	1:E:146:ARG:CD	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:GLY:N	1:E:309:ILE:HD11	2.23	0.54
1:E:35:ARG:O	1:E:37:THR:HG22	2.07	0.54
1:E:19:ARG:HD2	1:E:479:THR:HG21	1.89	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:F:421:PHE:N	1:F:421:PHE:HD2	2.04	0.54
1:F:87:THR:O	1:F:89:CYS:N	2.40	0.54
1:A:95:TYR:OH	1:A:145:THR:HG22	2.07	0.54
1:B:236:LEU:CD1	1:B:342:LYS:HB3	2.38	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: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: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
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.26	0.53
1:E:5:ASP:HB2	1:E:333:LYS:HE2	1.90	0.53
1:E:462:ARG:HE	1:E:466:ARG:NH2	2.06	0.53
1:E:95:TYR:OH	1:E:145:THR:HG22	2.07	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: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: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
1:B:19:ARG:HD2	1:B:479:THR:HG21	1.89	0.53
1:C:239:THR:HG23	1:C:240:PRO:N	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:E:391:HIS:C	4:E:507[A]:NAD:H4D	2.28	0.53
1:F:236:LEU:CD1	1:F:342:LYS:HB3	2.38	0.53
4:B:507[B]:NAD:N3A	1:F:488:LYS:HB3	2.23	0.53
1:A:189:HIS:CD2	1:E:154:LYS:HD2	2.43	0.53
1:B:238:MET:HE3	1:B:320:ASP:HB3	1.89	0.53
1:B:447:ASP:O	1:B:451:SER:HB3	2.08	0.53
1:C:236:LEU:CD1	1:C:342:LYS:HB3	2.38	0.53
1:C:34:THR:HG21	1:C:44:ARG:NH1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:HIS:CE1	1:F:87:THR:HG21	2.39	0.53
1:A:107:LEU:HB3	1:A:126:LYS:CG	2.30	0.53
1:A:17:PHE:HA	1:A:482:TYR:HD2	1.73	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: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:A:499:THR:CG2	1:D:64:PRO:HG2	2.39	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:117:VAL:HG23	1:B:485:ALA:HB2	1.91	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:C:447:ASP:O	1:C:451:SER:HB3	2.08	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:201:LYS:NZ	1:D:388:ASN:HD21	2.06	0.53
1:D:34:THR:HG21	1:D:44:ARG:NH1	2.23	0.53
1:D:447:ASP:O	1:D:451:SER:HB3	2.08	0.53
1:D:29:VAL:HA	1:D:45:VAL:HG21	1.90	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:B:33:LYS:HD3	1:B:41:LYS:HZ3	1.74	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:274:GLY:CA	1:D:314:ILE:HG13	2.39	0.53
1:D:5:ASP:HB2	1:D:333:LYS:HE2	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ASN:HD22	1:C:84:HIS:CD2	2.27	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: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:D:488:LYS:HB3	4:E:507[B]:NAD:N3A	2.23	0.53
1:F:310:TYR:CD1	1:F:311:GLU:N	2.75	0.53
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.74	0.53
1:F:462:ARG:HE	1:F:466:ARG:NH2	2.07	0.53
1:F:56:ASN:HD22	1:F:84:HIS:CD2	2.27	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
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:488:LYS:HB3	4:F:508[B]:NAD:N3A	2.23	0.53
1:A:9:PHE:CE1	1:A:107:LEU:HD13	2.34	0.53
1:A:5:ASP:HB2	1:A:333:LYS:HE2	1.90	0.53
1:A:19:ARG:NH2	1:A:478:ARG:HD2	2.24	0.53
1:B:360:PHE:CD2	1:B:365:ILE:HD12	2.44	0.53
1:B:340:LYS:N	1:B:363:ARG:HH22	2.05	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:319:CYS:O	1:E:341:ALA:HA	2.09	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: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:200:GLY:HA2	1:C:211:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HA	1:C:45:VAL:HG21	1.90	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:117:VAL:HG23	1:C:485:ALA:HB2	1.91	0.52
1:C:260:MET:HE2	1:C:288:PRO:HG3	1.90	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
1:C:46:ARG:HH11	1:C:46:ARG:CG	2.18	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
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:258:HIS:HA	1:C:261:ARG:HB2	1.91	0.52
1:C:303:GLY:N	1:C:309:ILE:HD11	2.23	0.52
1:C:48:ILE:O	1:C:52:ILE:HG13	2.09	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:117:VAL:HG23	1:E:485:ALA:HB2	1.91	0.52
1:E:34:THR:HG21	1:E:44:ARG:NH1	2.23	0.52
1:F:19:ARG:HD2	1:F:479:THR:HG21	1.89	0.52
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.36	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:A:56:ASN:HD22	1:A:84:HIS:CD2	2.27	0.52
1:C:5:ASP:HB2	1:C:333:LYS:HE2	1.90	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:D:87:THR:HG23	1:E:195:HIS:CE1	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:ALA:O	1:C:111:MET:HB2	2.09	0.52
1:C:66:ARG:NH1	1:C:70:GLY:HA2	2.25	0.52
1:D:246:THR:N	1:D:320:ASP:OD1	2.43	0.52
1:D:56:ASN:HD22	1:D:84:HIS:CD2	2.27	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
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.26	0.52
1:A:66:ARG:NH1	1:A:70:GLY:HA2	2.25	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:117:VAL:HG23	1:D:485:ALA:HB2	1.91	0.52
1:D:48:ILE:O	1:D:52:ILE:HG13	2.09	0.52
1:E:260:MET:HE1	1:E:288:PRO:HA	1.92	0.52
1:E:33:LYS:HD3	1:E:41:LYS:HZ3	1.74	0.52
1:F:319:CYS:O	1:F:341:ALA:HA	2.09	0.52
1:F:48:ILE:O	1:F:52:ILE:HG13	2.09	0.52
1:A:200:GLY:HA2	1:A:211:ARG:HD3	1.91	0.52
1:A:238:MET:HE2	1:A:245:LYS:HE2	1.92	0.52
1:A:117:VAL:HG23	1:A:485:ALA:HB2	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:413:VAL:O	1:E:417:LEU:HG	2.10	0.52
1:E:66:ARG:NH1	1:E:70:GLY:HA2	2.25	0.52
1:F:46:ARG:CG	1:F:46:ARG:HH11	2.18	0.52
1:F:44:ARG:CZ	1:F:494:ASN:HD21	2.23	0.52
1:F:66:ARG:NH1	1:F:70:GLY:HA2	2.25	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: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:B:108:ALA:O	1:B:111:MET:HB2	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:HA	1:A:43:ASN:HD22	1.74	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:B:48:ILE:O	1:B:52:ILE:HG13	2.09	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:246:THR:N	1:F:320:ASP:OD1	2.43	0.52
1:F:117:VAL:HG23	1:F:485:ALA:HB2	1.91	0.52
1:A:360:PHE:CD2	1:A:365:ILE:HD12	2.44	0.51
1:A:211:ARG:HG2	1:A:380:VAL:HG12	1.93	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:334:SER:O	1:C:338:ARG:NH2	2.43	0.51
1:C:44:ARG:NH1	1:C:494:ASN:HD21	2.08	0.51
1:E:200:GLY:HA2	1:E:211:ARG:HD3	1.91	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:C:282:ASN:HD21	1:C:284:ASP:HB2	1.74	0.51
1:C:252:PHE:HD2	1:C:295:LYS:HE3	1.76	0.51
1:C:44:ARG:CZ	1:C:494:ASN:HD21	2.23	0.51
1:D:260:MET:HE1	1:D:288:PRO:HA	1.90	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:B:138:ASP:HA	1:B:141:LEU:HD12	1.93	0.51
1:B:19:ARG:NH2	1:B:478:ARG:HD2	2.24	0.51
1:B:310:TYR:CD1	1:B:311:GLU:N	2.75	0.51
1:B:40:GLN:HA	1:B:43:ASN:HD22	1.74	0.51
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.71	0.51
1:D:348:ALA:HB3	1:D:351:PRO:HG3	1.91	0.51
1:D:44:ARG:NH1	1:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ARG:NH1	1:E:494:ASN:HD21	2.08	0.51
1:A:146:ARG:HE	1:A:182:THR:HG22	1.76	0.51
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: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: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:B:190:TYR:CE2	1:F:162:VAL:HG11	2.45	0.51
1:F:489:VAL:O	1:F:493:TYR:HD1	1.94	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:A:195:HIS:HE1	1:B:87:THR:HG21	1.72	0.51
1:C:319:CYS:O	1:C:341:ALA:HA	2.09	0.51
1:C:211:ARG:HG2	1:C:380:VAL:HG12	1.93	0.51
1:C:421:PHE:HE1	1:E:421:PHE:HE1	1.59	0.51
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.74	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:D:66:ARG:NH1	1:D:70:GLY:HA2	2.25	0.51
1:E:334:SER:O	1:E:338:ARG:NH2	2.43	0.51
1:E:66:ARG:HG3	1:E:72:TRP:CE2	2.46	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: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:310:TYR:CD1	1:E:311:GLU:N	2.75	0.51
1:E:59:LEU:CD2	1:E:61:LEU:HD11	2.41	0.51
1:F:339:VAL:H	1:F:363:ARG:NH2	2.08	0.51
1:F:211:ARG:HG2	1:F:380:VAL:HG12	1.93	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:A:138:ASP:HA	1:A:141:LEU:HD12	1.93	0.51
1:B:421:PHE:CE1	1:F:421:PHE:CE1	2.99	0.51
1:B:74:VAL:HG11	1:E:54:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:316:GLU:CD	1:F:338:ARG:HH11	2.14	0.51
1:A:210:GLY:O	1:A:214:ALA:HB2	2.11	0.51
1:A:59:LEU:CD2	1:A:61:LEU:HD11	2.41	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: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:C:316:GLU:CD	1:C:338:ARG:HH11	2.14	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:211:ARG:HG2	1:B:380:VAL:HG12	1.93	0.51
1:B:416:SER:HB3	1:F:430:ILE:CD1	2.41	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: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:A:316:GLU:CD	1:A:338:ARG:HH11	2.14	0.50
1:C:393:SER:HB3	4:C:507[B]:NAD:PA	2.51	0.50
1:D:59:LEU:CD2	1:D:61:LEU:HD11	2.41	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
1:E:44:ARG:CZ	1:E:494:ASN:HD21	2.23	0.50
4:C:507[B]:NAD:C6N	1:E:459:ARG:HH21	2.24	0.50
1:E:489:VAL:O	1:E:493:TYR:HD1	1.94	0.50
1:E:61:LEU:HD23	1:E:151:GLU:HB3	1.93	0.50
1:F:252:PHE:HD2	1:F:295:LYS:HE3	1.76	0.50
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.46	0.50
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:333:LYS:HB2	1:E:355:GLN:HB3	1.93	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:A:417:LEU:CD1	1:F:417:LEU:HD21	2.40	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:D:146:ARG:HE	1:D:182:THR:HG22	1.76	0.50
1:D:316:GLU:CD	1:D:338:ARG:HH11	2.15	0.50
1:D:346:GLU:HB3	1:D:370:ASP:HB3	1.93	0.50
1:D:44:ARG:CZ	1:D:494:ASN:HD21	2.23	0.50
1:F:260:MET:HE1	1:F:288:PRO:HA	1.94	0.50
1:A:489:VAL:O	1:A:493:TYR:HD1	1.94	0.50
1:C:66:ARG:HG3	1:C:72:TRP:CE2	2.46	0.50
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.31	0.50
1:D:66:ARG:HG3	1:D:72:TRP:CE2	2.46	0.50
1:E:252:PHE:HD2	1:E:295:LYS:HE3	1.76	0.50
1:E:316:GLU:CD	1:E:338:ARG:HH11	2.14	0.50
1:F:443:ALA:HB1	1:F:447:ASP:HB2	1.94	0.50
4:B:507[B]:NAD:C6N	1:F:459:ARG:HH21	2.24	0.50
1:B:443:ALA:HB1	1:B:447:ASP:HB2	1.94	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:A:459:ARG:HH21	4:F:508[B]:NAD:C6N	2.24	0.50
1:F:66:ARG:HG3	1:F:72:TRP:CE2	2.46	0.50
1:C:333:LYS:HB2	1:C:355:GLN:HB3	1.93	0.50
1:C:90:LYS:HD2	1:C:122:PHE:CE1	2.46	0.50
1:D:459:ARG:HH21	4:E:507[B]:NAD:C6N	2.24	0.50
1:D:61:LEU:HD23	1:D:151:GLU:HB3	1.93	0.50
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLY:HA3	1:D:373:LEU:HD23	1.94	0.50
1:E:222:GLY:HA3	1:E:373:LEU:HD23	1.94	0.50
1:E:211:ARG:HG2	1:E:380:VAL:HG12	1.92	0.50
1:E:17:PHE:HA	1:E:482:TYR:HD2	1.73	0.50
1:A:94:ARG:HE	1:A:168:ASN:ND2	2.10	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:A:14:GLU:O	1:A:17:PHE:HB3	2.12	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:B:316:GLU:CD	1:B:338:ARG:HH11	2.14	0.50
1:B:61:LEU:HD23	1:B:151:GLU:HB3	1.93	0.50
1:C:61:LEU:HD23	1:C:151:GLU:HB3	1.93	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:281:TRP:CH2	1:C:283:PRO:HG3	2.47	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
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:281:TRP:CH2	1:A:283:PRO:HG3	2.48	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:B:112:THR:HG22	1:B:124:GLY:CA	2.32	0.49
1:C:210:GLY:O	1:C:214:ALA:HB2	2.11	0.49
1:C:61:LEU:HD12	1:C:61:LEU:N	2.27	0.49
1:D:248:ALA:O	1:D:322:LEU:HD12	2.12	0.49
1:E:457:MET:CE	1:E:457:MET:HA	2.42	0.49
1:F:281:TRP:CH2	1:F:283:PRO:HG3	2.48	0.49
1:F:38:GLN:OE1	1:F:40:GLN:HB2	2.12	0.49
1:C:51:ILE:HA	1:F:74:VAL:CG2	2.42	0.49
1:B:107:LEU:CB	1:B:126:LYS:HG2	2.31	0.49
4:A:507[B]:NAD:C6N	1:B:459:ARG:HH21	2.24	0.49
1:B:462:ARG:NH2	1:B:466:ARG:HH22	2.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.93	0.49
1:D:93:ILE:HD11	1:D:165:PRO:HB3	1.94	0.49
1:E:93:ILE:HD11	1:E:165:PRO:HB3	1.94	0.49
1:F:391:HIS:C	4:F:508[A]:NAD:H4D	2.33	0.49
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.93	0.49
1:A:87:THR:O	1:A:88:PRO:C	2.50	0.49
1:B:222:GLY:HA3	1:B:373:LEU:CD2	2.42	0.49
1:D:211:ARG:HG2	1:D:380:VAL:HG12	1.93	0.49
1:D:94:ARG:HE	1:D:168:ASN:ND2	2.10	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: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:94:ARG:CZ	1:E:107:LEU:HD21	2.42	0.49
1:E:46:ARG:HH11	1:E:46:ARG:CG	2.18	0.49
1:F:344:ILE:HD12	1:F:367:VAL:HG22	1.95	0.49
1:F:93:ILE:HD11	1:F:165:PRO:HB3	1.94	0.49
1:B:2:ASP:OD2	1:B:5:ASP:HB3	2.13	0.49
1:B:315:LEU:HD11	1:B:330:GLN:HB3	1.93	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
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: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: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: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: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:F:138:ASP:HA	1:F:141:LEU:HD12	1.93	0.49
1:B:253:GLY:HA3	4:B:508:NAD:H4B	1.95	0.49
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.94	0.49
1:C:38:GLN:OE1	1:C:40:GLN:HB2	2.12	0.49
1:D:315:LEU:HD11	1:D:330:GLN:HB3	1.93	0.49
1:D:61:LEU:HD12	1:D:61:LEU:N	2.27	0.49
1:E:14:GLU:O	1:E:17:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:ILE:HD12	1:E:367:VAL:HG22	1.95	0.49
1:F:14:GLU:O	1:F:17:PHE:HB3	2.12	0.49
1:F:2:ASP:OD2	1:F:5:ASP:HB3	2.13	0.49
1:A:64:PRO:HG2	1:D:499:THR:CG2	2.37	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:F:87:THR:O	1:F:88:PRO:C	2.50	0.49
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.31	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:87:THR:O	1:D:88:PRO:C	2.50	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:331:LEU:HD12	1:E:352:THR:HG22	1.95	0.49
1:E:61:LEU:HD12	1:E:61:LEU:N	2.27	0.49
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.13	0.49
1:F:61:LEU:HD12	1:F:61:LEU:N	2.27	0.49
1:A:61:LEU:HD12	1:A:61:LEU:N	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:D:38:GLN:OE1	1:D:40:GLN:HB2	2.12	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:303:GLY:N	1:A:309:ILE:HD11	2.23	0.48
1:A:222:GLY:HA3	1:A:373:LEU:HD23	1.94	0.48
1:A:61:LEU:HD23	1:A:151:GLU:HB3	1.93	0.48
1:B:93:ILE:HD11	1:B:165:PRO:HB3	1.94	0.48
1:B:260:MET:HE1	1:B:288:PRO:HA	1.95	0.48
1:B:248:ALA:O	1:B:322:LEU:HD12	2.12	0.48
1:C:222:GLY:HA3	1:C:373:LEU:CD2	2.42	0.48
1:C:2:ASP:OD2	1:C:5:ASP:HB3	2.13	0.48
1:C:93:ILE:HD11	1:C:165:PRO:HB3	1.94	0.48
1:D:391:HIS:C	4:D:507[A]:NAD:H4D	2.33	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:B:87:THR:O	1:B:88:PRO:C	2.50	0.48
1:C:150:MET:SD	1:C:186:THR:HG21	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:253:GLY:HA3	4:C:508:NAD:H4B	1.95	0.48
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.13	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:443:ALA:HB1	1:A:447:ASP:HB2	1.94	0.48
1:A:457:MET:CE	1:A:457:MET:HA	2.42	0.48
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.13	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:222:GLY:HA3	1:D:373:LEU:CD2	2.42	0.48
1:D:443:ALA:HB1	1:D:447:ASP:HB2	1.94	0.48
1:D:59:LEU:HD23	1:D:61:LEU:HD11	1.96	0.48
1:E:443:ALA:HB1	1:E:447:ASP:HB2	1.94	0.48
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.13	0.48
1:B:275:GLU:HA	1:B:275:GLU:OE1	2.14	0.48
1:B:331:LEU:HD12	1:B:352:THR:HG22	1.95	0.48
1:C:94:ARG:HE	1:C:168:ASN:ND2	2.10	0.48
1:C:74:VAL:HG11	1:F:54:PRO:HG3	1.96	0.48
1:D:289:LYS:HG2	1:D:293:ASP:OD1	2.13	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:B:344:ILE:HD12	1:B:367:VAL:HG22	1.95	0.48
1:B:59:LEU:HD23	1:B:61:LEU:HD11	1.96	0.48
1:D:344:ILE:HD12	1:D:367:VAL:HG22	1.95	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:N	1:A:136:TYR:CD1	2.82	0.48
1:A:150:MET:SD	1:A:186:THR:HG21	2.53	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:B:61:LEU:HD12	1:B:61:LEU:N	2.27	0.48
1:C:136:TYR:CD1	1:C:136:TYR:N	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:HA	1:D:275:GLU:OE1	2.14	0.48
1:D:340:LYS:N	1:D:363:ARG:HH22	2.05	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:344:ILE:CG2	1:C:367:VAL:HG13	2.44	0.48
1:C:428:ILE:HG23	1:D:420:LYS:HZ2	1.78	0.48
1:C:59:LEU:HD23	1:C:61:LEU:HD11	1.96	0.48
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: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:B:136:TYR:CD1	1:B:136:TYR:N	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:93:ILE:HG12	1:F:127:ALA:HB3	1.96	0.48
1:F:17:PHE:HA	1:F:482:TYR:HD2	1.73	0.48
1:A:456:THR:HG21	1:F:396:ARG:HE	1.78	0.48
1:A:253:GLY:HA3	4:A:508:NAD:H4B	1.95	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:B:435:GLU:CD	1:B:435:GLU:H	2.18	0.47
1:C:275:GLU:HA	1:C:275:GLU:OE1	2.14	0.47
1:C:435:GLU:H	1:C:435:GLU:CD	2.18	0.47
1:C:87:THR:O	1:C:88:PRO:C	2.50	0.47
1:D:150:MET:SD	1:D:186:THR:HG21	2.53	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:HB3	1:E:333:LYS:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HD12	1:A:352:THR:HG22	1.95	0.47
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.45	0.47
1:E:353:THR:HG22	1:E:355:GLN:H	1.79	0.47
1:B:72:TRP:CH2	1:E:499:THR:HG22	2.49	0.47
1:A:369:PRO:CG	1:A:478:ARG:HA	2.44	0.47
1:B:333:LYS:HB3	1:B:333:LYS:HE2	1.65	0.47
1:C:107:LEU:HB3	1:C:126:LYS:CG	2.29	0.47
1:C:344:ILE:HD12	1:C:367:VAL:HG22	1.95	0.47
1:D:252:PHE:CE1	1:D:291:LEU:HD13	2.49	0.47
1:E:252:PHE:CE1	1:E:291:LEU:HD13	2.49	0.47
1:E:59:LEU:HD23	1:E:61:LEU:HD11	1.96	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:252:PHE:CE1	1:F:291:LEU:HD13	2.49	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:D:250:GLN:CD	1:D:315:LEU:HD21	2.35	0.47
1:E:275:GLU:HA	1:E:275:GLU:OE1	2.14	0.47
1:F:275:GLU:HA	1:F:275:GLU:OE1	2.14	0.47
1:F:344:ILE:CG2	1:F:367:VAL:HG13	2.44	0.47
1:F:457:MET:HA	1:F:457:MET:CE	2.42	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:D:136:TYR:CD1	1:D:136:TYR:N	2.82	0.47
1:C:456:THR:HG21	1:D:396:ARG:HE	1.80	0.47
1:E:82:HIS:CG	1:E:112:THR:HG21	2.48	0.47
1:A:275:GLU:HA	1:A:275:GLU:OE1	2.14	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:470:LYS:HE3	1:D:471:TYR:OH	2.15	0.47
1:D:393:SER:HB3	4:D:507[B]:NAD:PA	2.54	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:E:250:GLN:CD	1:E:315:LEU:HD21	2.35	0.47
1:A:252:PHE:CE1	1:A:291:LEU:HD13	2.49	0.47
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:282:ASN:C	1:B:282:ASN:ND2	2.68	0.47
1:B:313:SER:CB	1:B:316:GLU:HB2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LYS:HE3	1:B:471:TYR:CZ	2.50	0.47
1:C:33:LYS:HD3	1:C:41:LYS:NZ	2.30	0.47
1:C:393:SER:HB3	4:C:507[A]:NAD:O3	2.15	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: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:257:LEU:O	1:E:260:MET:HB3	2.14	0.47
1:E:343:ILE:HG12	1:E:366:MET:HE2	1.96	0.47
1:C:417:LEU:CD2	1:E:417:LEU:CD1	2.91	0.47
1:B:470:LYS:HE3	1:B:471:TYR:OH	2.15	0.47
1:C:333:LYS:HB3	1:C:333:LYS:HE2	1.65	0.47
1:C:350:GLY:N	1:C:351:PRO:HD3	2.29	0.47
1:D:257:LEU:O	1:D:260:MET:HB3	2.14	0.47
1:E:136:TYR:N	1:E:136:TYR:CD1	2.82	0.47
1:E:435:GLU:H	1:E:435:GLU:CD	2.18	0.47
1:E:381:SER:OG	3:E:506:AKG:O3	2.24	0.47
1:E:253:GLY:HA3	4:E:508:NAD:H4B	1.95	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: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:D:435:GLU:CD	1:D:435:GLU:H	2.18	0.47
1:E:282:ASN:C	1:E:282:ASN:ND2	2.68	0.47
1:A:313:SER:CB	1:A:316:GLU:HB2	2.42	0.47
1:A:33:LYS:HD3	1:A:41:LYS:NZ	2.30	0.47
1:A:469:MET:O	1:A:471:TYR:N	2.47	0.47
1:A:51:ILE:HA	1:D:74:VAL:CG2	2.45	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:B:250:GLN:CD	1:B:315:LEU:HD21	2.35	0.47
1:B:72:TRP:HZ3	1:E:499:THR:CG2	2.21	0.47
1:C:72:TRP:CZ2	1:F:498:VAL:HB	2.49	0.47
1:D:33:LYS:HD3	1:D:41:LYS:NZ	2.30	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:A:250:GLN:CD	1:A:315:LEU:HD21	2.35	0.47
1:A:53:LYS:O	1:A:82:HIS:HE1	1.98	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:B:64:PRO:HG2	1:E:499:THR:CB	2.45	0.47
1:F:246:THR:HG22	1:F:320:ASP:H	1.80	0.47
1:F:435:GLU:H	1:F:435:GLU:CD	2.18	0.47
1:A:169:MET:HE1	1:A:327:SER:HA	1.96	0.46
1:A:353:THR:HG22	1:A:355:GLN:H	1.79	0.46
1:B:174:ARG:NE	1:B:178:TRP:CH2	2.83	0.46
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.50	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:E:411:MET:HE3	1:E:415:GLU:HG3	1.97	0.46
1:F:220:PHE:HZ	1:F:266:PHE:CD2	2.33	0.46
1:F:250:GLN:CD	1:F:315:LEU:HD21	2.35	0.46
1:F:331:LEU:CD1	1:F:344:ILE:HD13	2.46	0.46
1:F:53:LYS:O	1:F:82:HIS:HE1	1.98	0.46
1:A:435:GLU:H	1:A:435:GLU:CD	2.18	0.46
1:A:489:VAL:HG12	1:A:489:VAL:O	2.15	0.46
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.96	0.46
1:D:406:ASN:HA	1:D:406:ASN:HD22	1.60	0.46
1:D:432:PRO:CB	1:D:436:PHE:HD2	2.28	0.46
1:D:457:MET:HA	1:D:457:MET:CE	2.42	0.46
1:D:53:LYS:O	1:D:82:HIS:HE1	1.98	0.46
1:E:40:GLN:HE21	1:E:40:GLN:HA	1.79	0.46
1:E:470:LYS:HE3	1:E:471:TYR:CZ	2.50	0.46
1:F:282:ASN:C	1:F:282:ASN:ND2	2.68	0.46
1:F:470:LYS:HE3	1:F:471:TYR:CZ	2.50	0.46
1:F:393:SER:HB3	4:F:508[B]:NAD:PA	2.55	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:A:260:MET:HE1	1:A:288:PRO:HA	1.96	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:331:LEU:HD22	1:F:339:VAL:HG11	1.98	0.46
1:F:33:LYS:HD3	1:F:41:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:NE	1:A:178:TRP:CH2	2.84	0.46
1:A:500:PHE:O	1:A:500:PHE:HD1	1.99	0.46
1:A:416:SER:HB3	1:B:430:ILE:HA	1.97	0.46
1:B:489:VAL:HG12	1:B:489:VAL:O	2.15	0.46
1:C:282:ASN:C	1:C:282:ASN:ND2	2.68	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
1:D:255:VAL:HG11	4:D:508:NAD:O4D	2.16	0.46
1:E:500:PHE:HD1	1:E:500:PHE:O	1.99	0.46
1:E:84:HIS:C	1:E:86:ARG:N	2.69	0.46
1:E:87:THR:O	1:E:88:PRO:C	2.50	0.46
1:F:470:LYS:HE3	1:F:471:TYR:OH	2.15	0.46
1:F:500:PHE:HD1	1:F:500:PHE:O	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:246:THR:HG22	1:B:320:ASP:H	1.80	0.46
1:B:33:LYS:HD3	1:B:33:LYS:HA	1.72	0.46
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.96	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:C:396:ARG:HE	1:E:456:THR:HG21	1.80	0.46
1:E:255:VAL:HG11	4:E:508:NAD:O4D	2.16	0.46
1:E:53:LYS:O	1:E:82:HIS:HE1	1.98	0.46
1:F:40:GLN:HA	1:F:40:GLN:HE21	1.79	0.46
1:F:489:VAL:HG12	1:F:489:VAL:O	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:A:282:ASN:C	1:A:282:ASN:ND2	2.68	0.46
1:A:84:HIS:C	1:A:86:ARG:N	2.69	0.46
1:C:238:MET:SD	1:C:342:LYS:HB2	2.56	0.46
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.71	0.46
1:D:9:PHE:CZ	1:D:328:GLU:HG2	2.51	0.46
1:D:331:LEU:HD22	1:D:339:VAL:HG11	1.98	0.46
1:D:84:HIS:C	1:D:86:ARG:N	2.69	0.46
1:E:315:LEU:HA	1:E:322:LEU:HD21	1.98	0.46
1:E:38:GLN:HB2	1:E:39:GLU:H	1.59	0.46
1:F:255:VAL:HG11	4:F:507:NAD:O4D	2.16	0.46
1:B:417:LEU:HD22	1:F:417:LEU:HD13	1.98	0.46
1:A:331:LEU:CD1	1:A:344:ILE:HD13	2.46	0.46
1:A:238:MET:SD	1:A:342:LYS:HB2	2.56	0.46
1:C:155:LYS:HD2	1:F:157:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PHE:CZ	1:C:328:GLU:HG2	2.51	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:331:LEU:CD1	1:B:344:ILE:HD13	2.46	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:C:82:HIS:CG	1:C:112:THR:HG21	2.48	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:D:282:ASN:HD21	1:D:284:ASP:CB	2.29	0.46
1:D:90:LYS:HD2	1:D:122:PHE:CD1	2.51	0.46
1:E:246:THR:HG22	1:E:320:ASP:H	1.80	0.46
1:E:33:LYS:HD3	1:E:41:LYS:NZ	2.30	0.46
1:F:90:LYS:HD2	1:F:122:PHE:CD1	2.51	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:169:MET:HE1	1:E:327:SER:HA	1.98	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:B:498:VAL:HB	1:E:72:TRP:CH2	2.51	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:B:61:LEU:HD23	1:B:151:GLU:CB	2.46	0.46
1:B:53:LYS:O	1:B:82:HIS:HE1	1.98	0.46
1:C:250:GLN:CD	1:C:315:LEU:HD21	2.35	0.46
1:A:500:PHE:CD1	1:D:147:ARG:NH1	2.84	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:282:ASN:HD21	1:A:284:ASP:CB	2.29	0.45
1:A:61:LEU:HD23	1:A:151:GLU:CB	2.46	0.45
1:B:500:PHE:HD1	1:B:500:PHE:O	1.99	0.45
1:B:255:VAL:HG11	4:B:508:NAD:O4D	2.16	0.45
1:C:255:VAL:HG11	4:C:508:NAD:O4D	2.16	0.45
1:C:84:HIS:C	1:C:86:ARG:N	2.69	0.45
1:D:10:PHE:O	1:D:14:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LEU:HA	1:D:322:LEU:HD21	1.98	0.45
1:D:40:GLN:HE21	1:D:40:GLN:HA	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: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:C:61:LEU:HD23	1:C:151:GLU:CB	2.46	0.45
1:C:489:VAL:HG12	1:C:489:VAL:O	2.15	0.45
1:C:90:LYS:HD2	1:C:122:PHE:CD1	2.51	0.45
1:E:379:THR:HG22	1:E:383:PHE:CZ	2.52	0.45
1:E:61:LEU:HD23	1:E:151:GLU:CB	2.46	0.45
1:E:8:ASN:OD1	1:E:11:LYS:HG3	2.16	0.45
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.98	0.45
1:A:336:ALA:O	1:A:339:VAL:HG13	2.16	0.45
1:B:331:LEU:HD22	1:B:339:VAL:HG11	1.98	0.45
1:B:84:HIS:C	1:B:86:ARG:N	2.69	0.45
1:C:282:ASN:ND2	1:C:284:ASP:N	2.60	0.45
1:C:495:GLU:OE1	1:D:204:SER:OG	2.11	0.45
1:E:168:ASN:ND2	1:E:169:MET:H	2.14	0.45
1:E:230:ALA:O	1:E:231:SER:C	2.55	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:443:ALA:HB2	1:F:401:TYR:CD2	2.51	0.45
1:F:84:HIS:C	1:F:86:ARG:N	2.69	0.45
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.99	0.45
1:A:8:ASN:OD1	1:A:11:LYS:HG3	2.16	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:A:90:LYS:HD2	1:A:122:PHE:CD1	2.51	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: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:HG12	1:D:489:VAL:O	2.15	0.45
1:E:336:ALA:O	1:E:339:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:PHE:CZ	1:F:328:GLU:HG2	2.51	0.45
1:A:230:ALA:O	1:A:231:SER:C	2.55	0.45
1:A:281:TRP:O	1:A:282:ASN:C	2.55	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:185:SER:HB2	1:F:500:PHE:CE2	2.51	0.45
1:B:230:ALA:O	1:B:231:SER:C	2.55	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:336:ALA:O	1:D:339:VAL:HG13	2.16	0.45
1:D:500:PHE:HD1	1:D:500:PHE:O	1.99	0.45
1:D:8:ASN:OD1	1:D:11:LYS:HG3	2.17	0.45
1:E:281:TRP:O	1:E:282:ASN:C	2.55	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:F:230:ALA:O	1:F:231:SER:C	2.55	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:C:362:GLU:C	1:C:364:ASN:H	2.20	0.45
1:B:336:ALA:O	1:B:339:VAL:HG13	2.16	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:C:230:ALA:O	1:C:231:SER:C	2.55	0.45
1:C:246:THR:HG22	1:C:320:ASP:H	1.80	0.45
1:C:281:TRP:O	1:C:282:ASN:C	2.55	0.45
1:C:370:ASP:HB2	1:C:374:ASN:ND2	2.20	0.45
1:D:230:ALA:O	1:D:231:SER:C	2.55	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:HG12	1:E:489:VAL:O	2.15	0.45
1:F:379:THR:HG22	1:F:383:PHE:CZ	2.52	0.45
1:B:416:SER:HB3	1:F:430:ILE:HD13	1.99	0.45
1:A:263:LEU:HD23	1:A:263:LEU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:401:TYR:CG	1:F:443:ALA:HB2	2.51	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:362:GLU:C	1:B:364:ASN:N	2.71	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
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: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: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:362:GLU:C	1:C:364:ASN:N	2.71	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:D:4:GLU:O	1:D:5:ASP:CB	2.65	0.44
1:E:321:ILE:HG23	1:E:343:ILE:HG22	1.99	0.44
1:E:362:GLU:C	1:E:364:ASN:H	2.20	0.44
1:F:112:THR:HB	1:F:124:GLY:H	1.82	0.44
1:F:377:GLY:O	1:F:381:SER:HB2	2.17	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:111:MET:HE2	1:B:111:MET:HB3	1.76	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: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:C:10:PHE:O	1:C:14:GLU:HB2	2.16	0.44
1:C:313:SER:CB	1:C:316:GLU:HB2	2.42	0.44
1:C:331:LEU:HD22	1:C:339:VAL:HG11	1.98	0.44
1:C:321:ILE:HG23	1:C:343:ILE:HG22	1.99	0.44
1:D:486:ILE:O	1:D:490:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.99	0.44
1:F:386:LEU:HD12	1:F:386:LEU:HA	1.80	0.44
1:B:282:ASN:H	1:B:307:ALA:HB1	1.82	0.44
1:B:391:HIS:C	4:B:507[A]:NAD:H4D	2.38	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:D:111:MET:HE2	1:D:111:MET:HB3	1.72	0.44
1:E:263:LEU:HA	1:E:263:LEU:HD23	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:F:362:GLU:C	1:F:364:ASN:N	2.70	0.44
1:A:355:GLN:HA	1:A:355:GLN:OE1	2.18	0.44
1:A:4:GLU:O	1:A:5:ASP:CB	2.65	0.44
1:B:112:THR:HB	1:B:124:GLY:H	1.82	0.44
1:B:355:GLN:HA	1:B:355:GLN:OE1	2.18	0.44
1:C:115:CYS:HB3	1:C:120:VAL:O	2.17	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:C:232:TYR:CE2	1:C:465:MET:HG2	2.52	0.44
1:C:391:HIS:C	4:C:507[A]:NAD:H4D	2.38	0.44
1:C:87:THR:HG21	1:D:195:HIS:CE1	2.48	0.44
1:D:67:ARG:NH1	1:D:136:TYR:HA	2.32	0.44
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.52	0.44
1:D:227:ILE:HG13	1:D:233:MET:SD	2.58	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:79:ARG:HD2	1:E:127:ALA:HB2	2.00	0.44
1:E:4:GLU:O	1:E:5:ASP:CB	2.65	0.44
1:F:281:TRP:O	1:F:282:ASN:C	2.55	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:C:62:SER:HB3	1:F:55:CYS:O	2.17	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:A:362:GLU:C	1:A:364:ASN:N	2.71	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:B:362:GLU:C	1:B:364:ASN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:SER:HB2	1:E:500:PHE:CE2	2.51	0.44
4:C:508:NAD:N7N	4:C:508:NAD:O2N	2.47	0.44
1:C:67:ARG:HH12	1:C:136:TYR:HA	1.83	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:E:67:ARG:NH1	1:E:136:TYR:HA	2.32	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
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:486:ILE:O	1:B:490:PHE:HB2	2.18	0.44
1:C:336:ALA:O	1:C:339:VAL:HG13	2.16	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:D:227:ILE:HA	1:D:233:MET:SD	2.57	0.44
1:D:362:GLU:C	1:D:364:ASN:H	2.20	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: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: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:A:111:MET:HE2	1:A:111:MET:HB3	1.79	0.44
1:A:333:LYS:HB3	1:A:333:LYS:HE2	1.65	0.44
1:D:235:ILE:HG13	1:D:235:ILE:H	1.69	0.44
1:D:282:ASN:ND2	1:D:282:ASN:C	2.68	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:E:473:LEU:HD12	1:E:480:ALA:HB2	2.00	0.44
1:E:371:LEU:HG	1:E:482:TYR:CE1	2.53	0.44
1:F:432:PRO:CB	1:F:436:PHE:HD2	2.28	0.44
1:F:4:GLU:O	1:F:5:ASP:CB	2.65	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:A:391:HIS:C	4:A:507[A]:NAD:H4D	2.38	0.44
1:B:377:GLY:O	1:B:381:SER:HB2	2.17	0.44
1:C:172:GLY:H	1:C:175:GLU:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:362:GLU:C	1:E:364:ASN:N	2.71	0.44
1:E:219:VAL:HG13	1:E:373:LEU:HD11	2.00	0.44
1:F:111:MET:HE2	1:F:111:MET:HB3	1.71	0.44
1:F:362:GLU:C	1:F:364:ASN:H	2.20	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:C:294:PHE:CE2	1:C:298:HIS:CE1	3.06	0.44
1:C:200:GLY:H	1:C:384:GLN:NE2	2.16	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:281:TRP:O	1:D:282:ASN:C	2.55	0.43
1:D:79:ARG:HD2	1:D:127:ALA:HB2	2.00	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:354:PRO:O	1:B:357:ASP:HB2	2.18	0.43
1:B:219:VAL:HG13	1:B:373:LEU:HD11	2.00	0.43
1:B:67:ARG:HH12	1:B:136:TYR:HA	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:349:ASN:C	1:C:351:PRO:HD3	2.39	0.43
1:D:294:PHE:CE2	1:D:298:HIS:CE1	3.06	0.43
1:D:349:ASN:C	1:D:351:PRO:HD3	2.39	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:F:227:ILE:HA	1:F:233:MET:SD	2.57	0.43
1:F:200:GLY:H	1:F:384:GLN:NE2	2.16	0.43
1:F:79:ARG:HD2	1:F:127:ALA:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLY:H	1:B:175:GLU:HG2	1.83	0.43
1:B:281:TRP:O	1:B:282:ASN:C	2.55	0.43
1:C:146:ARG:NE	1:C:182:THR:HG22	2.33	0.43
1:C:355:GLN:OE1	1:C:355:GLN:HA	2.18	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: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:HA	1:D:355:GLN:OE1	2.18	0.43
1:D:362:GLU:C	1:D:364:ASN:N	2.71	0.43
1:D:500:PHE:HE2	1:E:185:SER:CB	2.29	0.43
4:C:507[A]:NAD:N6A	1:E:120:VAL:O	2.49	0.43
1:C:190:TYR:CE2	1:E:162:VAL:HG11	2.54	0.43
1:E:227:ILE:HG13	1:E:233:MET:SD	2.58	0.43
1:C:401:TYR:CG	1:E:443:ALA:HB2	2.53	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:F:25:GLU:OE1	1:F:46:ARG:NE	2.51	0.43
1:B:321:ILE:HG23	1:B:343:ILE:HG22	1.99	0.43
1:B:66:ARG:HG3	1:B:72:TRP:CD2	2.54	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:D:391:HIS:CD2	4:D:507[A]:NAD:HO2N	2.12	0.43
1:E:146:ARG:NE	1:E:182:THR:HG22	2.33	0.43
1:E:90:LYS:HZ3	1:E:164:VAL:HG12	1.83	0.43
1:E:94:ARG:HE	1:E:168:ASN:HD22	1.66	0.43
1:F:349:ASN:C	1:F:351:PRO:HD3	2.39	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:473:LEU:HD12	1:A:480:ALA:HB2	2.00	0.43
1:A:396:ARG:HE	1:B:456:THR:HG21	1.83	0.43
1:C:473:LEU:HD12	1:C:480:ALA:HB2	2.00	0.43
1:D:354:PRO:O	1:D:357:ASP:HB2	2.18	0.43
1:D:84:HIS:O	1:D:86:ARG:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:499:THR:HG23	1:E:501:THR:N	2.33	0.43
1:F:146:ARG:NE	1:F:182:THR:HG22	2.33	0.43
1:F:84:HIS:O	1:F:86:ARG:N	2.51	0.43
1:A:394:TYR:CE1	1:A:448:ILE:HG13	2.54	0.43
1:A:190:TYR:CD2	1:B:162:VAL:HG11	2.52	0.43
1:B:4:GLU:O	1:B:5:ASP:HB3	2.19	0.43
1:C:112:THR:HB	1:C:124:GLY:H	1.82	0.43
1:C:5:ASP:OD1	1:C:353:THR:HG21	2.19	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:A:499:THR:CB	1:D:64:PRO:HG2	2.49	0.43
1:E:37:THR:HG21	1:E:41:LYS:HG3	2.00	0.43
1:F:355:GLN:HA	1:F:355:GLN:OE1	2.18	0.43
1:A:349:ASN:C	1:A:351:PRO:HD3	2.39	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:B:266:PHE:CD1	1:B:266:PHE:N	2.87	0.43
1:B:57:HIS:HE1	1:E:151:GLU:OE1	2.02	0.43
1:C:111:MET:HE2	1:C:111:MET:HB3	1.70	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:D:57:HIS:CD2	1:D:84:HIS:NE2	2.87	0.43
1:E:486:ILE:O	1:E:490:PHE:HB2	2.18	0.43
1:E:66:ARG:HG3	1:E:72:TRP:CD2	2.54	0.43
1:A:500:PHE:CE2	1:F:185:SER:HB2	2.48	0.43
1:F:219:VAL:HG13	1:F:373:LEU:HD11	2.00	0.43
1:F:235:ILE:HG13	1:F:235:ILE:H	1.69	0.43
1:F:281:TRP:CG	1:F:310:TYR:HD2	2.36	0.43
1:F:275:GLU:C	4:F:507:NAD:C2A	2.87	0.43
1:A:362:GLU:C	1:A:364:ASN:H	2.20	0.43
1:B:370:ASP:CB	1:B:374:ASN:HD21	2.21	0.43
1:B:501:THR:HG22	1:E:66:ARG:H	1.83	0.43
1:C:266:PHE:CD1	1:C:266:PHE:N	2.87	0.43
1:C:302:LEU:HA	1:C:302:LEU:HD23	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:275:GLU:C	4:D:508:NAD:C2A	2.87	0.43
1:D:394:TYR:CE1	1:D:448:ILE:HG13	2.54	0.43
1:E:219:VAL:O	1:E:223:ILE:HG13	2.19	0.43
1:E:349:ASN:C	1:E:351:PRO:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:HIS:O	1:E:86:ARG:N	2.51	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:B:396:ARG:HE	1:F:456:THR:HG21	1.84	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:D:162:VAL:HG11	1:E:190:TYR:CE2	2.53	0.43
1:D:2:ASP:O	1:D:3:ARG:C	2.58	0.43
1:E:25:GLU:OE1	1:E:46:ARG:NE	2.51	0.43
4:E:508:NAD:N7N	4:E:508:NAD:O2N	2.47	0.43
1:F:294:PHE:CE2	1:F:298:HIS:CE1	3.06	0.43
1:F:57:HIS:CD2	1:F:84:HIS:NE2	2.87	0.43
1:C:499:THR:CG2	1:F:64:PRO:HG2	2.44	0.43
1:A:146:ARG:NE	1:A:182:THR:HG22	2.34	0.43
1:A:86:ARG:CZ	4:F:508[A]:NAD:C4N	2.97	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: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:C:23:ILE:HD12	1:C:479:THR:OG1	2.19	0.43
1:C:275:GLU:C	4:C:508:NAD:C2A	2.87	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:169:MET:HE1	1:D:327:SER:HA	2.01	0.43
1:D:473:LEU:HD12	1:D:480:ALA:HB2	2.00	0.43
1:E:238:MET:SD	1:E:342:LYS:HB3	2.59	0.43
1:E:275:GLU:C	4:E:508:NAD:C2A	2.87	0.43
1:E:23:ILE:HD12	1:E:479:THR:OG1	2.19	0.43
1:F:238:MET:SD	1:F:342:LYS:HB3	2.59	0.43
1:F:2:ASP:O	1:F:3:ARG:C	2.57	0.43
1:A:219:VAL:O	1:A:223:ILE:HG13	2.19	0.42
1:A:23:ILE:HD12	1:A:479:THR:OG1	2.19	0.42
1:A:275:GLU:C	4:A:508:NAD:C2A	2.87	0.42
1:B:169:MET:HE1	1:B:327:SER:HA	2.00	0.42
1:B:432:PRO:CB	1:B:436:PHE:HD2	2.28	0.42
1:B:57:HIS:CD2	1:B:84:HIS:NE2	2.87	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
1:C:5:ASP:HB2	1:C:333:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:5:ASP:HB2	1:E:333:LYS:NZ	2.34	0.42
4:C:507[A]:NAD:C4N	1:E:86:ARG:CZ	2.97	0.42
4:F:507:NAD:N7N	4:F:507:NAD:O2N	2.47	0.42
1:F:66:ARG:HG3	1:F:72:TRP:CD2	2.54	0.42
1:A:185:SER:HB2	1:B:500:PHE:CE2	2.51	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:371:LEU:HG	1:B:482:TYR:CE1	2.53	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:C:25:GLU:OE1	1:C:46:ARG:NE	2.51	0.42
1:C:4:GLU:O	1:C:5:ASP:HB3	2.19	0.42
1:D:5:ASP:OD1	1:D:353:THR:HG21	2.19	0.42
1:D:4:GLU:O	1:D:5:ASP:HB3	2.19	0.42
1:E:33:LYS:HA	1:E:41:LYS:HZ1	1.84	0.42
1:F:219:VAL:O	1:F:223:ILE:HG13	2.19	0.42
1:F:5:ASP:HB2	1:F:333:LYS:NZ	2.34	0.42
1:A:224:GLU:HB2	1:A:242:PHE:HE2	1.84	0.42
1:A:90:LYS:O	1:A:111:MET:HE2	2.19	0.42
1:B:146:ARG:NE	1:B:182:THR:HG22	2.34	0.42
1:B:275:GLU:C	4:B:508:NAD:C2A	2.87	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:C:406:ASN:HA	1:C:406:ASN:HD22	1.60	0.42
1:C:86:ARG:NH2	4:D:507[A]:NAD:C5N	2.83	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:C:157:PHE:CE1	1:F:155:LYS:HD2	2.55	0.42
1:F:242:PHE:CD1	1:F:263:LEU:HD22	2.54	0.42
1:F:266:PHE:CD1	1:F:266:PHE:N	2.87	0.42
1:B:421:PHE:CZ	1:F:421:PHE:HD1	2.37	0.42
1:A:219:VAL:HG13	1:A:373:LEU:HD11	2.00	0.42
1:A:266:PHE:CD1	1:A:266:PHE:N	2.87	0.42
1:A:242:PHE:HB2	1:A:266:PHE:O	2.20	0.42
1:A:4:GLU:O	1:A:5:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:HG22	1:B:187:ILE:N	2.35	0.42
1:B:242:PHE:O	1:B:268:ALA:HA	2.18	0.42
1:A:392:VAL:HG13	1:B:386:LEU:HD21	2.02	0.42
1:B:394:TYR:CE1	1:B:448:ILE:HG13	2.54	0.42
1:B:23:ILE:HD12	1:B:479:THR:OG1	2.19	0.42
1:C:282:ASN:H	1:C:307:ALA:HB1	1.82	0.42
1:C:33:LYS:HD3	1:C:33:LYS:HA	1.72	0.42
1:C:29:VAL:CA	1:C: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:D:29:VAL:CA	1:D:45:VAL:HG21	2.50	0.42
1:E:266:PHE:N	1:E:266:PHE:CD1	2.87	0.42
1:E:5:ASP:OD1	1:E:353:THR:HG21	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:F:4:GLU:O	1:F:5:ASP:HB3	2.19	0.42
4:B:507[A]:NAD:C5N	1:F:86:ARG:NH2	2.83	0.42
1:A:66:ARG:HG3	1:A:72:TRP:CD2	2.54	0.42
1:B:281:TRP:CG	1:B:310:TYR:HD2	2.36	0.42
1:B:349:ASN:C	1:B:351:PRO:HD3	2.39	0.42
1:B:5:ASP:HB2	1:B:333:LYS:NZ	2.34	0.42
1:C:242:PHE:CD1	1:C:263:LEU:HD22	2.54	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:D:224:GLU:HB2	1:D:242:PHE:HE2	1.84	0.42
1:E:242:PHE:HB2	1:E:266:PHE:O	2.20	0.42
1:D:86:ARG:NH2	4:E:507[A]:NAD:C5N	2.82	0.42
1:E:57:HIS:CD2	1:E:84:HIS:NE2	2.87	0.42
1:A:386:LEU:HD21	1:F:392:VAL:HG13	2.00	0.42
4:B:507[A]:NAD:C4N	1:F:86:ARG:CZ	2.97	0.42
1:A:110:LEU:O	1:A:114:LYS:HB2	2.20	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.91	0.42
1:B:2:ASP:O	1:B:3:ARG:C	2.58	0.42
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.83	0.42
1:F:158:ILE:HG13	1:F:165:PRO:CD	2.50	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:A:57:HIS:CD2	1:A:84:HIS:NE2	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:5:ASP:HB2	1:D:333:LYS:NZ	2.34	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: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:F:5:ASP:OD1	1:F:353:THR:HG21	2.19	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:B:411:MET:HE3	1:B:415:GLU:HG3	2.01	0.42
1:C:235:ILE:HG13	1:C:235:ILE:H	1.69	0.42
1:D:428:ILE:H	1:D:428:ILE:HD13	1.84	0.42
1:D:86:ARG:CZ	4:E:507[A]:NAD:C4N	2.97	0.42
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.84	0.42
1:E:42:ARG:O	1:E:46:ARG:N	2.53	0.42
1:F:23:ILE:HD12	1:F:479:THR:OG1	2.19	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:F:32:LEU:CD1	1:F:44:ARG:HH11	2.33	0.42
1:A:29:VAL:HG22	1:A:42:ARG:HA	2.02	0.42
1:A:2:ASP:O	1:A:3:ARG:C	2.58	0.42
1:A:5:ASP:HB2	1:A:333:LYS:NZ	2.34	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:406:ASN:HB3	1:B:440:ILE:HD11	2.02	0.42
4:A:507[A]:NAD:C5N	1:B:86:ARG:NH2	2.83	0.42
1:C:120:VAL:O	4:D:507[A]:NAD:N6A	2.49	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: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:HA	1:F:110:LEU:HD23	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:186:THR:HG22	1:C:187:ILE:N	2.34	0.42
1:C:38:GLN:HB2	1:C:39:GLU:H	1.59	0.42
1:D:186:THR:HG22	1:D:187:ILE:N	2.35	0.42
1:D:32:LEU:HD11	1:D:44:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:LYS:HD3	1:D:33:LYS:HA	1.72	0.42
1:D:450:HIS:CE1	5:D:514:HOH:O	2.72	0.42
1:E:33:LYS:HD3	1:E:33:LYS:HA	1.72	0.42
1:E:321:ILE:HG23	1:E:343:ILE:CG2	2.50	0.42
1:F:110:LEU:O	1:F:114:LYS:HB2	2.20	0.42
1:F:29:VAL:HG22	1:F:42:ARG:HA	2.02	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
1:D:406:ASN:HB3	1:D:440:ILE:HD11	2.02	0.41
1:E:158:ILE:HG13	1:E:165:PRO:CD	2.50	0.41
1:F:169:MET:CE	1:F:327:SER:HA	2.51	0.41
1:F:336:ALA:N	1:F:337:PRO:CD	2.83	0.41
1:F:113:TYR:HB2	1:F:371:LEU:HD21	2.02	0.41
1:F:42:ARG:O	1:F:46:ARG:N	2.53	0.41
1:A:186:THR:HG22	1:A:187:ILE:N	2.35	0.41
1:A:32:LEU:CD1	1:A:44:ARG:HH11	2.33	0.41
1:B:5:ASP:CB	1:B:333:LYS:HE2	2.51	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:A:147:ARG:NH1	1:D:500:PHE:CD1	2.88	0.41
1:C:401:TYR:CD2	1:E:443:ALA:HB2	2.55	0.41
1:E:67:ARG:HH12	1:E:136:TYR:HA	1.83	0.41
1:F:239:THR:HG23	1:F:240:PRO:O	2.20	0.41
1:A:239:THR:HG23	1:A:240:PRO:O	2.20	0.41
1:A:321:ILE:HA	1:A:343:ILE:O	2.20	0.41
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.50	0.41
1:A:428:ILE:HG23	1:F:420:LYS:HZ2	1.85	0.41
1:A:32:LEU:HD11	1:A:44:ARG:HH11	1.85	0.41
1:B:94:ARG:HE	1:B:168:ASN:HD22	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ILE:HD12	1:D:286:ILE:N	2.35	0.41
1:D:169:MET:CE	1:D:327:SER:HA	2.51	0.41
1:D:32:LEU:CD1	1:D:44:ARG:NH1	2.83	0.41
1:D:336:ALA:N	1:D:337:PRO:CD	2.83	0.41
1:A:498:VAL:HB	1:D:72:TRP:CZ2	2.55	0.41
1:E:169:MET:CE	1:E:327:SER:HA	2.51	0.41
1:E:276:SER:N	4:E:508:NAD:C2A	2.84	0.41
1:E:2:ASP:O	1:E:3:ARG:C	2.58	0.41
1:E:5:ASP:HB2	1:E:333:LYS:CE	2.50	0.41
1:E:336:ALA:N	1:E:337:PRO:CD	2.83	0.41
1:E:4:GLU:O	1:E:5:ASP:HB3	2.19	0.41
1:E:393:SER:HB3	4:E:507[A]:NAD:O3	2.20	0.41
1:A:86:ARG:NH2	4:F:508[A]:NAD:C5N	2.83	0.41
1:A:111:MET:HE1	1:A:378:VAL:CG1	2.50	0.41
1:A:175:GLU:HA	1:A:178:TRP:CE3	2.56	0.41
1:A:42:ARG:O	1:A:46:ARG:N	2.53	0.41
1:A:276:SER:N	4:A:508:NAD:C2A	2.84	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:3:ARG:HB2	1:B:4:GLU:H	1.72	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:CD1	1:F:44:ARG:NH1	2.84	0.41
1:F:32:LEU:HD11	1:F:44:ARG:HH11	1.85	0.41
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.48	0.41
1:B:204:SER:OG	1:F:495:GLU:OE1	2.18	0.41
1:F:276:SER:N	4:F:507:NAD:C2A	2.84	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:B:321:ILE:HG23	1:B:343:ILE:CG2	2.50	0.41
1:B:32:LEU:CD1	1:B:44:ARG:NH1	2.84	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
1:C:5:ASP:CB	1:C:333:LYS:HE2	2.51	0.41
1:C:5:ASP:HB2	1:C:333:LYS:CE	2.50	0.41
1:E:286:ILE:HD12	1:E:286:ILE:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:507[A]:NAD:C5N	1:E:86:ARG:NH2	2.83	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:A:5:ASP:CB	1:A:333:LYS:HE2	2.51	0.41
1:B:113:TYR:HB2	1:B:371:LEU:HD21	2.02	0.41
1:C:169:MET:CE	1:C:327:SER:HA	2.51	0.41
1:C:246:THR:CG2	1:C:319:CYS:HA	2.51	0.41
1:C:242:PHE:HB2	1:C:266:PHE:O	2.20	0.41
1:C:321:ILE:HA	1:C:343:ILE:O	2.20	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:D:29:VAL:HG22	1:D:42:ARG:HA	2.02	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:38:GLN:HB2	1:F:39:GLU:H	1.59	0.41
1:F:29:VAL:CA	1:F:45:VAL:HG21	2.50	0.41
1:A:15:GLY:O	1:A:18:ASP:N	2.54	0.41
1:A:386:LEU:HA	1:A:386:LEU:HD12	1.80	0.41
1:B:110:LEU:O	1:B:114:LYS:HB2	2.20	0.41
1:C:110:LEU:O	1:C:114:LYS:HB2	2.20	0.41
1:C:2:ASP:O	1:C:3:ARG:C	2.58	0.41
1:C:32:LEU:CD1	1:C:44:ARG:NH1	2.84	0.41
1:D:331:LEU:HD13	1:D:344:ILE:HD13	2.03	0.41
1:D:42:ARG:O	1:D:46:ARG:N	2.53	0.41
3:D:506:AKG:O2	4:D:508:NAD:C6N	2.68	0.41
1:E:110:LEU:O	1:E:114:LYS:HB2	2.20	0.41
1:B:155:LYS:HD2	1:E:157:PHE:CE1	2.56	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:32:LEU:HD11	1:E:44:ARG:HH11	1.85	0.41
1:F:167:PRO:HG3	1:F:176:MET:CG	2.51	0.41
1:F:13:VAL:HA	1:F:16:PHE:CD1	2.55	0.41
1:F:175:GLU:HA	1:F:178:TRP:CE3	2.56	0.41
1:A:495:GLU:HB2	1:F:205:GLN:HE21	1.86	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
1:F:33:LYS:HA	1:F:41:LYS:HZ3	1.85	0.41
1:B:421:PHE:CZ	1:F:421:PHE:CD1	3.09	0.41
1:B:401:TYR:CD1	1:F:443:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:506:AKG:O2	4:F:507:NAD:C6N	2.68	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
1:A:5:ASP:HB2	1:A:333:LYS:CE	2.50	0.41
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
1:C:15:GLY:O	1:C:18:ASP:N	2.54	0.41
1:C:360:PHE:HB3	1:C:365:ILE:HB	2.03	0.41
1:C:344:ILE:HB	1:C:367:VAL:HA	2.03	0.41
3:C:506:AKG:O2	4:C:508:NAD:C6N	2.68	0.41
1:D:370:ASP:HB2	1:D:374:ASN:ND2	2.20	0.41
1:D:5:ASP:HB2	1:D:333:LYS:CE	2.50	0.41
1:E:428:ILE:HD13	1:E:428:ILE:H	1.84	0.41
1:E:32:LEU:CD1	1:E:44:ARG:NH1	2.83	0.41
4:B:507[A]:NAD:N6A	1:F:120:VAL:O	2.49	0.41
1:F:23:ILE:CD1	1:F:473:LEU:HD21	2.47	0.41
1:A:13:VAL:HA	1:A:16:PHE:CD1	2.55	0.41
1:A:227:ILE:HD11	1:A:245:LYS:HG2	2.03	0.41
1:A:360:PHE:HB3	1:A:365:ILE:HB	2.03	0.41
1:A:87:THR:HG21	1:F:195:HIS:CE1	2.51	0.41
1:B:15:GLY:O	1:B:18:ASP:N	2.54	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: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: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:E:239:THR:HG23	1:E:240:PRO:O	2.20	0.41
1:E:29:VAL:CA	1:E:45:VAL:HG21	2.50	0.41
1:E:86:ARG:HD2	1:E:86:ARG:HA	1.85	0.41
1:F:321:ILE:HA	1:F:343:ILE:O	2.20	0.41
1:F:413:VAL:O	1:F:416:SER:HB2	2.21	0.41
1:A:238:MET:HE3	1:A:320:ASP:HB3	2.03	0.41
1:A:32:LEU:CD1	1:A:44:ARG:NH1	2.84	0.41
1:A:409:LEU:HD12	1:B:436:PHE:HZ	1.83	0.41
1:B:286:ILE:N	1:B:286:ILE:HD12	2.36	0.41
1:B:32:LEU:HD11	1:B:44:ARG:HH11	1.85	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:498:VAL:HB	1:F:72:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HA	1:C:127:ALA:HB3	2.03	0.41
1:D:94:ARG:HE	1:D:168:ASN:HD22	1.67	0.41
1:D:298:HIS:O	1:D:299:GLY:C	2.60	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
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.56	0.41
1:B:169:MET:CE	1:B:327:SER:HA	2.51	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:B:90:LYS:O	1:B:111:MET:HE2	2.21	0.41
1:C:298:HIS:O	1:C:299:GLY:C	2.59	0.41
1:C:32:LEU:HD11	1:C:44:ARG:HH11	1.85	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: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:D:26:ASP:HA	1:D:42:ARG:HH12	1.86	0.41
1:E:294:PHE:CD2	1:E:298:HIS:ND1	2.88	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: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:C:55:CYS:O	1:F:62:SER:HB3	2.21	0.41
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.69	0.40
1:B:298:HIS:O	1:B:299:GLY:C	2.60	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: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:D:113:TYR:HB2	1:D:371:LEU:HD21	2.02	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: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:C:499:THR:CB	1:F:64:PRO:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HA	1:F:127:ALA:HB3	2.04	0.40
1:A:205:GLN:HE21	1:B:495:GLU:HB2	1.86	0.40
1:A:113:TYR:HB2	1:A:371:LEU:HD21	2.02	0.40
1:B:167:PRO:HG3	1:B:176:MET:CG	2.51	0.40
1:B:238:MET:HE2	1:B:245:LYS:HE2	2.03	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:167:PRO:HG3	1:C:176:MET:CG	2.51	0.40
1:C:406:ASN:HB3	1:C:440:ILE:HD11	2.02	0.40
1:C:457:MET:CE	1:C:457:MET:HA	2.42	0.40
1:D:386:LEU:HA	1:D:386:LEU:HD12	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:C:54:PRO:HG3	1:F:74:VAL:HG11	2.02	0.40
1:A:26:ASP:HA	1:A:42:ARG:HH12	1.86	0.40
1:B:336:ALA:N	1:B:337:PRO:CD	2.83	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: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:C:23:ILE:CD1	1:C:473:LEU:HD21	2.47	0.40
1:D:333:LYS:HB3	1:D:333:LYS:HE2	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:E:469:MET:O	1:E:470:LYS:C	2.60	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:346:GLU:OE2	1:F:369:PRO:HA	2.22	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:A:23:ILE:CD1	1:A:473:LEU:HD21	2.47	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:411:MET:HE3	1:D:415:GLU:HG3	2.02	0.40
1:E:110:LEU:HA	1:E:110:LEU:HD23	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:24:VAL:O	1:F:25:GLU:C	2.60	0.40
1:F:273:VAL:HG21	1:F:291:LEU:HD11	2.03	0.40
1:A:169:MET:CE	1:A:327:SER:HA	2.51	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: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:B:309:ILE:CG1	1:C:284:ASP:OD1[2_545]	2.14	0.06
1:A:3:ARG:CZ	1:E:298:HIS:NE2[2_556]	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%)	3	21
1	B	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	21
1	C	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	21
1	D	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	21
1	F	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3	21
All	All	2994/3006 (100%)	2502 (84%)	354 (12%)	138 (5%)	3	21

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%)	359 (86%)	58 (14%)	4	19
1	B	417/417 (100%)	359 (86%)	58 (14%)	4	19
1	C	417/417 (100%)	359 (86%)	58 (14%)	4	19
1	D	417/417 (100%)	359 (86%)	58 (14%)	4	19
1	E	417/417 (100%)	359 (86%)	58 (14%)	4	19
1	F	417/417 (100%)	359 (86%)	58 (14%)	4	19
All	All	2502/2502 (100%)	2154 (86%)	348 (14%)	4	19

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	26	ASP
1	A	38	GLN
1	A	40	GLN
1	A	46	ARG
1	A	86	ARG
1	A	90	LYS
1	A	102	ASP
1	A	107	LEU
1	A	112	THR
1	A	130	LYS
1	A	132	ASN
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	211	ARG
1	A	231	SER
1	A	236	LEU
1	A	239	THR
1	A	245	LYS
1	A	246	THR
1	A	249	VAL
1	A	255	VAL
1	A	275	GLU
1	A	291	LEU
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
1	A	385	ILE
1	A	386	LEU
1	A	392	VAL
1	A	393	SER

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Mol	Chain	Res	Type
1	A	394	TYR
1	A	396	ARG
1	A	402	GLU
1	A	405	SER
1	A	406	ASN
1	A	421	PHE
1	A	423	LYS
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	500	PHE
1	A	501	THR
1	B	3	ARG
1	B	26	ASP
1	B	38	GLN
1	B	40	GLN
1	B	46	ARG
1	B	86	ARG
1	B	90	LYS
1	B	102	ASP
1	B	107	LEU
1	B	112	THR
1	B	130	LYS
1	B	132	ASN
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	211	ARG
1	B	231	SER
1	B	236	LEU
1	B	239	THR
1	B	245	LYS
1	B	246	THR
1	B	249	VAL
1	B	255	VAL
1	B	275	GLU

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Mol	Chain	Res	Type
1	B	291	LEU
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	394	TYR
1	B	396	ARG
1	B	402	GLU
1	B	405	SER
1	B	406	ASN
1	B	421	PHE
1	B	423	LYS
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	500	PHE
1	B	501	THR
1	C	3	ARG
1	C	26	ASP
1	C	38	GLN
1	C	40	GLN
1	C	46	ARG
1	C	86	ARG
1	C	90	LYS
1	C	102	ASP
1	C	107	LEU
1	C	112	THR
1	C	130	LYS

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Mol	Chain	Res	Type
1	C	132	ASN
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	211	ARG
1	C	231	SER
1	C	236	LEU
1	C	239	THR
1	C	245	LYS
1	C	246	THR
1	C	249	VAL
1	C	255	VAL
1	C	275	GLU
1	C	291	LEU
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
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	394	TYR
1	C	396	ARG
1	C	402	GLU
1	C	405	SER
1	C	406	ASN
1	C	421	PHE
1	C	423	LYS
1	C	428	ILE
1	C	437	GLN
1	C	451	SER

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Mol	Chain	Res	Type
1	C	458	GLU
1	C	469	MET
1	C	479	THR
1	C	500	PHE
1	C	501	THR
1	D	3	ARG
1	D	26	ASP
1	D	38	GLN
1	D	40	GLN
1	D	46	ARG
1	D	86	ARG
1	D	90	LYS
1	D	102	ASP
1	D	107	LEU
1	D	112	THR
1	D	130	LYS
1	D	132	ASN
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	211	ARG
1	D	231	SER
1	D	236	LEU
1	D	239	THR
1	D	245	LYS
1	D	246	THR
1	D	249	VAL
1	D	255	VAL
1	D	275	GLU
1	D	291	LEU
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

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Mol	Chain	Res	Type
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	394	TYR
1	D	396	ARG
1	D	402	GLU
1	D	405	SER
1	D	406	ASN
1	D	421	PHE
1	D	423	LYS
1	D	428	ILE
1	D	437	GLN
1	D	451	SER
1	D	458	GLU
1	D	469	MET
1	D	479	THR
1	D	500	PHE
1	D	501	THR
1	E	3	ARG
1	E	26	ASP
1	E	38	GLN
1	E	40	GLN
1	E	46	ARG
1	E	86	ARG
1	E	90	LYS
1	E	102	ASP
1	E	107	LEU
1	E	112	THR
1	E	130	LYS
1	E	132	ASN
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	211	ARG
1	E	231	SER
1	E	236	LEU

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Mol	Chain	Res	Type
1	E	239	THR
1	E	245	LYS
1	E	246	THR
1	E	249	VAL
1	E	255	VAL
1	E	275	GLU
1	E	291	LEU
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
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	394	TYR
1	E	396	ARG
1	E	402	GLU
1	E	405	SER
1	E	406	ASN
1	E	421	PHE
1	E	423	LYS
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	500	PHE
1	E	501	THR
1	F	3	ARG
1	F	26	ASP
1	F	38	GLN
1	F	40	GLN
1	F	46	ARG

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Mol	Chain	Res	Type
1	F	86	ARG
1	F	90	LYS
1	F	102	ASP
1	F	107	LEU
1	F	112	THR
1	F	130	LYS
1	F	132	ASN
1	F	138	ASP
1	F	145	THR
1	F	162	VAL
1	F	170	SER
1	F	175	GLU
1	F	182	THR
1	F	211	ARG
1	F	231	SER
1	F	236	LEU
1	F	239	THR
1	F	245	LYS
1	F	246	THR
1	F	249	VAL
1	F	255	VAL
1	F	275	GLU
1	F	291	LEU
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	394	TYR
1	F	396	ARG
1	F	402	GLU
1	F	405	SER

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Mol	Chain	Res	Type
1	F	406	ASN
1	F	421	PHE
1	F	423	LYS
1	F	428	ILE
1	F	437	GLN
1	F	451	SER
1	F	458	GLU
1	F	469	MET
1	F	479	THR
1	F	500	PHE
1	F	501	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) 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	282	ASN
1	A	388	ASN
1	A	391	HIS
1	A	406	ASN
1	A	450	HIS
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

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Mol	Chain	Res	Type
1	B	254	ASN
1	B	258	HIS
1	B	282	ASN
1	B	388	ASN
1	B	391	HIS
1	B	406	ASN
1	B	450	HIS
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	282	ASN
1	C	388	ASN
1	C	391	HIS
1	C	406	ASN
1	C	450	HIS
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	209	HIS
1	D	254	ASN
1	D	258	HIS
1	D	282	ASN
1	D	388	ASN
1	D	391	HIS
1	D	406	ASN
1	D	450	HIS
1	D	494	ASN

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Mol	Chain	Res	Type
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	209	HIS
1	E	254	ASN
1	E	258	HIS
1	E	282	ASN
1	E	388	ASN
1	E	391	HIS
1	E	406	ASN
1	E	450	HIS
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	209	HIS
1	F	254	ASN
1	F	258	HIS
1	F	282	ASN
1	F	388	ASN
1	F	391	HIS
1	F	406	ASN
1	F	450	HIS
1	F	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	502	-	4,4,4	1.14	0	6,6,6	0.77	0
2	PO4	A	503	-	4,4,4	1.12	0	6,6,6	0.77	0
2	PO4	A	504	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	A	505	-	4,4,4	1.83	2 (50%)	6,6,6	0.76	0
3	AKG	A	506	-	3,9,9	1.11	0	4,11,11	3.40	3 (75%)
4	NAD	A	507[A]	-	41,48,48	2.23	10 (24%)	43,73,73	2.59	13 (30%)
4	NAD	A	507[B]	-	41,48,48	2.43	11 (26%)	43,73,73	2.27	13 (30%)
4	NAD	A	508	-	41,48,48	2.14	12 (29%)	43,73,73	2.60	13 (30%)
2	PO4	B	502	-	4,4,4	1.12	0	6,6,6	0.77	0
2	PO4	B	503	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	B	504	-	4,4,4	1.83	2 (50%)	6,6,6	0.75	0
2	PO4	B	505	-	4,4,4	1.13	0	6,6,6	0.76	0
3	AKG	B	506	-	3,9,9	1.09	0	4,11,11	3.39	3 (75%)
4	NAD	B	507[A]	-	41,48,48	2.22	10 (24%)	43,73,73	2.59	14 (32%)
4	NAD	B	507[B]	-	41,48,48	2.43	10 (24%)	43,73,73	2.27	13 (30%)
4	NAD	B	508	-	41,48,48	2.14	12 (29%)	43,73,73	2.59	13 (30%)
2	PO4	C	502	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	C	503	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	C	504	-	4,4,4	1.84	2 (50%)	6,6,6	0.76	0
2	PO4	C	505	-	4,4,4	1.13	0	6,6,6	0.77	0
3	AKG	C	506	-	3,9,9	1.11	0	4,11,11	3.40	3 (75%)
4	NAD	C	507[A]	-	41,48,48	2.23	10 (24%)	43,73,73	2.59	14 (32%)
4	NAD	C	507[B]	-	41,48,48	2.42	11 (26%)	43,73,73	2.27	13 (30%)
4	NAD	C	508	-	41,48,48	2.14	12 (29%)	43,73,73	2.60	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	502	-	4,4,4	1.12	0	6,6,6	0.76	0
2	PO4	D	503	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	D	504	-	4,4,4	1.13	0	6,6,6	0.77	0
2	PO4	D	505	-	4,4,4	1.82	2 (50%)	6,6,6	0.75	0
3	AKG	D	506	-	3,9,9	1.09	0	4,11,11	3.40	3 (75%)
4	NAD	D	507[A]	-	41,48,48	2.22	10 (24%)	43,73,73	2.59	14 (32%)
4	NAD	D	507[B]	-	41,48,48	2.43	11 (26%)	43,73,73	2.27	13 (30%)
4	NAD	D	508	-	41,48,48	2.15	12 (29%)	43,73,73	2.60	13 (30%)
2	PO4	E	502	-	4,4,4	1.11	0	6,6,6	0.76	0
2	PO4	E	503	-	4,4,4	1.14	0	6,6,6	0.77	0
2	PO4	E	504	-	4,4,4	1.13	0	6,6,6	0.76	0
2	PO4	E	505	-	4,4,4	1.83	2 (50%)	6,6,6	0.75	0
3	AKG	E	506	-	3,9,9	1.13	0	4,11,11	3.41	3 (75%)
4	NAD	E	507[A]	-	41,48,48	2.23	10 (24%)	43,73,73	2.58	14 (32%)
4	NAD	E	507[B]	-	41,48,48	2.43	11 (26%)	43,73,73	2.27	13 (30%)
4	NAD	E	508	-	41,48,48	2.15	12 (29%)	43,73,73	2.60	13 (30%)
2	PO4	F	502	-	4,4,4	1.14	0	6,6,6	0.77	0
2	PO4	F	503	-	4,4,4	1.12	0	6,6,6	0.77	0
2	PO4	F	504	-	4,4,4	1.14	0	6,6,6	0.77	0
2	PO4	F	505	-	4,4,4	1.83	2 (50%)	6,6,6	0.76	0
3	AKG	F	506	-	3,9,9	1.13	0	4,11,11	3.41	3 (75%)
4	NAD	F	507	-	41,48,48	2.15	12 (29%)	43,73,73	2.59	13 (30%)
4	NAD	F	508[A]	-	41,48,48	2.23	10 (24%)	43,73,73	2.59	14 (32%)
4	NAD	F	508[B]	-	41,48,48	2.43	11 (26%)	43,73,73	2.27	13 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	-	-	0/0/0/0	0/0/0/0
2	PO4	A	505	-	-	0/0/0/0	0/0/0/0
3	AKG	A	506	-	-	0/3/9/9	0/0/0/0
4	NAD	A	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	A	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	A	508	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	PO4	B	503	-	-	0/0/0/0	0/0/0/0
2	PO4	B	504	-	-	0/0/0/0	0/0/0/0
2	PO4	B	505	-	-	0/0/0/0	0/0/0/0
3	AKG	B	506	-	-	0/3/9/9	0/0/0/0
4	NAD	B	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	B	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	B	508	-	-	0/22/62/62	0/5/5/5
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	C	503	-	-	0/0/0/0	0/0/0/0
2	PO4	C	504	-	-	0/0/0/0	0/0/0/0
2	PO4	C	505	-	-	0/0/0/0	0/0/0/0
3	AKG	C	506	-	-	0/3/9/9	0/0/0/0
4	NAD	C	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	C	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	C	508	-	-	0/22/62/62	0/5/5/5
2	PO4	D	502	-	-	0/0/0/0	0/0/0/0
2	PO4	D	503	-	-	0/0/0/0	0/0/0/0
2	PO4	D	504	-	-	0/0/0/0	0/0/0/0
2	PO4	D	505	-	-	0/0/0/0	0/0/0/0
3	AKG	D	506	-	-	0/3/9/9	0/0/0/0
4	NAD	D	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	D	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	D	508	-	-	0/22/62/62	0/5/5/5
2	PO4	E	502	-	-	0/0/0/0	0/0/0/0
2	PO4	E	503	-	-	0/0/0/0	0/0/0/0
2	PO4	E	504	-	-	0/0/0/0	0/0/0/0
2	PO4	E	505	-	-	0/0/0/0	0/0/0/0
3	AKG	E	506	-	-	0/3/9/9	0/0/0/0
4	NAD	E	507[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	E	507[B]	-	-	0/22/62/62	0/5/5/5
4	NAD	E	508	-	-	0/22/62/62	0/5/5/5
2	PO4	F	502	-	-	0/0/0/0	0/0/0/0
2	PO4	F	503	-	-	0/0/0/0	0/0/0/0
2	PO4	F	504	-	-	0/0/0/0	0/0/0/0
2	PO4	F	505	-	-	0/0/0/0	0/0/0/0
3	AKG	F	506	-	-	0/3/9/9	0/0/0/0
4	NAD	F	507	-	-	0/22/62/62	0/5/5/5
4	NAD	F	508[A]	-	-	0/22/62/62	0/5/5/5
4	NAD	F	508[B]	-	-	0/22/62/62	0/5/5/5

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	507[B]	NAD	C2N-C3N	-4.31	1.32	1.39
4	B	507[B]	NAD	C2N-C3N	-4.31	1.32	1.39
4	E	507[B]	NAD	C2N-C3N	-4.29	1.32	1.39
4	F	508[B]	NAD	C2N-C3N	-4.29	1.32	1.39
4	C	507[B]	NAD	C2N-C3N	-4.27	1.32	1.39
4	D	507[B]	NAD	C2N-C3N	-4.25	1.32	1.39
4	E	508	NAD	C2N-C3N	-3.67	1.33	1.39
4	D	508	NAD	C2N-C3N	-3.67	1.33	1.39
4	F	507	NAD	C2N-C3N	-3.66	1.33	1.39
4	C	508	NAD	C2N-C3N	-3.66	1.33	1.39
4	A	508	NAD	C2N-C3N	-3.65	1.33	1.39
4	B	508	NAD	C2N-C3N	-3.62	1.33	1.39
4	A	507[A]	NAD	C2N-C3N	-3.45	1.33	1.39
4	F	508[A]	NAD	C2N-C3N	-3.45	1.33	1.39
4	C	507[A]	NAD	C2N-C3N	-3.45	1.33	1.39
4	E	507[A]	NAD	C2N-C3N	-3.44	1.33	1.39
4	B	507[A]	NAD	C2N-C3N	-3.43	1.33	1.39
4	D	507[A]	NAD	C2N-C3N	-3.41	1.33	1.39
4	E	507[A]	NAD	PA-O5B	-3.13	1.45	1.59
4	D	507[A]	NAD	PA-O5B	-3.12	1.45	1.59
4	A	507[A]	NAD	PA-O5B	-3.12	1.45	1.59
4	F	508[A]	NAD	PA-O5B	-3.12	1.45	1.59
4	C	507[A]	NAD	PA-O5B	-3.12	1.45	1.59
4	B	507[A]	NAD	PA-O5B	-3.11	1.45	1.59
4	E	507[A]	NAD	PN-O1N	-2.98	1.39	1.50
4	C	507[A]	NAD	PN-O1N	-2.98	1.39	1.50
4	A	507[A]	NAD	PN-O1N	-2.97	1.39	1.50
4	F	508[A]	NAD	PN-O1N	-2.97	1.39	1.50
4	B	507[A]	NAD	PN-O1N	-2.97	1.39	1.50
4	D	507[A]	NAD	PN-O1N	-2.96	1.39	1.50
4	D	507[B]	NAD	PA-O5B	-2.95	1.46	1.59
4	F	508[B]	NAD	PA-O5B	-2.95	1.46	1.59
4	B	507[B]	NAD	PA-O5B	-2.94	1.46	1.59
4	E	507[B]	NAD	PA-O5B	-2.94	1.46	1.59
4	C	507[B]	NAD	PA-O5B	-2.94	1.46	1.59
4	A	507[B]	NAD	PA-O5B	-2.94	1.46	1.59
4	D	508	NAD	PA-O5B	-2.77	1.47	1.59
4	C	508	NAD	PA-O5B	-2.77	1.47	1.59
4	B	508	NAD	PA-O5B	-2.75	1.47	1.59
4	A	508	NAD	PA-O5B	-2.75	1.47	1.59
4	F	507	NAD	PA-O5B	-2.75	1.47	1.59
4	E	508	NAD	PA-O5B	-2.74	1.47	1.59
4	E	507[B]	NAD	PN-O1N	-2.31	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	507[B]	NAD	PN-O1N	-2.31	1.42	1.50
4	F	508[B]	NAD	PN-O1N	-2.31	1.42	1.50
4	C	507[B]	NAD	PN-O1N	-2.30	1.42	1.50
4	A	507[B]	NAD	PN-O1N	-2.30	1.42	1.50
4	B	507[B]	NAD	PN-O1N	-2.28	1.42	1.50
4	E	508	NAD	C3D-C4D	-2.13	1.47	1.53
4	D	508	NAD	C3D-C4D	-2.13	1.47	1.53
4	F	507	NAD	C3D-C4D	-2.13	1.47	1.53
4	A	508	NAD	C3D-C4D	-2.12	1.47	1.53
4	C	508	NAD	C3D-C4D	-2.12	1.47	1.53
4	B	508	NAD	C3D-C4D	-2.11	1.47	1.53
4	D	507[B]	NAD	O3B-C3B	2.03	1.47	1.43
4	E	507[B]	NAD	O3B-C3B	2.03	1.47	1.43
4	F	508[B]	NAD	O3B-C3B	2.04	1.47	1.43
4	A	507[B]	NAD	O3B-C3B	2.06	1.47	1.43
4	C	507[B]	NAD	O3B-C3B	2.08	1.47	1.43
2	E	505	PO4	P-O1	2.10	1.55	1.50
2	D	505	PO4	P-O1	2.10	1.55	1.50
2	B	504	PO4	P-O1	2.10	1.55	1.50
2	A	505	PO4	P-O1	2.11	1.55	1.50
4	C	507[B]	NAD	C6N-N1N	2.12	1.40	1.35
4	E	507[B]	NAD	C6N-N1N	2.12	1.40	1.35
4	A	507[A]	NAD	C6N-N1N	2.12	1.40	1.35
2	F	505	PO4	P-O1	2.12	1.55	1.50
4	D	507[A]	NAD	C6N-N1N	2.13	1.41	1.35
4	F	508[A]	NAD	C6N-N1N	2.14	1.41	1.35
4	C	507[A]	NAD	C6N-N1N	2.14	1.41	1.35
4	B	507[A]	NAD	C6N-N1N	2.14	1.41	1.35
4	B	507[B]	NAD	C6N-N1N	2.14	1.41	1.35
4	D	507[B]	NAD	C6N-N1N	2.14	1.41	1.35
4	E	507[A]	NAD	C6N-N1N	2.14	1.41	1.35
4	F	508[B]	NAD	C6N-N1N	2.15	1.41	1.35
2	C	504	PO4	P-O1	2.15	1.55	1.50
4	A	507[B]	NAD	C6N-N1N	2.16	1.41	1.35
4	B	508	NAD	C3B-C4B	2.17	1.58	1.53
4	C	508	NAD	C3B-C4B	2.17	1.58	1.53
4	A	508	NAD	C3B-C4B	2.19	1.58	1.53
4	E	508	NAD	C3B-C4B	2.19	1.58	1.53
4	D	508	NAD	C3B-C4B	2.19	1.58	1.53
4	F	507	NAD	C3B-C4B	2.20	1.58	1.53
4	F	507	NAD	C5N-C4N	2.45	1.43	1.38
4	C	508	NAD	C5N-C4N	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	508	NAD	C5N-C4N	2.46	1.43	1.38
4	A	508	NAD	C5N-C4N	2.47	1.43	1.38
4	D	508	NAD	C5N-C4N	2.47	1.43	1.38
4	B	508	NAD	C5N-C4N	2.49	1.43	1.38
4	B	507[A]	NAD	O2D-C2D	2.50	1.48	1.43
4	D	507[A]	NAD	O2D-C2D	2.51	1.48	1.43
4	C	507[A]	NAD	O2D-C2D	2.52	1.48	1.43
4	E	507[A]	NAD	O2D-C2D	2.52	1.48	1.43
4	F	508[A]	NAD	O2D-C2D	2.53	1.48	1.43
4	A	507[A]	NAD	O2D-C2D	2.54	1.48	1.43
4	C	507[B]	NAD	C5N-C4N	2.84	1.44	1.38
4	B	507[B]	NAD	C5N-C4N	2.85	1.44	1.38
4	F	508[B]	NAD	C5N-C4N	2.86	1.44	1.38
4	D	507[B]	NAD	C5N-C4N	2.87	1.44	1.38
4	F	507	NAD	C6N-N1N	2.87	1.42	1.35
4	E	508	NAD	C6N-N1N	2.87	1.42	1.35
4	E	507[B]	NAD	C5N-C4N	2.88	1.44	1.38
4	A	507[B]	NAD	C5N-C4N	2.89	1.44	1.38
4	B	508	NAD	C6N-N1N	2.89	1.42	1.35
4	A	508	NAD	C6N-N1N	2.90	1.42	1.35
4	D	508	NAD	C6N-N1N	2.91	1.43	1.35
4	C	508	NAD	C6N-N1N	2.91	1.43	1.35
2	D	505	PO4	P-O4	2.92	1.64	1.54
2	F	505	PO4	P-O4	2.92	1.64	1.54
2	A	505	PO4	P-O4	2.92	1.64	1.54
2	B	504	PO4	P-O4	2.93	1.64	1.54
2	E	505	PO4	P-O4	2.93	1.64	1.54
2	C	504	PO4	P-O4	2.94	1.64	1.54
4	B	508	NAD	C3N-C7N	3.12	1.55	1.50
4	C	508	NAD	C3N-C7N	3.12	1.55	1.50
4	B	508	NAD	C7N-N7N	3.15	1.39	1.33
4	F	507	NAD	C3N-C7N	3.16	1.55	1.50
4	C	508	NAD	C7N-N7N	3.16	1.39	1.33
4	A	508	NAD	C3N-C7N	3.16	1.55	1.50
4	A	508	NAD	C7N-N7N	3.16	1.39	1.33
4	F	507	NAD	C7N-N7N	3.18	1.39	1.33
4	D	508	NAD	C2A-N3A	3.18	1.37	1.32
4	D	508	NAD	C3N-C7N	3.18	1.55	1.50
4	E	508	NAD	C7N-N7N	3.19	1.39	1.33
4	D	508	NAD	C7N-N7N	3.19	1.39	1.33
4	A	508	NAD	C2A-N3A	3.20	1.37	1.32
4	E	508	NAD	C3N-C7N	3.20	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	508	NAD	C2A-N3A	3.22	1.37	1.32
4	E	508	NAD	C2A-N3A	3.22	1.37	1.32
4	F	507	NAD	C2A-N3A	3.23	1.37	1.32
4	B	508	NAD	C2A-N3A	3.24	1.37	1.32
4	D	507[A]	NAD	C4A-N3A	4.11	1.41	1.35
4	A	507[A]	NAD	C4A-N3A	4.13	1.41	1.35
4	B	507[A]	NAD	C4A-N3A	4.14	1.41	1.35
4	F	508[A]	NAD	C4A-N3A	4.15	1.41	1.35
4	C	507[A]	NAD	C4A-N3A	4.15	1.41	1.35
4	E	507[A]	NAD	C4A-N3A	4.17	1.41	1.35
4	B	507[B]	NAD	C4A-N3A	4.49	1.42	1.35
4	C	507[B]	NAD	C4A-N3A	4.52	1.42	1.35
4	F	508[B]	NAD	C4A-N3A	4.53	1.42	1.35
4	A	507[B]	NAD	C4A-N3A	4.55	1.42	1.35
4	D	507[B]	NAD	C4A-N3A	4.57	1.42	1.35
4	E	507[A]	NAD	C3N-C7N	4.59	1.57	1.50
4	B	507[A]	NAD	C3N-C7N	4.60	1.57	1.50
4	C	507[A]	NAD	C3N-C7N	4.60	1.57	1.50
4	E	507[B]	NAD	C4A-N3A	4.61	1.42	1.35
4	F	508[A]	NAD	C3N-C7N	4.62	1.57	1.50
4	D	507[A]	NAD	C3N-C7N	4.64	1.57	1.50
4	A	507[A]	NAD	C3N-C7N	4.67	1.57	1.50
4	D	508	NAD	PA-O1A	4.95	1.69	1.50
4	C	508	NAD	PA-O1A	4.96	1.69	1.50
4	A	508	NAD	PA-O1A	4.96	1.69	1.50
4	B	508	NAD	PA-O1A	4.97	1.69	1.50
4	E	508	NAD	PA-O1A	4.98	1.69	1.50
4	F	507	NAD	PA-O1A	4.98	1.69	1.50
4	E	507[A]	NAD	C2A-N3A	4.99	1.40	1.32
4	D	507[A]	NAD	C2A-N3A	5.00	1.40	1.32
4	C	507[A]	NAD	C2A-N3A	5.01	1.40	1.32
4	B	507[A]	NAD	C2A-N3A	5.03	1.40	1.32
4	F	508[A]	NAD	C2A-N3A	5.03	1.40	1.32
4	A	507[A]	NAD	C2A-N3A	5.04	1.40	1.32
4	B	507[A]	NAD	C7N-N7N	5.18	1.43	1.33
4	E	507[A]	NAD	C7N-N7N	5.18	1.43	1.33
4	D	507[A]	NAD	C7N-N7N	5.19	1.43	1.33
4	F	508[A]	NAD	C7N-N7N	5.19	1.43	1.33
4	A	507[B]	NAD	C3N-C7N	5.20	1.58	1.50
4	A	507[A]	NAD	C7N-N7N	5.21	1.43	1.33
4	C	507[A]	NAD	C7N-N7N	5.24	1.43	1.33
4	B	507[B]	NAD	C3N-C7N	5.25	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	507[B]	NAD	C3N-C7N	5.25	1.58	1.50
4	C	507[B]	NAD	C3N-C7N	5.25	1.58	1.50
4	F	508[B]	NAD	C3N-C7N	5.26	1.58	1.50
4	D	507[B]	NAD	C3N-C7N	5.28	1.58	1.50
4	B	508	NAD	O4B-C1B	5.38	1.48	1.41
4	A	507[B]	NAD	C2A-N3A	5.38	1.41	1.32
4	F	507	NAD	O4B-C1B	5.40	1.48	1.41
4	A	508	NAD	O4B-C1B	5.41	1.48	1.41
4	D	507[B]	NAD	C2A-N3A	5.42	1.41	1.32
4	D	508	NAD	O4B-C1B	5.42	1.48	1.41
4	E	507[B]	NAD	C2A-N3A	5.42	1.41	1.32
4	C	508	NAD	O4B-C1B	5.43	1.48	1.41
4	C	507[B]	NAD	C2A-N3A	5.43	1.41	1.32
4	F	508[B]	NAD	C2A-N3A	5.45	1.41	1.32
4	E	508	NAD	O4B-C1B	5.45	1.48	1.41
4	B	507[B]	NAD	C2A-N3A	5.48	1.41	1.32
4	C	508	NAD	C4A-N3A	5.60	1.43	1.35
4	B	508	NAD	C4A-N3A	5.61	1.43	1.35
4	A	508	NAD	C4A-N3A	5.65	1.43	1.35
4	E	508	NAD	C4A-N3A	5.65	1.43	1.35
4	F	507	NAD	C4A-N3A	5.68	1.43	1.35
4	D	508	NAD	C4A-N3A	5.70	1.43	1.35
4	C	507[B]	NAD	PA-O1A	5.82	1.72	1.50
4	B	507[B]	NAD	PA-O1A	5.83	1.72	1.50
4	F	508[B]	NAD	PA-O1A	5.83	1.72	1.50
4	E	507[B]	NAD	PA-O1A	5.83	1.72	1.50
4	A	507[B]	NAD	PA-O1A	5.83	1.72	1.50
4	D	507[B]	NAD	PA-O1A	5.84	1.72	1.50
4	D	507[A]	NAD	PA-O1A	5.94	1.73	1.50
4	A	507[A]	NAD	PA-O1A	5.95	1.73	1.50
4	F	508[A]	NAD	PA-O1A	5.95	1.73	1.50
4	C	507[A]	NAD	PA-O1A	5.96	1.73	1.50
4	B	507[A]	NAD	PA-O1A	5.97	1.73	1.50
4	E	507[A]	NAD	PA-O1A	5.97	1.73	1.50
4	D	507[B]	NAD	C7N-N7N	6.80	1.46	1.33
4	C	507[B]	NAD	C7N-N7N	6.80	1.46	1.33
4	A	507[B]	NAD	C7N-N7N	6.81	1.46	1.33
4	F	508[B]	NAD	C7N-N7N	6.81	1.46	1.33
4	B	507[B]	NAD	C7N-N7N	6.82	1.46	1.33
4	E	507[B]	NAD	C7N-N7N	6.84	1.46	1.33

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	507	NAD	N3A-C2A-N1A	-9.95	120.20	128.86
4	D	508	NAD	N3A-C2A-N1A	-9.94	120.20	128.86
4	C	508	NAD	N3A-C2A-N1A	-9.93	120.21	128.86
4	A	508	NAD	N3A-C2A-N1A	-9.93	120.21	128.86
4	B	508	NAD	N3A-C2A-N1A	-9.92	120.22	128.86
4	E	508	NAD	N3A-C2A-N1A	-9.92	120.22	128.86
4	B	507[A]	NAD	N3A-C2A-N1A	-8.87	121.13	128.86
4	C	507[A]	NAD	N3A-C2A-N1A	-8.85	121.15	128.86
4	F	508[A]	NAD	N3A-C2A-N1A	-8.80	121.19	128.86
4	D	507[A]	NAD	N3A-C2A-N1A	-8.79	121.21	128.86
4	E	507[A]	NAD	N3A-C2A-N1A	-8.78	121.21	128.86
4	A	507[A]	NAD	N3A-C2A-N1A	-8.77	121.22	128.86
4	C	507[B]	NAD	N3A-C2A-N1A	-8.05	121.85	128.86
4	B	507[B]	NAD	N3A-C2A-N1A	-8.05	121.85	128.86
4	F	508[B]	NAD	N3A-C2A-N1A	-8.04	121.86	128.86
4	A	507[B]	NAD	N3A-C2A-N1A	-8.04	121.86	128.86
4	E	507[B]	NAD	N3A-C2A-N1A	-8.02	121.87	128.86
4	D	507[B]	NAD	N3A-C2A-N1A	-8.00	121.89	128.86
4	C	507[A]	NAD	C4B-O4B-C1B	-5.01	104.43	109.77
4	F	508[A]	NAD	C4B-O4B-C1B	-4.99	104.46	109.77
4	D	507[A]	NAD	C4B-O4B-C1B	-4.99	104.46	109.77
4	B	507[A]	NAD	C4B-O4B-C1B	-4.98	104.47	109.77
4	E	507[A]	NAD	C4B-O4B-C1B	-4.97	104.48	109.77
4	A	507[A]	NAD	C4B-O4B-C1B	-4.95	104.50	109.77
4	C	508	NAD	C5N-C6N-N1N	-4.89	112.88	120.40
4	E	508	NAD	C5N-C6N-N1N	-4.88	112.90	120.40
4	A	508	NAD	C5N-C6N-N1N	-4.88	112.90	120.40
4	F	507	NAD	C5N-C6N-N1N	-4.88	112.91	120.40
4	D	508	NAD	C5N-C6N-N1N	-4.87	112.91	120.40
4	B	508	NAD	C5N-C6N-N1N	-4.86	112.93	120.40
4	A	507[B]	NAD	C5N-C6N-N1N	-4.76	113.09	120.40
4	F	508[B]	NAD	C5N-C6N-N1N	-4.75	113.10	120.40
4	C	507[B]	NAD	C5N-C6N-N1N	-4.74	113.11	120.40
4	E	507[B]	NAD	C5N-C6N-N1N	-4.74	113.12	120.40
4	D	507[B]	NAD	C5N-C6N-N1N	-4.72	113.14	120.40
4	B	507[B]	NAD	C5N-C6N-N1N	-4.72	113.15	120.40
4	C	507[A]	NAD	C5N-C6N-N1N	-4.59	113.34	120.40
4	E	507[A]	NAD	C5N-C6N-N1N	-4.59	113.35	120.40
4	A	507[A]	NAD	C5N-C6N-N1N	-4.58	113.35	120.40
4	F	508[A]	NAD	C5N-C6N-N1N	-4.58	113.37	120.40
4	D	507[A]	NAD	C5N-C6N-N1N	-4.55	113.41	120.40
4	B	507[A]	NAD	C5N-C6N-N1N	-4.54	113.42	120.40
4	D	507[B]	NAD	C5N-C4N-C3N	-4.48	115.08	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	507[B]	NAD	C5N-C4N-C3N	-4.47	115.09	120.35
4	F	508[B]	NAD	C5N-C4N-C3N	-4.45	115.12	120.35
4	C	507[B]	NAD	C5N-C4N-C3N	-4.44	115.13	120.35
4	B	507[B]	NAD	C5N-C4N-C3N	-4.43	115.13	120.35
4	E	507[B]	NAD	C5N-C4N-C3N	-4.42	115.15	120.35
4	A	507[A]	NAD	C5N-C4N-C3N	-4.36	115.22	120.35
4	C	507[A]	NAD	C5N-C4N-C3N	-4.36	115.22	120.35
4	F	508[A]	NAD	C5N-C4N-C3N	-4.35	115.23	120.35
4	D	507[A]	NAD	C5N-C4N-C3N	-4.33	115.25	120.35
4	B	507[A]	NAD	C5N-C4N-C3N	-4.32	115.27	120.35
4	E	507[A]	NAD	C5N-C4N-C3N	-4.31	115.28	120.35
4	A	507[A]	NAD	C3N-C7N-N7N	-3.97	113.24	117.77
4	F	508[A]	NAD	C3N-C7N-N7N	-3.94	113.28	117.77
4	B	507[A]	NAD	C3N-C7N-N7N	-3.93	113.28	117.77
4	C	507[A]	NAD	C3N-C7N-N7N	-3.93	113.29	117.77
4	D	507[A]	NAD	C3N-C7N-N7N	-3.93	113.29	117.77
4	E	507[A]	NAD	C3N-C7N-N7N	-3.89	113.33	117.77
4	E	508	NAD	C5N-C4N-C3N	-3.83	115.84	120.35
4	A	508	NAD	C5N-C4N-C3N	-3.80	115.87	120.35
4	B	508	NAD	C5N-C4N-C3N	-3.79	115.89	120.35
4	F	507	NAD	C5N-C4N-C3N	-3.79	115.90	120.35
4	D	508	NAD	C5N-C4N-C3N	-3.78	115.90	120.35
4	C	508	NAD	C5N-C4N-C3N	-3.77	115.92	120.35
4	E	508	NAD	C4B-O4B-C1B	-3.60	105.93	109.77
4	C	508	NAD	C4B-O4B-C1B	-3.60	105.94	109.77
4	D	508	NAD	C4B-O4B-C1B	-3.60	105.94	109.77
4	A	508	NAD	C4B-O4B-C1B	-3.58	105.96	109.77
4	B	508	NAD	C4B-O4B-C1B	-3.57	105.96	109.77
4	F	507	NAD	C4B-O4B-C1B	-3.52	106.02	109.77
4	D	507[B]	NAD	C3N-C7N-N7N	-3.30	114.01	117.77
4	B	507[B]	NAD	C3N-C7N-N7N	-3.30	114.01	117.77
4	C	507[B]	NAD	C3N-C7N-N7N	-3.28	114.03	117.77
4	F	508[B]	NAD	C3N-C7N-N7N	-3.27	114.04	117.77
4	E	507[B]	NAD	C3N-C7N-N7N	-3.26	114.05	117.77
4	A	507[B]	NAD	C3N-C7N-N7N	-3.26	114.05	117.77
4	A	507[A]	NAD	C3N-C2N-N1N	-2.83	117.58	120.43
4	D	507[A]	NAD	C3N-C2N-N1N	-2.82	117.59	120.43
4	C	507[A]	NAD	C3N-C2N-N1N	-2.81	117.60	120.43
4	B	507[A]	NAD	C3N-C2N-N1N	-2.79	117.62	120.43
4	F	508[A]	NAD	C3N-C2N-N1N	-2.78	117.63	120.43
4	E	507[A]	NAD	C3N-C2N-N1N	-2.75	117.66	120.43
4	C	508	NAD	O7N-C7N-C3N	-2.34	116.89	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	508	NAD	O7N-C7N-C3N	-2.31	116.92	119.62
4	A	508	NAD	O7N-C7N-C3N	-2.31	116.93	119.62
4	D	508	NAD	O7N-C7N-C3N	-2.30	116.93	119.62
4	F	507	NAD	O7N-C7N-C3N	-2.29	116.95	119.62
4	E	508	NAD	O7N-C7N-C3N	-2.28	116.95	119.62
4	F	507	NAD	C4D-O4D-C1D	-2.15	107.48	109.77
4	C	508	NAD	C4D-O4D-C1D	-2.14	107.49	109.77
4	D	508	NAD	C4D-O4D-C1D	-2.12	107.52	109.77
4	A	508	NAD	C4D-O4D-C1D	-2.11	107.52	109.77
4	B	508	NAD	C4D-O4D-C1D	-2.10	107.53	109.77
4	E	508	NAD	C4D-O4D-C1D	-2.10	107.53	109.77
4	B	507[A]	NAD	C1B-N9A-C4A	-2.03	123.13	126.64
4	E	507[A]	NAD	C1B-N9A-C4A	-2.02	123.14	126.64
4	F	508[A]	NAD	C1B-N9A-C4A	-2.02	123.14	126.64
4	C	507[A]	NAD	C1B-N9A-C4A	-2.01	123.17	126.64
4	D	507[A]	NAD	C1B-N9A-C4A	-2.00	123.17	126.64
4	D	507[B]	NAD	N6A-C6A-N1A	2.01	122.75	118.77
4	C	507[B]	NAD	N6A-C6A-N1A	2.03	122.78	118.77
4	F	508[B]	NAD	N6A-C6A-N1A	2.03	122.80	118.77
4	E	507[A]	NAD	O4B-C4B-C5B	2.04	116.30	109.40
4	D	507[A]	NAD	O4B-C4B-C5B	2.04	116.31	109.40
4	B	507[A]	NAD	O4B-C4B-C5B	2.04	116.31	109.40
4	A	507[B]	NAD	N6A-C6A-N1A	2.05	122.83	118.77
4	F	508[A]	NAD	O4B-C4B-C5B	2.05	116.32	109.40
4	E	507[B]	NAD	N6A-C6A-N1A	2.05	122.83	118.77
4	C	507[A]	NAD	O4B-C4B-C5B	2.05	116.33	109.40
4	B	507[B]	NAD	N6A-C6A-N1A	2.06	122.84	118.77
4	A	507[A]	NAD	O4B-C4B-C5B	2.06	116.35	109.40
4	B	507[B]	NAD	O2B-C2B-C3B	2.11	118.59	111.83
4	E	507[B]	NAD	O2B-C2B-C3B	2.12	118.61	111.83
4	D	507[B]	NAD	O2B-C2B-C3B	2.12	118.62	111.83
4	F	508[B]	NAD	O2B-C2B-C3B	2.12	118.63	111.83
4	A	507[B]	NAD	O7N-C7N-N7N	2.12	125.60	122.58
4	C	507[B]	NAD	O2B-C2B-C3B	2.13	118.65	111.83
4	E	507[B]	NAD	O7N-C7N-N7N	2.13	125.61	122.58
4	C	507[B]	NAD	O7N-C7N-N7N	2.13	125.62	122.58
4	A	507[B]	NAD	O2B-C2B-C3B	2.14	118.69	111.83
4	F	508[B]	NAD	O7N-C7N-N7N	2.15	125.64	122.58
4	B	508	NAD	O2N-PN-O1N	2.16	123.44	112.28
4	E	508	NAD	O2N-PN-O1N	2.16	123.44	112.28
4	C	508	NAD	O2N-PN-O1N	2.16	123.45	112.28
4	A	508	NAD	O2N-PN-O1N	2.16	123.46	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	507	NAD	O2N-PN-O1N	2.16	123.46	112.28
4	B	508	NAD	O7N-C7N-N7N	2.16	125.66	122.58
4	D	508	NAD	O2N-PN-O1N	2.16	123.47	112.28
4	C	507[A]	NAD	O5B-C5B-C4B	2.16	116.68	109.00
4	B	507[B]	NAD	O7N-C7N-N7N	2.17	125.67	122.58
4	A	507[A]	NAD	O5B-C5B-C4B	2.17	116.70	109.00
4	F	508[A]	NAD	O5B-C5B-C4B	2.17	116.71	109.00
4	A	508	NAD	O7N-C7N-N7N	2.18	125.68	122.58
4	B	507[A]	NAD	O5B-C5B-C4B	2.18	116.73	109.00
4	F	507	NAD	O7N-C7N-N7N	2.18	125.69	122.58
4	E	507[A]	NAD	O5B-C5B-C4B	2.18	116.74	109.00
4	C	508	NAD	O7N-C7N-N7N	2.19	125.69	122.58
4	E	508	NAD	O7N-C7N-N7N	2.19	125.69	122.58
4	D	507[A]	NAD	O5B-C5B-C4B	2.19	116.76	109.00
4	D	507[B]	NAD	O7N-C7N-N7N	2.19	125.69	122.58
4	D	508	NAD	O7N-C7N-N7N	2.19	125.70	122.58
4	C	507[B]	NAD	C2D-C3D-C4D	2.24	106.99	102.62
4	D	507[B]	NAD	C2D-C3D-C4D	2.25	107.00	102.62
4	F	508[B]	NAD	C2D-C3D-C4D	2.25	107.00	102.62
4	E	507[B]	NAD	C2D-C3D-C4D	2.25	107.01	102.62
4	A	507[B]	NAD	C2D-C3D-C4D	2.27	107.03	102.62
4	B	507[B]	NAD	C2D-C3D-C4D	2.27	107.04	102.62
4	C	507[B]	NAD	O2N-PN-O1N	2.37	124.56	112.28
4	D	507[B]	NAD	O2N-PN-O1N	2.37	124.57	112.28
4	F	508[B]	NAD	O2N-PN-O1N	2.38	124.58	112.28
4	A	507[B]	NAD	O2N-PN-O1N	2.38	124.58	112.28
4	E	507[B]	NAD	O2N-PN-O1N	2.38	124.59	112.28
4	B	507[B]	NAD	O2N-PN-O1N	2.38	124.62	112.28
4	C	507[B]	NAD	C2B-C3B-C4B	2.45	107.38	102.62
4	F	507	NAD	N6A-C6A-N1A	2.45	123.62	118.77
4	F	508[B]	NAD	C2B-C3B-C4B	2.45	107.39	102.62
4	B	507[B]	NAD	C2B-C3B-C4B	2.45	107.39	102.62
4	E	507[B]	NAD	C2B-C3B-C4B	2.45	107.39	102.62
4	A	507[B]	NAD	C2B-C3B-C4B	2.45	107.40	102.62
4	D	507[B]	NAD	C2B-C3B-C4B	2.46	107.42	102.62
4	C	508	NAD	N6A-C6A-N1A	2.47	123.66	118.77
4	A	508	NAD	N6A-C6A-N1A	2.48	123.68	118.77
4	B	508	NAD	N6A-C6A-N1A	2.49	123.69	118.77
4	D	508	NAD	N6A-C6A-N1A	2.49	123.71	118.77
4	E	508	NAD	N6A-C6A-N1A	2.50	123.72	118.77
3	D	506	AKG	C4-C3-C2	2.58	118.99	113.04
3	B	506	AKG	C4-C3-C2	2.58	118.99	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	AKG	C4-C3-C2	2.59	119.01	113.04
3	F	506	AKG	C4-C3-C2	2.59	119.03	113.04
3	E	506	AKG	C4-C3-C2	2.59	119.03	113.04
3	C	506	AKG	C4-C3-C2	2.60	119.05	113.04
4	C	507[A]	NAD	O7N-C7N-N7N	2.92	126.74	122.58
4	E	507[A]	NAD	O7N-C7N-N7N	2.95	126.78	122.58
4	D	507[A]	NAD	O7N-C7N-N7N	2.96	126.79	122.58
4	F	508[A]	NAD	O7N-C7N-N7N	2.96	126.79	122.58
4	B	507[A]	NAD	O7N-C7N-N7N	2.96	126.80	122.58
4	A	507[A]	NAD	O7N-C7N-N7N	2.98	126.82	122.58
4	D	507[A]	NAD	C6N-C5N-C4N	3.12	124.15	119.44
4	B	507[A]	NAD	C6N-C5N-C4N	3.13	124.17	119.44
4	F	508[A]	NAD	C6N-C5N-C4N	3.15	124.19	119.44
4	C	507[A]	NAD	C6N-C5N-C4N	3.15	124.20	119.44
4	E	507[A]	NAD	C6N-C5N-C4N	3.16	124.20	119.44
4	A	507[A]	NAD	C6N-C5N-C4N	3.16	124.20	119.44
4	E	507[B]	NAD	C6N-C5N-C4N	3.21	124.28	119.44
4	B	507[B]	NAD	C6N-C5N-C4N	3.23	124.31	119.44
4	C	507[B]	NAD	C6N-C5N-C4N	3.24	124.33	119.44
4	F	508[B]	NAD	C6N-C5N-C4N	3.25	124.34	119.44
4	A	507[B]	NAD	C6N-C5N-C4N	3.26	124.36	119.44
4	D	507[B]	NAD	C6N-C5N-C4N	3.26	124.36	119.44
4	B	508	NAD	C4A-C5A-N7A	3.28	112.58	109.41
4	A	508	NAD	C4A-C5A-N7A	3.32	112.62	109.41
4	F	507	NAD	C4A-C5A-N7A	3.33	112.62	109.41
4	D	508	NAD	C4A-C5A-N7A	3.33	112.63	109.41
4	C	508	NAD	C4A-C5A-N7A	3.36	112.65	109.41
4	E	508	NAD	C4A-C5A-N7A	3.36	112.66	109.41
4	A	507[A]	NAD	C2D-C3D-C4D	3.42	109.27	102.62
4	C	507[A]	NAD	C2D-C3D-C4D	3.42	109.28	102.62
4	E	507[A]	NAD	C2D-C3D-C4D	3.43	109.29	102.62
4	F	508[A]	NAD	C2D-C3D-C4D	3.43	109.30	102.62
4	B	507[A]	NAD	C2D-C3D-C4D	3.44	109.31	102.62
4	D	507[A]	NAD	C2D-C3D-C4D	3.44	109.32	102.62
3	D	506	AKG	C3-C4-C5	3.46	118.58	112.66
3	B	506	AKG	C3-C4-C5	3.47	118.60	112.66
3	A	506	AKG	C3-C4-C5	3.49	118.63	112.66
3	E	506	AKG	C3-C4-C5	3.50	118.64	112.66
3	C	506	AKG	C3-C4-C5	3.51	118.66	112.66
3	F	506	AKG	C3-C4-C5	3.51	118.66	112.66
4	D	508	NAD	C6N-C5N-C4N	3.80	125.16	119.44
4	B	508	NAD	C6N-C5N-C4N	3.80	125.17	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	507	NAD	C6N-C5N-C4N	3.80	125.18	119.44
4	A	508	NAD	C6N-C5N-C4N	3.82	125.20	119.44
4	C	508	NAD	C6N-C5N-C4N	3.83	125.22	119.44
4	E	508	NAD	C6N-C5N-C4N	3.83	125.22	119.44
4	B	507[B]	NAD	C2N-C3N-C4N	3.93	122.74	118.26
4	A	507[B]	NAD	C2N-C3N-C4N	3.94	122.76	118.26
4	C	507[B]	NAD	C2N-C3N-C4N	3.94	122.76	118.26
4	F	508[B]	NAD	C2N-C3N-C4N	3.95	122.76	118.26
4	D	507[B]	NAD	C2N-C3N-C4N	3.95	122.77	118.26
4	E	507[B]	NAD	C2N-C3N-C4N	3.95	122.77	118.26
4	C	508	NAD	C2N-C3N-C4N	4.02	122.85	118.26
4	B	508	NAD	C2N-C3N-C4N	4.04	122.87	118.26
4	A	508	NAD	C2N-C3N-C4N	4.06	122.89	118.26
4	F	507	NAD	C2N-C3N-C4N	4.08	122.92	118.26
4	D	508	NAD	C2N-C3N-C4N	4.09	122.92	118.26
4	E	508	NAD	C2N-C3N-C4N	4.10	122.94	118.26
4	E	507[A]	NAD	C2N-C3N-C4N	4.64	123.56	118.26
4	B	507[A]	NAD	C2N-C3N-C4N	4.67	123.58	118.26
4	F	508[A]	NAD	C2N-C3N-C4N	4.68	123.60	118.26
4	C	507[A]	NAD	C2N-C3N-C4N	4.69	123.61	118.26
4	D	507[B]	NAD	C2A-N1A-C6A	4.70	127.00	118.77
4	A	507[A]	NAD	C2N-C3N-C4N	4.71	123.63	118.26
4	D	507[A]	NAD	C2N-C3N-C4N	4.71	123.63	118.26
4	A	507[B]	NAD	C2A-N1A-C6A	4.72	127.02	118.77
4	C	507[B]	NAD	C2A-N1A-C6A	4.72	127.03	118.77
4	F	508[B]	NAD	C2A-N1A-C6A	4.72	127.03	118.77
4	E	507[B]	NAD	C2A-N1A-C6A	4.72	127.03	118.77
4	B	507[B]	NAD	C2A-N1A-C6A	4.74	127.07	118.77
3	C	506	AKG	O5-C2-C3	4.86	128.98	120.32
3	B	506	AKG	O5-C2-C3	4.87	129.00	120.32
4	D	507[A]	NAD	C2A-N1A-C6A	4.88	127.30	118.77
3	A	506	AKG	O5-C2-C3	4.88	129.01	120.32
3	E	506	AKG	O5-C2-C3	4.88	129.01	120.32
4	A	507[A]	NAD	C2A-N1A-C6A	4.88	127.31	118.77
4	F	508[A]	NAD	C2A-N1A-C6A	4.88	127.31	118.77
3	F	506	AKG	O5-C2-C3	4.89	129.03	120.32
4	C	507[A]	NAD	C2A-N1A-C6A	4.89	127.33	118.77
4	E	507[A]	NAD	C2A-N1A-C6A	4.89	127.33	118.77
4	B	507[A]	NAD	C2A-N1A-C6A	4.90	127.35	118.77
3	D	506	AKG	O5-C2-C3	4.91	129.06	120.32
4	F	507	NAD	C2A-N1A-C6A	6.08	129.40	118.77
4	B	508	NAD	C2A-N1A-C6A	6.09	129.42	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	508	NAD	C2A-N1A-C6A	6.09	129.42	118.77
4	A	508	NAD	C2A-N1A-C6A	6.09	129.43	118.77
4	E	508	NAD	C2A-N1A-C6A	6.10	129.44	118.77
4	D	508	NAD	C2A-N1A-C6A	6.11	129.46	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	PO4	2	0
2	A	503	PO4	1	0
2	A	504	PO4	2	0
2	A	505	PO4	1	0
3	A	506	AKG	6	0
4	A	507[A]	NAD	16	0
4	A	507[B]	NAD	6	0
4	A	508	NAD	10	0
2	B	502	PO4	1	0
2	B	503	PO4	2	0
2	B	504	PO4	1	0
2	B	505	PO4	2	0
3	B	506	AKG	7	0
4	B	507[A]	NAD	17	0
4	B	507[B]	NAD	7	0
4	B	508	NAD	11	0
2	C	502	PO4	1	0
2	C	503	PO4	2	0
2	C	504	PO4	1	0
2	C	505	PO4	2	0
3	C	506	AKG	7	0
4	C	507[A]	NAD	19	0
4	C	507[B]	NAD	7	0
4	C	508	NAD	12	0
2	D	502	PO4	1	0
2	D	503	PO4	2	0
2	D	504	PO4	2	0
2	D	505	PO4	1	0
3	D	506	AKG	7	0
4	D	507[A]	NAD	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	507[B]	NAD	7	0
4	D	508	NAD	11	0
2	E	502	PO4	1	0
2	E	503	PO4	2	0
2	E	504	PO4	2	0
2	E	505	PO4	1	0
3	E	506	AKG	7	0
4	E	507[A]	NAD	12	0
4	E	507[B]	NAD	7	0
4	E	508	NAD	11	0
2	F	502	PO4	2	0
2	F	503	PO4	1	0
2	F	504	PO4	2	0
2	F	505	PO4	1	0
3	F	506	AKG	7	0
4	F	507	NAD	12	0
4	F	508[A]	NAD	14	0
4	F	508[B]	NAD	7	0

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.