



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:56 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

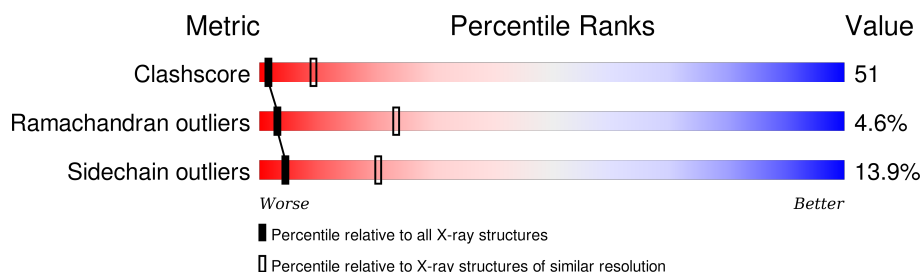
1 Overall quality at a glance

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (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 criteria:

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:

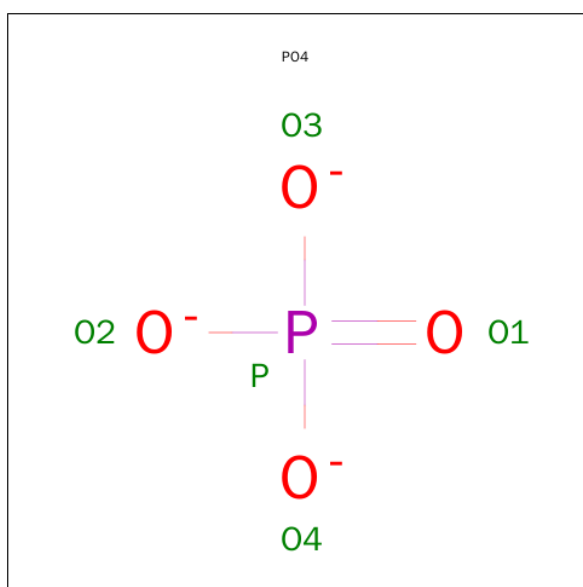
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO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

Continued on next page...

Continued from previous page...

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: O₄P).



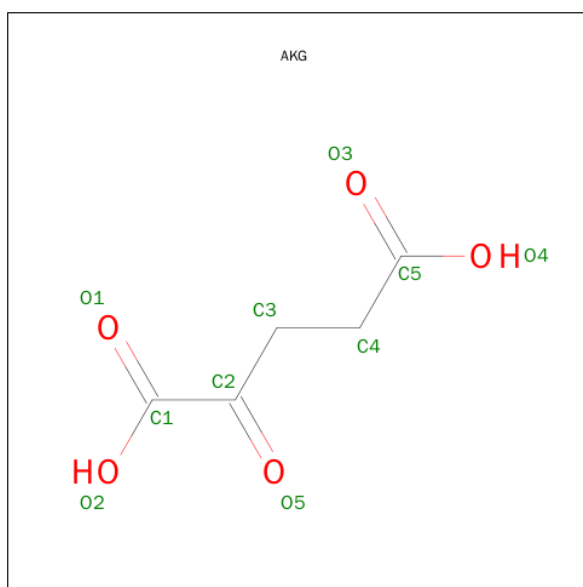
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

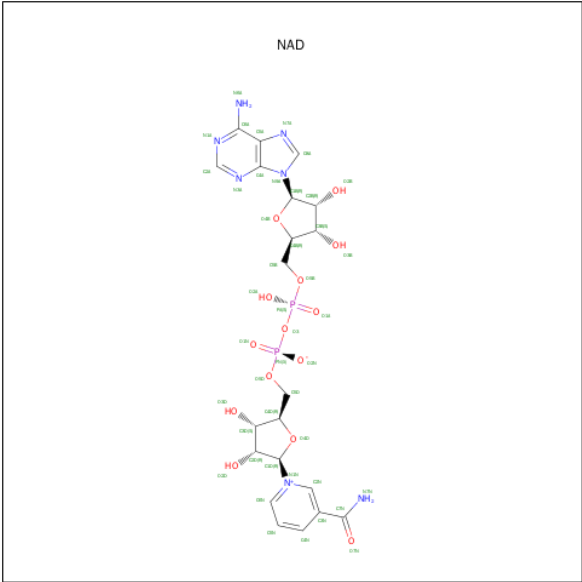
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total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

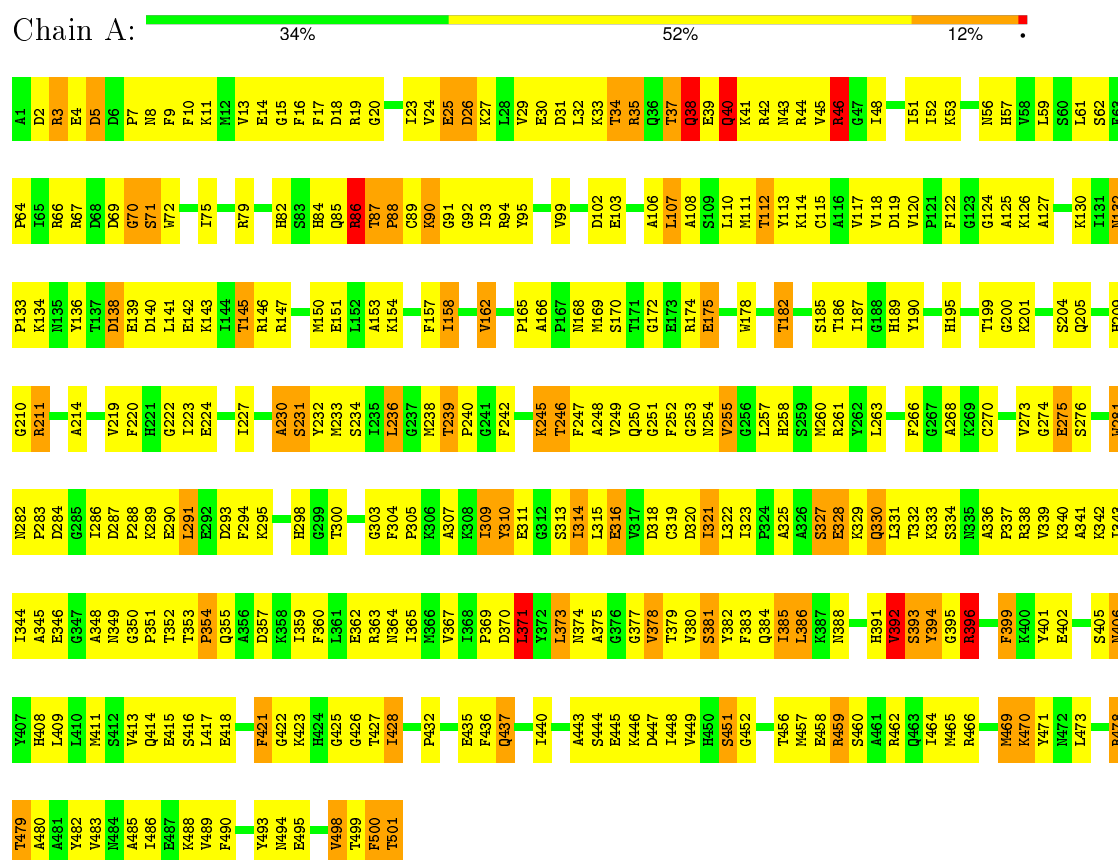
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	6	Total 6	O 6	0	0
5	C	6	Total 6	O 6	0	0
5	D	6	Total 6	O 6	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0

3 Residue-property plots

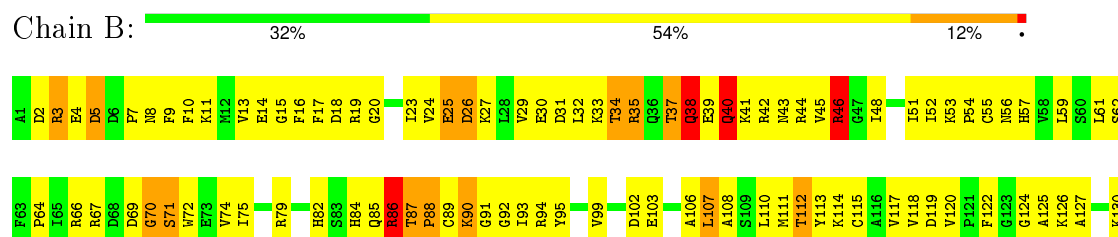
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

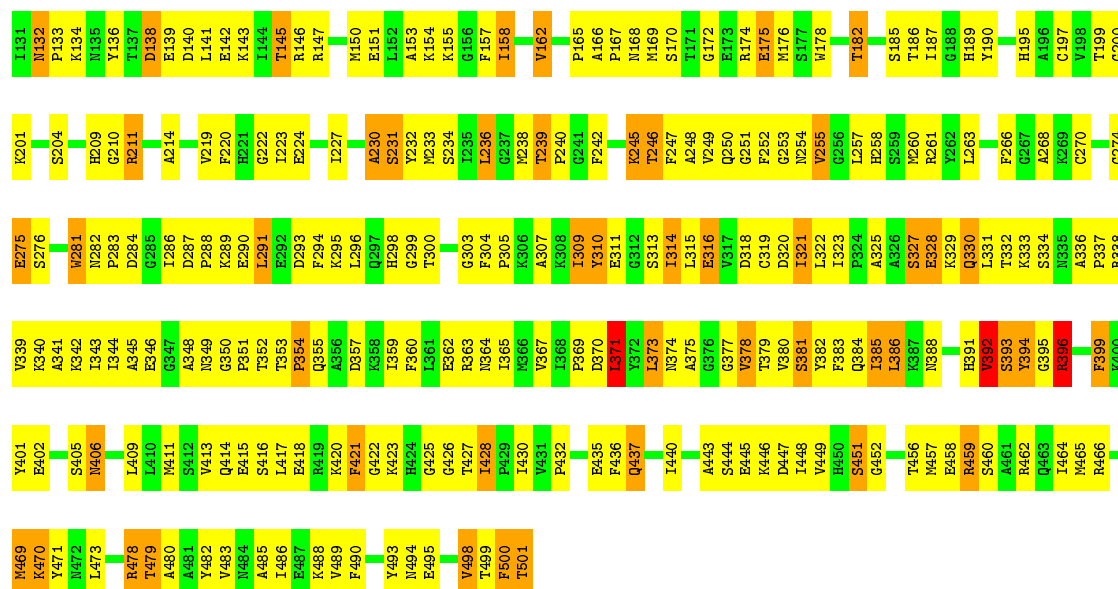
Note EDS was not executed.

• Molecule 1: GLUTAMATE DEHYDROGENASE

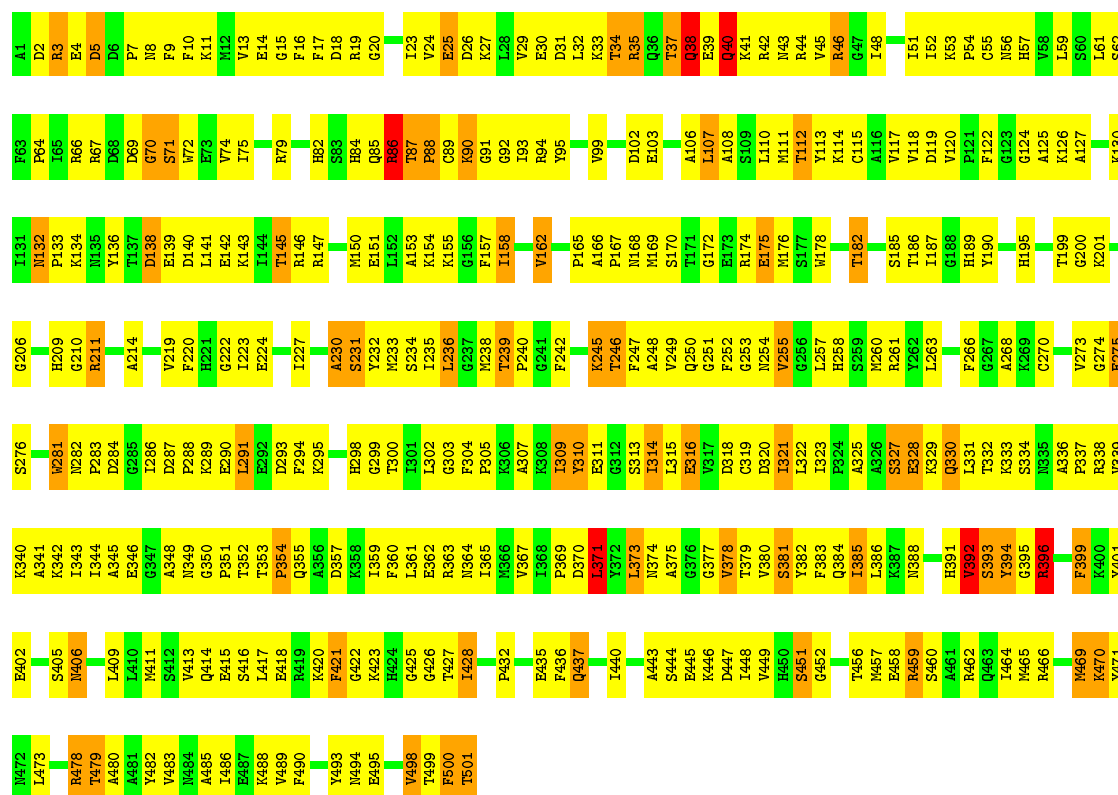


• Molecule 1: GLUTAMATE DEHYDROGENASE

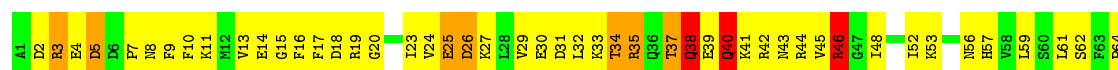


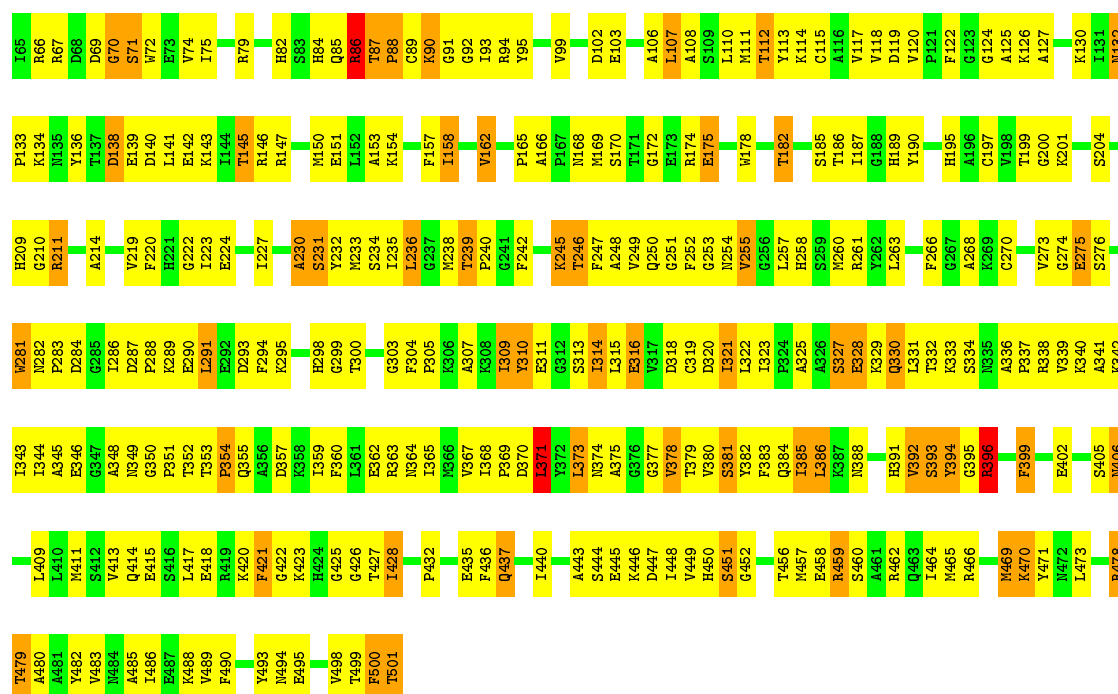


- Molecule 1: GLUTAMATE DEHYDROGENASE



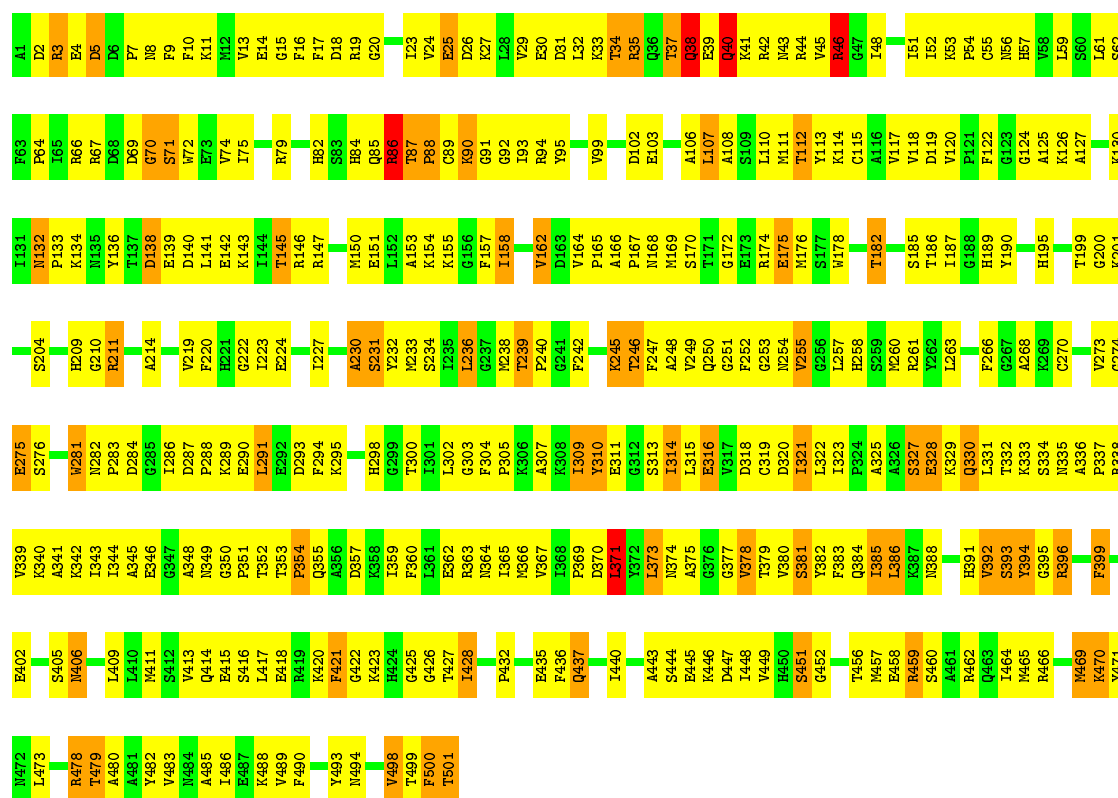
- Molecule 1: GLUTAMATE DEHYDROGENASE





• 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	D2
Y471	A341	A341	N281	H209	P133	I65	R3
N472	S405	K342	N282	G210	K134	R66	E4
L473	N406	I343	P283	R211	N135	R67	D5
	L409	I344	D284		Y136	D68	D6
R478	L410	A345	G285	A214	T137	D69	P7
T479	A346	E346	I286		D138	G70	N8
A480	M411	G347	D287	V219	E139	S71	F10
A481	A412	A348	D287	F220	D140	W72	F11
Y482	V413	N349	P288	H221	L141	E73	K11
V483	Q414	G350	K289	G222	E142	V74	K11
M484	E415	P351	E290	I223	L144	I75	V13
A485	S416	T352	L291	I224	T145		E14
L486	L417	T353	E292	E224	R146	R79	F16
E487	E418	P354	D293		R147		F17
K488	R419	Q355	F294	I227	M150	H82	D18
V489	K420	K356	K295		E151	S83	R19
F490	F421	D357		A230	L152	R84	G10
	G422	K358	H298	S231	A153	Q85	R20
Y493	K423	I359	G299	Y232	K154	R86	V24
N494	H424	F360	T300	M233	K155	P88	E25
E495	G425	L361	I301	S234	G156	C89	D26
	G426	E362	L302	I235	F157	G91	K27
V498	T427	R363	G303	L236	T158	G92	L28
T499	L428	N364	F304	G237		R93	V29
F500	P429	I365	P305	M238	V162	R94	E30
	L430	K366	K306	T239		D91	D31
T501	V431	V367	A307	P240	P165	Y95	
	P432	L366	K308	G241	A166		
		P369	I309	F242	P167	V99	
	E435	D370	Y310		K245	D102	K33
	F436	L371	E311	R246	N168	E103	T34
	Q437	Y372	G312	F247	M169	A106	R35
		L373	S313	A248	S170	L107	Q36
	L440	N374	I314	V249	T171	E108	T37
		A375	L315			S109	Q38
	A443	G376	E316	Q250	G172	L110	E39
	S444	G377	V317	G251	E173	M111	K41
	E445	V378	D318	F252	E175	L112	R42
	K446	T379	C319	G253	M176	K114	M43
	D447	V380	D320	N254	S177	Y113	M44
	L448	S381	I321	V255	H178	G115	V45
	V449	Y382	L322	G256	T182	E116	R46
	H450	F383	I323	L287		V117	G47
	S451	Q384	P324	H258	S185	I118	I48
	G452	L385	A325	S259	T186	D119	
		L386	A326	K260	G188	V120	K53
	T456	F387	S327	R261	H189	P121	P54
	M457	N388	E328	Y262	Y190	F122	C55
	E458		K329	L263	H195	G123	N56
	R459	H391	Q330	F266	T199	A124	F58
	S460	V392	L331	G267	G200	K126	S60
	L461	S393	T332	K269	K201	A127	L61
	R462	I394	K333	A268			S62
	Q463	G395	S334	K269			
	L464	R396	A335	C270			
	M465			V273			
	R466	F399	P337	G274			
		L469	R339	C273			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

Continued on next page...

Continued from previous page...

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:F:391:HIS:HA	4:F:508[A]:NAD:O3D	0.80	0.98
1:D:153:ALA:HB1	1:D:187:ILE:HD11	1.41	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:378:VAL:HG12	3:C:506:AKG:O4	1.65	0.96
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.46	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:B:107:LEU:HB3	1:B:126:LYS:HG2	1.46	0.95
1:A:378:VAL:HG12	3:A:506:AKG:O4	1.65	0.95

Continued on next page...

Continued from previous page...

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:209:HIS:HD2	2:A:502:PO4:O3	1.51	0.93
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.51	0.93
1:D:209:HIS:HD2	2:D:503:PO4:O3	1.51	0.93
2:F:502:PO4:O4	5:F:513:HOH:O	1.86	0.93
1:F:209:HIS:HD2	2:F:504:PO4:O3	1.51	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:417:LEU:HD21	1:F:417:LEU:CD1	2.00	0.92
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.51	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: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:C:82:HIS:CD2	1:C: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:D:219:VAL:HG22	1:D:373:LEU:HD13	1.55	0.89
1:A:219:VAL:HG22	1:A: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:F:462:ARG:HH21	1:F:466:ARG:HH22	1.21	0.88
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
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

Continued on next page...

Continued from previous page...

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
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
2:B:505:PO4:O3	5:B:510:HOH:O	1.91	0.88
1:E:370:ASP:HB2	1:E:374:ASN:HD21	1.39	0.88
2:A:505:PO4:O2	5:A:510:HOH:O	1.93	0.87
1:B:142:GLU:HG2	1:B:146:ARG:HD2	1.55	0.87
1:B:370:ASP:HB2	1:B:374:ASN:HD21	1.39	0.87
1:D:323:ILE:HG12	1:D:345:ALA:HB3	1.53	0.87
1:C:462:ARG:HH21	1:C:466:ARG:HH22	1.21	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
2:E:505:PO4:O2	5:E:512:HOH:O	1.93	0.87
1:E:323:ILE:HG12	1:E:345:ALA:HB3	1.53	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:C:209:HIS:CD2	2:C:503:PO4:O3	2.29	0.86
1:B:462:ARG:HH21	1:B:466:ARG:HH22	1.21	0.86
2:D:505:PO4:O2	5:D:510:HOH:O	1.93	0.86
1:F:209:HIS:CD2	2:F:504:PO4:O3	2.29	0.86
1:A:462:ARG:HH21	1:A:466:ARG:HH22	1.21	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:D:209:HIS:CD2	2:D:503:PO4:O3	2.29	0.85
2:C:504:PO4:O2	5:C:510:HOH:O	1.93	0.85
1:B:72:TRP:CZ3	1:E:499:THR:HG22	2.12	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

Continued on next page...

Continued from previous page...

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:B:9:PHE:HE1	1:B:107:LEU:HD13	1.43	0.84
1:A:141:LEU:O	1:A:145:THR:HG23	1.77	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:D:118:VAL:HG21	1:D:375:ALA:HB1	1.59	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: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:118:VAL:HG21	1:C:375:ALA:CB	2.09	0.83
1:C:141:LEU:O	1:C:145:THR:HG23	1.77	0.83
1: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:D:391:HIS:HD2	4:D:507[A]:NAD:HO2N	1.26	0.83
1:A:118:VAL:HG21	1:A:375:ALA:CB	2.09	0.83
2:B:502:PO4:O2	5:B:512:HOH:O	1.95	0.82
1:D:87:THR:H	4:E:507[A]:NAD:H72N	1.27	0.82
1:B:118:VAL:HG21	1:B:375:ALA:CB	2.09	0.82
1:D:118:VAL:HG21	1:D:375:ALA:CB	2.09	0.82
1:E:118:VAL:HG21	1:E:375:ALA:CB	2.09	0.82
1:C:46:ARG:HH11	1:C:46:ARG:HG3	1.44	0.82
1:E:9:PHE:HE1	1:E:107:LEU:HD13	1.43	0.82
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.44	0.82
2:A:504:PO4:O3	5:A:514:HOH:O	1.97	0.82
1:B:141:LEU:O	1:B:145:THR:HG23	1.77	0.82
1: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:118:VAL:HG21	1:C:375:ALA:HB1	1.59	0.82
1:C:242:PHE:HB3	1:C:268:ALA:HB2	1.62	0.82
1:C:87:THR:H	4:D:507[A]:NAD:H72N	1.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:507[A]:NAD:H72N	1:E:87:THR:H	1.27	0.81
1:C:87:THR:CG2	1:D:195:HIS:HE1	1.93	0.81
4:A:507[A]:NAD:H72N	1:B:87:THR:H	1.27	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:46:ARG:HH11	1:F:46:ARG:HG3	1.44	0.80
1:F:242:PHE:HB3	1:F:268:ALA:HB2	1.62	0.80
1:F:391:HIS:HA	4:F:508[A]:NAD:C3D	2.11	0.80
3:A:506:AKG:O2	4:A:508:NAD:C5N	2.29	0.80
3:F:506:AKG:O2	4:F:507:NAD:C5N	2.29	0.80
1:B:242:PHE:HB3	1:B:268:ALA:HB2	1.62	0.80
1:E:242:PHE:HB3	1:E:268:ALA:HB2	1.62	0.80
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:A:87:THR:H	4:F:508[A]:NAD:H72N	1.27	0.79
1:D:275:GLU:OE1	4:D:508:NAD:H1B	1.83	0.79
1:C:275:GLU:OE1	4:C:508:NAD:H1B	1.83	0.79
1: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:C:282:ASN:ND2	1:C:284:ASP:H	1.84	0.75
1:A:313:SER:HB3	1:A:316:GLU:HB2	1.68	0.75

Continued on next page...

Continued from previous page...

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:D:282:ASN:ND2	1:D:284:ASP:H	1.84	0.75
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.69	0.75
1:B:298:HIS:O	1:B:300:THR:HG22	1.87	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:457:MET:HA	1:C:457:MET:HE2	1.69	0.74
1:C:2:ASP:HB3	1:C:5:ASP:O	1.88	0.74
1:C:195:HIS:HE1	1:E:87:THR:HG23	1.52	0.74
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.69	0.74
1:D:313:SER:HB3	1:D:316:GLU:HB2	1.68	0.74
1:A:391:HIS:HA	4:A:507[A]:NAD:C3D	2.15	0.74
1:D:298:HIS:O	1:D:300:THR:HG22	1.87	0.73
1:E:2:ASP:HB3	1:E:5:ASP:O	1.87	0.73
1:A:24:VAL:HG13	1:A:483:VAL:HG22	1.70	0.73
1:E:313:SER:HB3	1:E:316:GLU:HB2	1.68	0.73
1:C:313:SER:HB3	1:C:316:GLU:HB2	1.68	0.73
1:F:282:ASN:ND2	1:F:284:ASP:H	1.84	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:C:391:HIS:HA	4:C:507[A]:NAD:C3D	2.16	0.73
1:A:195:HIS:HE1	1:B:87:THR:CG2	2.01	0.73
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.69	0.73
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.69	0.73
1:A:457:MET:HA	1:A:457:MET:HE2	1.71	0.73
1:E:24:VAL:HG13	1:E:483:VAL:HG22	1.71	0.73
1:F:24:VAL:HG13	1:F:483:VAL:HG22	1.71	0.73
1:F:2:ASP:HB3	1:F:5:ASP:O	1.88	0.73
1:E:20:GLY:O	1:E:24:VAL:HG22	1.89	0.73
1:B:195:HIS:CE1	1:F:87:THR:HG23	2.24	0.72
1:D:20:GLY:O	1:D:24:VAL:HG22	1.89	0.72
1:B:195:HIS:HE1	1:F:87:THR:HG23	1.51	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:HIS:CE1	1:E:87:THR:HG23	2.24	0.72
1:D:87:THR:CG2	1:E:195:HIS:HE1	2.02	0.72
1:B:20:GLY:O	1:B:24:VAL:HG22	1.89	0.72
1:D:457:MET:HE2	1:D:457:MET:HA	1.71	0.72
1:A:20:GLY:O	1:A:24:VAL:HG22	1.89	0.72
1:A:499:THR:HG22	1:D:72:TRP:CZ3	2.23	0.72
1:F:20:GLY:O	1:F:24:VAL:HG22	1.89	0.72
1:A:66:ARG:H	1:D:501:THR:HG22	1.55	0.72
1:B:303:GLY:H	1:B:309:ILE:HD11	1.55	0.72
1:C:72:TRP:CZ3	1:F:499:THR:HG22	2.23	0.72
1:D:24:VAL:HG13	1:D:483:VAL:HG22	1.70	0.72
1:C:239:THR:HG22	1:C:245:LYS:HE3	1.72	0.72
1:A:391:HIS:HA	4:A:507[A]:NAD:HO3N	0.91	0.72
1:A:239:THR:HG22	1:A:245:LYS:HE3	1.72	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:B:195:HIS:HE1	1:F:87:THR:HG21	1.54	0.71
1:C:303:GLY:H	1:C:309:ILE:HD11	1.55	0.71
1:A:417:LEU:HD21	1:B:417:LEU:CD1	2.20	0.71
1:C:310:TYR:HD1	1:C:311:GLU:N	1.88	0.71
1:F:310:TYR:HD1	1:F:311:GLU:N	1.88	0.71
1:E:418:GLU:OE2	1:E:427:THR:HA	1.91	0.71
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.71	0.71
1:A:418:GLU:OE2	1:A:427:THR:HA	1.91	0.71
1:F:136:TYR:HB3	1:F:140:ASP:HB2	1.72	0.71
1:A:136:TYR:HB3	1:A:140:ASP:HB2	1.72	0.71
1:A:391:HIS:CA	4:A:507[A]:NAD:HO3N	1.74	0.71
1:D:23:ILE:HD13	1:D:473:LEU:HD21	1.73	0.71
1:B:418:GLU:OE2	1:B:427:THR:HA	1.91	0.71
1:B:421:PHE:HE1	1:F:421:PHE:HE1	1.38	0.71
1: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: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
3:E:506:AKG:C1	4:E:508:NAD:C5N	2.69	0.71
1:E:23:ILE:HD13	1:E:473:LEU:HD21	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:H	1:A:309:ILE:HD11	1.55	0.71
1:B:7:PRO:HD2	1:B:329:LYS:HD2	1.73	0.71
1:E:310:TYR:HD1	1:E:311:GLU:N	1.88	0.71
1:E:239:THR:HG22	1:E:245:LYS:HE3	1.72	0.71
1:A:7:PRO:HD2	1:A:329:LYS:HD2	1.73	0.71
1:D:7:PRO:HD2	1:D:329:LYS:HD2	1.73	0.71
1:C:136:TYR:HB3	1:C:140:ASP:HB2	1.72	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:B:417:LEU:CD2	1:F:417:LEU:CD1	2.69	0.70
1:D:310:TYR:HD1	1:D:311:GLU:N	1.88	0.70
1:F:23:ILE:HD13	1:F:473:LEU:HD21	1.73	0.70
1:B:310:TYR:HD1	1:B:311:GLU:N	1.88	0.70
1:D:500:PHE:HE2	1:E:185:SER:HB2	1.56	0.70
1:C:418:GLU:OE2	1:C:427:THR:HA	1.91	0.70
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.73	0.70
1:F:239:THR:HG22	1:F:245:LYS:HE3	1.72	0.70
1:C:417:LEU:HD21	1:E:417:LEU:CD1	2.20	0.70
3:C:506:AKG:C1	4:C:508:NAD:C5N	2.69	0.70
3:A:506:AKG:C1	4:A:508:NAD:C5N	2.69	0.70
3:F:506:AKG:C1	4:F:507:NAD:C5N	2.69	0.70
1:D:418:GLU:OE2	1:D:427:THR:HA	1.91	0.70
1:D:378:VAL:CG1	3:D:506:AKG:O4	2.39	0.70
3:B:506:AKG:C1	4:B:508:NAD:C5N	2.69	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:F:87:THR:OG1	1:F:88:PRO:HD3	1.92	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:D:239:THR:HG22	1:D:245:LYS:HE3	1.72	0.69
1:D:132:ASN:HD21	1:D:134:LYS:HG3	1.56	0.69
1:C:7:PRO:HD2	1:C:329:LYS:HD2	1.73	0.69

Continued on next page...

Continued from previous page...

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: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:17:PHE:HA	1:A:482:TYR:CD2	2.28	0.69
1:A:25:GLU:O	1:A:29:VAL:HG23	1.92	0.69
1:A:428:ILE:N	1:A:428:ILE:HD13	2.07	0.69
1:E:132:ASN:HD21	1:E:134:LYS:HG3	1.56	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:D:428:ILE:N	1:D:428:ILE:HD13	2.08	0.69
1:D:87:THR:OG1	1:D:88:PRO:HD3	1.92	0.69
1:B:239:THR:HG22	1:B:245:LYS:HE3	1.72	0.69
1:E:460:SER:O	1:E:464:ILE:HG13	1.92	0.69
1:A:444:SER:OG	1:A:446:LYS:HG2	1.93	0.69
1:E:17:PHE:HA	1:E:482:TYR:CD2	2.28	0.69
1:B:25:GLU:O	1:B:29:VAL:HG23	1.92	0.69
1:C:46:ARG:HG3	1:C:46:ARG:NH1	2.07	0.69
1:A:72:TRP:CZ3	1:D:499:THR:HG22	2.28	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:17:PHE:HA	1:B:482:TYR:CD2	2.28	0.69
1:F:391:HIS:N	4:F:508[A]:NAD:O3D	2.25	0.69
1:E:391:HIS:HD2	4:E:507[A]:NAD:HO2N	1.39	0.69
1:E:428:ILE:N	1:E:428:ILE:HD13	2.07	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:303:GLY:H	1:E:309:ILE:HD11	1.55	0.69
1:D:136:TYR:HB3	1:D:140:ASP:HB2	1.72	0.69
1:A:132:ASN:HD21	1:A:134:LYS:HG3	1.56	0.69
1:A:87:THR:OG1	1:A:88:PRO:HD3	1.92	0.69
4:B:507[B]:NAD:H2D	1:F:459:ARG:NH2	2.07	0.69
1:B:444:SER:OG	1:B:446:LYS:HG2	1.93	0.69
1:F:378:VAL:CG1	3:F:506:AKG:O4	2.39	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:F:428:ILE:N	1:F:428:ILE:HD13	2.07	0.69
1:F:17:PHE:HA	1:F:482:TYR:CD2	2.28	0.69
1:B:499:THR:HG22	1:E:72:TRP:CZ3	2.26	0.69
1:F:31:ASP:O	1:F:33:LYS:HG2	1.93	0.68
1:C:428:ILE:HD13	1:C:428:ILE:N	2.07	0.68
1:B:460:SER:O	1:B:464:ILE:HG13	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HA	1:A:75:ILE:O	1.93	0.68
1:D:460:SER:O	1:D:464:ILE:HG13	1.92	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:87:THR:HG23	1:F:195:HIS:HE1	1.57	0.68
1:C:499:THR:HG22	1:F:72:TRP:HZ3	1.57	0.68
1:A:460:SER:O	1:A:464:ILE:HG13	1.92	0.68
1:F:62:SER:HA	1:F:75:ILE:O	1.93	0.68
1:D:17:PHE:HA	1:D:482:TYR:CD2	2.28	0.68
1:C:87:THR:OG1	1:C:88:PRO:HD3	1.92	0.68
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.07	0.68
1:D:29:VAL:HG21	1:D:42:ARG:HG2	1.76	0.68
1:C:444:SER:OG	1:C:446:LYS:HG2	1.93	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:E:31:ASP:O	1:E:33:LYS:HG2	1.93	0.68
1:D:444:SER:OG	1:D:446: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:F:391:HIS:HD2	4:F:508[A]:NAD:HO2N	1.40	0.67
1:C:142:GLU:O	1:C:146:ARG:HG3	1.94	0.67
1:B:195:HIS:CE1	1:F:87:THR:CG2	2.74	0.67
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.07	0.67
1:A:499:THR:HG22	1:D:72:TRP:HZ3	1.60	0.67
1:D:142:GLU:O	1:D:146:ARG:HG3	1.94	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:E:142:GLU:O	1:E:146:ARG:HG3	1.94	0.67
1:D:62:SER:HA	1:D:75:ILE:O	1.93	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

Continued on next page...

Continued from previous page...

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:F:32:LEU:HD11	1:F:34:THR:OG1	1.94	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:142:GLU:O	1:F:146:ARG:HG3	1.94	0.67
1:B:378:VAL:CG1	3:B:506:AKG:O4	2.39	0.67
1:B:32:LEU:HD11	1:B:34:THR:OG1	1.95	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:32:LEU:HD11	1:C:34:THR:OG1	1.94	0.67
1:C:29:VAL:HG21	1:C:42:ARG:HG2	1.76	0.67
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.24	0.67
1:D:417:LEU:CD1	1:E:417:LEU:HD21	2.25	0.67
1: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:D:339:VAL:HG22	1:D:363:ARG:HH21	1.61	0.66
1:A:190:TYR:CE2	1:B:162:VAL:HG11	2.31	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: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:C:72:TRP:HZ3	1:F:499:THR:HG22	1.59	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:87:THR:HG21	1:D:195:HIS:HE1	1.61	0.65
1:E:281:TRP:HB2	1:E:310:TYR:CD2	2.28	0.65
1:D:339:VAL:HG22	1:D:363:ARG:NH2	2.12	0.65
1:E:353:THR:HG23	1:E:354:PRO:HD2	1.79	0.65
1:A:411:MET:CE	1:A:415:GLU:HG3	2.26	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

Continued on next page...

Continued from previous page...

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:F:46:ARG:HG3	1:F:46:ARG:NH1	2.07	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:E:339:VAL:HG22	1:E:363:ARG:NH2	2.12	0.65
1:A:339:VAL:HG22	1:A:363:ARG:NH2	2.12	0.65
1:A:339:VAL:HG22	1:A:363:ARG:HH21	1.61	0.65
1:E:79:ARG:HG2	1:E:157:PHE:HB3	1.79	0.65
1:A:204:SER:OG	1:B:495:GLU:OE1	2.07	0.65
1:C:339:VAL:HG22	1:C:363:ARG:NH2	2.12	0.65
1:A:353:THR:HG23	1:A:354:PRO:HD2	1.79	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:D:40:GLN:NE2	1:D:40:GLN:HA	2.12	0.64
1:B:132:ASN:ND2	1:B:134:LYS:HG3	2.12	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:A:501:THR:HG22	1:D:66:ARG:H	1.61	0.64
1:D:87:THR:HG21	1:E:195:HIS:HE1	1.62	0.64
1:B:79:ARG:HG2	1:B:157:PHE:HB3	1.79	0.64
1:B:391:HIS:N	4:B:507[A]:NAD:O3D	2.29	0.64
1:A:153:ALA:HB1	1:A:187:ILE:CD1	2.25	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:B:411:MET:CE	1:B:415:GLU:HG3	2.26	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:40:GLN:NE2	1:A:40:GLN:HA	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:VAL:HG13	3:F:506:AKG:H31	1.81	0.63
1:C:40:GLN:HA	1:C:40:GLN:NE2	2.13	0.63
1:B:353:THR:HG23	1:B:354:PRO:HD2	1.79	0.63
1:E:378:VAL:HG13	3:E:506:AKG:H31	1.81	0.63
1:B:46:ARG:NH1	1:B:46:ARG:HG3	2.07	0.63
1:A:500:PHE:HE2	1:F:185:SER:HB2	1.63	0.63
1:D:79:ARG:HG2	1:D:157:PHE:HB3	1.79	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:C:107:LEU:HG	1:C:126:LYS:HE2	1.80	0.63
1:B:40:GLN:NE2	1:B:40:GLN:HA	2.12	0.63
1:E:107:LEU:HG	1:E: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:A:87:THR:HG23	1:F:195:HIS:CE1	2.33	0.63
1:C:391:HIS:C	4:C:507[A]:NAD:O3D	2.35	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:F:142:GLU:CG	1:F:146:ARG:HD2	2.29	0.62
1:E:281:TRP:CB	1:E:310:TYR:HD2	2.11	0.62
1:B:27:LYS:HA	1:B:30:GLU:HB3	1.81	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: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:B:64:PRO:HG2	1:E:499:THR:HG21	1.79	0.62
1:B:281:TRP:CB	1:B:310:TYR:HD2	2.11	0.62
1:F:5:ASP:OD2	1:F:332:THR:HB	1.99	0.62
1:A:409:LEU:HD11	1:B:409:LEU:HD22	1.81	0.62
1:D:391:HIS:C	4:D:507[A]:NAD:O3D	2.36	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:E:5:ASP:OD2	1:E:332:THR:HB	1.99	0.62
1:E:27:LYS:HA	1:E:30:GLU:HB3	1.81	0.62
1:A:378:VAL:HG13	3:A:506:AKG:H31	1.81	0.62
1:B:391:HIS:C	4:B:507[A]:NAD:O3D	2.35	0.62
1:D:107:LEU:HG	1:D:126:LYS:HE2	1.80	0.62
1:E:142:GLU:CG	1:E:146:ARG:HD2	2.29	0.62
1:C:27:LYS:HA	1:C:30:GLU:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

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
1:C:391:HIS:HA	4:C:507[A]:NAD:HO3N	0.79	0.61
4:A:507[B]:NAD:O1N	4:A:507[B]:NAD:H2B	2.01	0.61
1:B:224:GLU:HA	1:B:227:ILE:HG22	1.82	0.61
1:D:452:GLY:O	1:D:456:THR:HG23	2.00	0.61
1:C:378:VAL:HG13	3:C:506:AKG:H31	1.81	0.61
1:A:281:TRP:CB	1:A:310:TYR:HD2	2.11	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
4:D:507[B]:NAD:H2B	4:D:507[B]:NAD:O1N	2.00	0.61
4:C:507[B]:NAD:H2B	4:C:507[B]:NAD:O1N	2.01	0.61
1:B:378:VAL:HG13	3:B:506:AKG:H31	1.81	0.61
1:E:32:LEU:HG	1:E:41:LYS:HG2	1.82	0.61
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.31	0.61
1:B:51:ILE:HA	1:E:74:VAL:CG2	2.31	0.61
1:F:360:PHE:HD2	1:F:365:ILE:HD12	1.66	0.61
1:B:154:LYS:HD2	1:C:189:HIS:CD2	2.36	0.61
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.36	0.61
1:B:452:GLY:O	1:B:456:THR:HG23	2.00	0.61
4:B:507[B]:NAD:H2B	4:B:507[B]:NAD:O1N	2.00	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
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:C:24:VAL:CG1	1:C:483:VAL:HG13	2.31	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:B:281:TRP:HB2	1:B:310:TYR:CD2	2.28	0.61
1:A:411:MET:HE2	1:A:415:GLU:HG3	1.81	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:F:224:GLU:HA	1:F:227:ILE:HG22	1.82	0.61
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.31	0.61
1:D:393:SER:HB3	4:D:507[A]:NAD:PA	2.41	0.61
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.36	0.61

Continued on next page...

Continued from previous page...

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:E:252:PHE:CZ	1:E:291:LEU:HD13	2.36	0.60
1:D:360:PHE:HD2	1:D:365:ILE:HD12	1.66	0.60
1:A:281:TRP:CG	1:A:281:TRP:O	2.54	0.60
1:C:281:TRP:O	1:C:281:TRP:CG	2.54	0.60
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.36	0.60
4:E:507[B]:NAD:H2B	4:E:507[B]:NAD:O1N	2.00	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
1:C:360:PHE:HD2	1:C:365:ILE:HD12	1.66	0.60
4:F:508[B]:NAD:H2B	4:F:508[B]:NAD:O1N	2.01	0.60
1:E:219:VAL:HG22	1:E:373:LEU:CD1	2.30	0.60
1:A:224:GLU:HA	1:A:227:ILE:HG22	1.82	0.60
1:C:420:LYS:HZ2	1:E:428:ILE:HG23	1.66	0.60
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.36	0.60
1:F:391:HIS:C	4:F:508[A]:NAD:O3D	2.36	0.60
1:C:391:HIS:HD2	4:C:507[A]:NAD:HO2N	1.47	0.60
1:F:94:ARG:HH21	1:F:168:ASN:HD21	1.50	0.60
1:A:142:GLU:CG	1:A:146:ARG:HD2	2.29	0.60
1:D:281:TRP:O	1:D:281:TRP:CG	2.54	0.60
1:A:33:LYS:HA	1:A:41:LYS:NZ	2.16	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:B:69:ASP:O	1:B:71:SER:N	2.35	0.60
1:A:69:ASP:O	1:A:71:SER:N	2.35	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:F:393:SER:HB3	4:F:508[A]:NAD:PA	2.42	0.60
1:E:281:TRP:CG	1:E:281:TRP:O	2.54	0.60
1:E:94:ARG:HH21	1:E:168:ASN:HD21	1.49	0.60
1:C:33:LYS:HA	1:C:41:LYS:NZ	2.16	0.60
1:C:32:LEU:HG	1:C:41:LYS:HG2	1.82	0.60
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.31	0.60
1:D:69:ASP:O	1:D:71:SER:N	2.35	0.60
1:A:452:GLY:O	1:A:456:THR:HG23	2.00	0.60
1:C:87:THR:CG2	1:D:195:HIS:CE1	2.82	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:A:136:TYR:HB3	1:A:140:ASP:CB	2.32	0.60
1:F:258:HIS:HD2	1:F:261:ARG:NH1	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PHE:HD2	1:B:365:ILE:HD12	1.66	0.60
1:E:258:HIS:HD2	1:E:261:ARG:NH1	2.00	0.60
1:F:153:ALA:HB1	1:F:187:ILE:CD1	2.25	0.59
1:E:33:LYS:HA	1:E:41:LYS:NZ	2.16	0.59
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.31	0.59
1:C:411:MET:HE2	1:C:415:GLU:HG3	1.84	0.59
1:E:393:SER:HB3	4:E:507[A]:NAD:PA	2.42	0.59
1:C:136:TYR:HB3	1:C:140:ASP:CB	2.32	0.59
1:E:69:ASP:O	1:E:71:SER:N	2.35	0.59
1: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:142:GLU:CG	1:B:146:ARG:HD2	2.29	0.59
1:B:136:TYR:HB3	1:B:140:ASP:CB	2.32	0.59
1:E:360:PHE:HD2	1:E:365:ILE:HD12	1.66	0.59
1:C:276:SER:N	4:C:508:NAD:N3A	2.51	0.59
1:C:421:PHE:N	1:C:421:PHE:CD2	2.70	0.59
1:C:195:HIS:CE1	1:E:87:THR:HG21	2.35	0.59
1:D:459:ARG:NH2	4:E:507[B]:NAD:H6N	2.18	0.59
1:D:153:ALA:HB1	1:D:187:ILE:CD1	2.25	0.59
1:F:33:LYS:HA	1:F:41:LYS:NZ	2.16	0.59
1:B:411:MET:HE2	1:B:415:GLU:HG3	1.84	0.59
1:A:459:ARG:NH2	4:F:508[B]:NAD:H6N	2.18	0.59
1:E:178:TRP:O	1:E:182:THR:HG23	2.03	0.59
1:F:421:PHE:N	1:F:421:PHE:CD2	2.70	0.59
1:E:247:PHE:CZ	1:E:270:CYS:HB2	2.38	0.59
4:A:507[B]:NAD:H6N	1:B:459:ARG:NH2	2.18	0.59
1:D:219:VAL:HG22	1:D:373:LEU:CD1	2.30	0.59
1:C:178:TRP:O	1:C:182:THR:HG23	2.03	0.59
1:B:178:TRP:O	1:B:182:THR:HG23	2.03	0.59
1:C:500:PHE:HE2	1:D:185:SER:HB2	1.68	0.59
1:A:258:HIS:HD2	1:A:261:ARG:NH1	2.00	0.59
1:C:258:HIS:HD2	1:C:261:ARG:NH1	2.00	0.59
1:B:421:PHE:CD2	1:B:421:PHE:N	2.70	0.59
1:D:276:SER:N	4:D:508:NAD:N3A	2.51	0.59
1:A:178:TRP:O	1:A:182:THR:HG23	2.03	0.59
1:B:74:VAL:CG2	1:E:51:ILE:HA	2.32	0.59
1:D:411:MET:HE2	1:D:415:GLU:HG3	1.83	0.59
1:D:421:PHE:CD2	1:D:421:PHE:N	2.70	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:B:391:HIS:HD2	4:B:507[A]:NAD:HO2N	1.46	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:TRP:CB	1:F:310:TYR:HD2	2.11	0.58
1:A:238:MET:SD	1:A:342:LYS:CB	2.91	0.58
1:E:238:MET:SD	1:E:342:LYS:CB	2.91	0.58
1:D:238:MET:SD	1:D:342:LYS:CB	2.91	0.58
1:B:247:PHE:CZ	1:B:270:CYS:HB2	2.38	0.58
1:D:258:HIS:HD2	1:D:261:ARG:NH1	2.00	0.58
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.38	0.58
1:F:276:SER:N	4:F:507:NAD:N3A	2.51	0.58
1:D:142:GLU:CG	1:D:146:ARG:HD2	2.29	0.58
1:C:185:SER:HB2	1:E:500:PHE:HE2	1.68	0.58
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.68	0.58
1:A:185:SER:HB2	1:B:500:PHE:HE2	1.67	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:F:178:TRP:O	1:F:182:THR:HG23	2.03	0.58
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.68	0.58
1:B:260:MET:HE2	1:B:288:PRO:HG3	1.85	0.58
1:B:276:SER:N	4:B:508:NAD:N3A	2.51	0.58
1:A:276:SER:N	4:A:508:NAD:N3A	2.51	0.58
1:F:136:TYR:HB3	1:F:140:ASP:CB	2.32	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:C:92:GLY:HA2	1:C:166:ALA:O	2.04	0.58
1:B:185:SER:HB2	1:F:500:PHE:HE2	1.69	0.58
1:D:92:GLY:HA2	1:D:166:ALA:O	2.04	0.58
4:C:507[B]:NAD:H6N	1:E:459:ARG:NH2	2.18	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
1:F:437:GLN:O	1:F:440:ILE:HG22	2.04	0.58
1:E:92:GLY:HA2	1:E:166:ALA:O	2.04	0.58
1:C:459:ARG:NH2	4:D:507[B]:NAD:H6N	2.18	0.58
1:C:238:MET:SD	1:C:342:LYS:CB	2.92	0.58
1:B:51:ILE:HD11	1:E:72:TRP:HB3	1.84	0.58
1:E:421:PHE:CD2	1:E:421:PHE:N	2.70	0.58
1:D:258:HIS:CD2	1:D:261:ARG:NH1	2.72	0.58
1:A:437:GLN:O	1:A:440:ILE:HG22	2.04	0.58
4:B:507[B]:NAD:H6N	1:F:459:ARG:NH2	2.18	0.58
1:E:91:GLY:HA3	1:E:125:ALA:O	2.04	0.58
1:E:238:MET:HE3	1:E:320:ASP:HB3	1.86	0.58
1:D:136:TYR:HB3	1:D:140:ASP:CB	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:HIS:CD2	1:F:261:ARG:NH1	2.72	0.58
1:B:258:HIS:CD2	1:B:261:ARG:NH1	2.72	0.58
1:F:260:MET:HE2	1:F:288:PRO:HG3	1.86	0.58
1:D:247:PHE:CZ	1:D:270:CYS:HB2	2.38	0.58
1:B:395:GLY:HA3	1:B:399:PHE:CZ	2.39	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:C:91:GLY:HA3	1:C:125:ALA:O	2.04	0.58
1:E:276:SER:N	4:E:508:NAD:N3A	2.51	0.58
1:C:233:MET:HA	1:C:236:LEU:HB2	1.86	0.58
1:F:238:MET:SD	1:F:342:LYS:CB	2.91	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:E:258:HIS:CD2	1:E:261:ARG:NH1	2.72	0.58
1:C:258:HIS:CD2	1:C:261:ARG:NH1	2.72	0.58
1:D:395:GLY:HA3	1:D:399:PHE:CZ	2.39	0.58
1:B:91:GLY:HA3	1:B:125:ALA:O	2.04	0.57
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.69	0.57
1:A:258:HIS:CD2	1:A:261:ARG:NH1	2.72	0.57
1:E:395:GLY:HA3	1:E:399:PHE:CZ	2.39	0.57
1:F:395:GLY:HA3	1:F:399:PHE:CZ	2.39	0.57
1:D:437:GLN:O	1:D:440:ILE:HG22	2.04	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:B:94:ARG:HH21	1:B:168:ASN:HD21	1.50	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:C:409:LEU:HD22	1:D:409:LEU:HD11	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:E:41:LYS:O	1:E:45:VAL:HG23	2.05	0.57
1:D:233:MET:HA	1:D:236:LEU:HB2	1.86	0.57
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.87	0.57
1:F:219:VAL:HG22	1:F:373:LEU:CD1	2.30	0.57
1:A:233:MET:HA	1:A:236:LEU:HB2	1.86	0.57
1:A:92:GLY:HA2	1:A:166:ALA:O	2.04	0.57
1:E:153:ALA:HB1	1:E:187:ILE:CD1	2.25	0.57
1:C:94:ARG:HH21	1:C:168:ASN:HD21	1.50	0.57
1:B:219:VAL:HG22	1:B:373:LEU:CD1	2.30	0.57
1:B:250:GLN:O	1:B:325:ALA:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

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:D:91:GLY:HA3	1:D:125:ALA:O	2.04	0.57
1:C:41:LYS:O	1:C:45:VAL:HG23	2.05	0.57
1:F:233:MET:HA	1:F:236:LEU:HB2	1.86	0.57
1:B:233:MET:HA	1:B:236:LEU:HB2	1.86	0.57
1:D:238:MET:HE3	1:D:320:ASP:HB3	1.87	0.57
1:C:66:ARG:HG2	1:C:70:GLY:O	2.04	0.57
1:A:91:GLY:HA3	1:A:125:ALA:O	2.04	0.57
1:B:142:GLU:HG2	1:B:146:ARG:CD	2.33	0.57
1:C:37:THR:HG21	1:C:41:LYS:HE3	1.87	0.57
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.57
1: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:A:421:PHE:CD2	1:A:421:PHE:N	2.70	0.57
1:C:395:GLY:HA3	1:C:399:PHE:CZ	2.39	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:D:250:GLN:O	1:D:325:ALA:HB3	2.05	0.57
1:F:91:GLY:HA3	1:F:125:ALA:O	2.04	0.56
1:B:66:ARG:HG2	1:B:70:GLY:O	2.04	0.56
1:F:33:LYS:HD3	1:F:41:LYS:HZ3	1.69	0.56
1:C:72:TRP:HB3	1:F:51:ILE:HD11	1.86	0.56
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.69	0.56
1:E:437:GLN:O	1:E:440:ILE:HG22	2.04	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: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:B:139:GLU:OE2	1:B:143:LYS:HE3	2.05	0.56
1:E:250:GLN:O	1:E:325:ALA:HB3	2.05	0.56
1:C:153:ALA:HB1	1:C:187:ILE:CD1	2.25	0.56
1:F:254:ASN:HB3	4:F:507:NAD:O2N	2.06	0.56
1:A:37:THR:HG21	1:A:41:LYS:HE3	1.87	0.56
1:F:29:VAL:HG13	1:F:41:LYS:HB3	1.87	0.56
1:C:409:LEU:HD11	1:E:409:LEU:HD22	1.87	0.56
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.87	0.56
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.87	0.56
1:E:139:GLU:OE2	1:E:143:LYS:HE3	2.06	0.56
1: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ASN:HB3	4:E:508:NAD:O2N	2.06	0.56
1:A:41:LYS:O	1:A:45:VAL:HG23	2.05	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:337:PRO:HD3	1:D:359:ILE:HD13	1.88	0.56
1:B:117:VAL:HG21	1:B:371:LEU:HD13	1.87	0.56
1:F:117:VAL:HG21	1:F:371:LEU:HD13	1.87	0.56
1:E:411:MET:HE2	1:E:415:GLU:HG3	1.88	0.56
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.41	0.56
1:D:139:GLU:OE2	1:D:143:LYS:HE3	2.06	0.56
1:B:393:SER:HB3	4:B:507[A]:NAD:PA	2.45	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:B:421:PHE:HE1	1:F:421:PHE:CE1	2.21	0.56
1:E:260:MET:HE2	1:E:288:PRO:HG3	1.88	0.56
1:F:9:PHE:CE1	1:F:107:LEU:HD13	2.34	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: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:250:GLN:O	1:A:325:ALA:HB3	2.05	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:A:304:PHE:CD1	1:A:305:PRO:HD2	2.41	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:D:254:ASN:HB3	4:D:508:NAD:O2N	2.06	0.56
1:C:337:PRO:HD3	1:C:359:ILE:HD13	1.88	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: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:117:VAL:HG21	1:C:371:LEU:HD13	1.87	0.55
1:A:421:PHE:HD2	1:A:421:PHE:N	2.04	0.55
1:C:304:PHE:CD1	1:C:305:PRO:HD2	2.41	0.55
1:A:39:GLU:O	1:A:42:ARG:HB2	2.06	0.55
1:A:337:PRO:HD3	1:A:359:ILE:HD13	1.88	0.55
1:E:117:VAL:HG21	1:E:371:LEU:HD13	1.87	0.55
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASN:HB3	4:A:508:NAD:O2N	2.06	0.55
1:F:107:LEU:HB3	1:F:126:LYS:CG	2.30	0.55
1:B:118:VAL:HG12	1:B:118:VAL:O	2.06	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:C:238:MET:HE3	1:C:320:ASP:HB3	1.88	0.55
1:A:236:LEU:HD13	1:A:342:LYS:HB3	1.88	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:139:GLU:OE2	1:A:143:LYS:HE3	2.06	0.55
1:D:87:THR:HG23	1:E:195:HIS:HE1	1.70	0.55
1:D:9:PHE:CE1	1:D:107:LEU:HD13	2.34	0.55
1:A:35:ARG:O	1:A:37:THR:HG22	2.07	0.55
1:A:118:VAL:HG12	1:A:118:VAL:O	2.06	0.55
1:C:39:GLU:O	1:C:42:ARG:HB2	2.06	0.55
1:F:238:MET:HE3	1:F:320:ASP:HB3	1.88	0.55
1:E:337:PRO:HD3	1:E:359:ILE:HD13	1.88	0.55
1:B:254:ASN:HB3	4:B:508:NAD:O2N	2.06	0.55
1:D:112:THR:HG22	1:D:124:GLY:CA	2.32	0.55
1:B:35:ARG:O	1:B:37:THR:HG22	2.07	0.55
1:D:29:VAL:HG13	1:D:41:LYS:HB3	1.88	0.55
1:A:147:ARG:NH1	1:D:501:THR:OXT	2.40	0.55
1:C:250:GLN:OE1	1:C:315:LEU:HD21	2.07	0.55
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.41	0.55
1:F:462:ARG:NH2	1:F:466:ARG:HH22	2.00	0.55
1:F:369:PRO:HG2	1:F:478:ARG:HA	1.89	0.55
1:A:46:ARG:CG	1:A:46:ARG:HH11	2.18	0.55
1:A:436:PHE:CZ	1:F:409:LEU:HD12	2.42	0.55
1:D:33:LYS:HD3	1:D:41:LYS:HZ3	1.71	0.55
1:C:24:VAL:HG11	1:C:483:VAL:HG13	1.89	0.55
1:A:117:VAL:HG21	1:A:371:LEU:HD13	1.87	0.55
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.41	0.55
1:F:118:VAL:O	1:F:118:VAL:HG12	2.06	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:B:425:GLY:O	1:B:427:THR:N	2.40	0.55
1:E:250:GLN:OE1	1:E:315:LEU:HD21	2.07	0.55
1:F:122:PHE:HZ	1:F:385:ILE:HG21	1.72	0.55
1:E:39:GLU:O	1:E:42:ARG:HB2	2.06	0.55
1:A:72:TRP:HZ3	1:D:499:THR:HG22	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LEU:HD13	1:E:342:LYS:HB3	1.88	0.55
1:E:24:VAL:HG11	1:E:483:VAL:HG13	1.89	0.55
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.89	0.55
1:C:74:VAL:CG2	1:F:51:ILE:HA	2.37	0.55
1:E:425:GLY:O	1:E:427:THR:N	2.40	0.55
1:F:425:GLY:O	1:F:427:THR:N	2.40	0.55
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.05	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:F:95:TYR:OH	1:F:145:THR:HG22	2.07	0.54
1:F:35:ARG:O	1:F:37:THR:HG22	2.07	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:C:51:ILE:HD11	1:F:72:TRP:HB3	1.88	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:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.42	0.54
1:D:95:TYR:OH	1:D:145:THR:HG22	2.07	0.54
1:D:46:ARG:CG	1:D:46:ARG:HH11	2.18	0.54
1:D:236:LEU:HD13	1:D:342:LYS:HB3	1.88	0.54
1:B:421:PHE:HD2	1:B:421:PHE:N	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:250:GLN:OE1	1:D:315:LEU:HD21	2.07	0.54
4:B:507[A]:NAD:H6N	4:B:507[A]:NAD:O5D	2.08	0.54
1:E:87:THR:O	1:E:89:CYS:N	2.40	0.54
1:A:462:ARG:NH2	1:A:466:ARG:HH22	2.00	0.54
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.42	0.54
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.88	0.54
1:A:369:PRO:HG2	1:A:478:ARG:HA	1.89	0.54
1:B:250:GLN:OE1	1:B:315:LEU:HD21	2.07	0.54
1:C:122:PHE:HZ	1:C:385:ILE:HG21	1.72	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:A:33:LYS:HD3	1:A:41:LYS:HZ3	1.71	0.54
1:C:35:ARG:O	1:C:37:THR:HG22	2.07	0.54
1:F:29:VAL:HA	1:F:45:VAL:HG21	1.90	0.54
1:B:369:PRO:HG2	1:B:478:ARG:HA	1.89	0.54
1:C:369:PRO:HG2	1:C:478:ARG:HA	1.89	0.54
1:A:19:ARG:HD2	1:A:479:THR:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:PHE:CE1	1:E:155:LYS:HD2	2.42	0.54
1:C:260:MET:HE1	1:C:288:PRO:HA	1.89	0.54
1:A:250:GLN:OE1	1:A:315:LEU:HD21	2.07	0.54
1:F:250:GLN:OE1	1:F:315:LEU:HD21	2.07	0.54
1:B:122:PHE:HZ	1:B:385:ILE:HG21	1.72	0.54
1:D:87:THR:O	1:D:89:CYS:N	2.40	0.54
1:D:142:GLU:HG2	1:D:146:ARG:CD	2.33	0.54
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.42	0.54
1:D:425:GLY:O	1:D:427:THR:N	2.40	0.54
1:B:498:VAL:HB	1:E:72:TRP:CZ2	2.43	0.54
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.05	0.54
4:E:507[A]:NAD:H6N	4:E:507[A]:NAD:O5D	2.08	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
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:A:459:ARG:NH2	4:F:508[B]:NAD:C6N	2.71	0.54
4:B:507[B]:NAD:C6N	1:F:459:ARG:NH2	2.71	0.54
4:C:507[B]:NAD:C6N	1:E:459:ARG:NH2	2.71	0.54
1:F:112:THR:HG22	1:F:124:GLY:CA	2.32	0.54
1:C:310:TYR:CD1	1:C:311:GLU:N	2.75	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:C:201:LYS:NZ	1:C:388:ASN:HD21	2.05	0.54
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.06	0.54
1:C:459:ARG:NH2	4:D:507[B]:NAD:C6N	2.71	0.54
4:F:508[A]:NAD:O5D	4:F:508[A]:NAD:H6N	2.08	0.54
4:C:507[A]:NAD:H6N	4:C:507[A]:NAD:O5D	2.08	0.54
1:D:39:GLU:O	1:D:42:ARG:HB2	2.06	0.54
1:F:34:THR:HG21	1:F:44:ARG:NH1	2.23	0.54
1:C:318:ASP:HA	1:C:340:LYS:HG3	1.90	0.54
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.26	0.54
1:F:87:THR:O	1:F:89:CYS:N	2.40	0.54
4:C:507[B]:NAD:N3A	1:E:488:LYS:HB3	2.23	0.54
4:A:507[A]:NAD:O5D	4:A:507[A]:NAD:H6N	2.08	0.54
4:A:507[B]:NAD:C6N	1:B:459:ARG:NH2	2.71	0.54
1:D:459:ARG:NH2	4:E:507[B]:NAD:C6N	2.71	0.54
1:E:142:GLU:HG2	1:E:146:ARG:CD	2.34	0.54
1:E:19:ARG:HD2	1:E:479:THR:HG21	1.89	0.54
1:A:34:THR:HG21	1:A:44:ARG:NH1	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HA	1:A:45:VAL:HG21	1.90	0.54
1:E:35:ARG:O	1:E:37:THR:HG22	2.07	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:F:421:PHE:N	1:F:421:PHE:HD2	2.04	0.54
1:E:303:GLY:N	1:E:309:ILE:HD11	2.23	0.54
1:B:189:HIS:CD2	1:C:154:LYS:HD2	2.43	0.54
1:C:87:THR:O	1:C:89:CYS:N	2.40	0.54
4:A:507[B]:NAD:N3A	1:B:488:LYS:HB3	2.23	0.54
1:A:95:TYR:OH	1:A:145:THR:HG22	2.07	0.54
1:C:95:TYR:OH	1:C:145:THR:HG22	2.07	0.54
1:B:236:LEU:CD1	1:B:342:LYS:HB3	2.38	0.54
1:B:5:ASP:HB2	1:B:333:LYS:HE2	1.90	0.54
1:F:303:GLY:N	1:F:309:ILE:HD11	2.23	0.54
4:D:507[A]:NAD:H6N	4:D:507[A]:NAD:O5D	2.08	0.53
1:E:95:TYR:OH	1:E:145:THR:HG22	2.07	0.53
1:E:462:ARG:HE	1:E:466:ARG:NH2	2.06	0.53
1:D:318:ASP:HA	1:D:340:LYS:HG3	1.90	0.53
1:B:339:VAL:N	1:B:363:ARG:NH2	2.56	0.53
1:E:5:ASP:HB2	1:E:333:LYS:HE2	1.90	0.53
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.26	0.53
4:B:507[B]:NAD:N3A	1:F:488:LYS:HB3	2.23	0.53
1:E:391:HIS:C	4:E:507[A]:NAD:H4D	2.28	0.53
1:A:122:PHE:HZ	1:A:385:ILE:HG21	1.72	0.53
3:A:506:AKG:C1	4:A:508:NAD:H5N	2.39	0.53
1:F:236:LEU:CD1	1:F:342:LYS:HB3	2.38	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:C:239:THR:HG23	1:C:240:PRO:N	2.23	0.53
1:B:19:ARG:HD2	1:B:479:THR:HG21	1.89	0.53
1:D:17:PHE:HA	1:D:482:TYR:HD2	1.73	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
1:E:122:PHE:HZ	1:E:385:ILE:HG21	1.72	0.53
1:B:195:HIS:CE1	1:F:87:THR:HG21	2.39	0.53
1:E:369:PRO:HG2	1:E:478:ARG:HA	1.89	0.53
1:C:34:THR:HG21	1:C:44:ARG:NH1	2.23	0.53
1:C:236:LEU:CD1	1:C:342:LYS:HB3	2.38	0.53
1:B:238:MET:HE3	1:B:320:ASP:HB3	1.89	0.53
1:D:258:HIS:HA	1:D:261:ARG:HB2	1.91	0.53
1:B:447:ASP:O	1:B:451:SER:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:HIS:CD2	1:E:154:LYS:HD2	2.43	0.53
1:A:107:LEU:HB3	1:A:126:LYS:CG	2.30	0.53
1:E:112:THR:HG22	1:E:124:GLY:CA	2.32	0.53
1:A:462:ARG:HE	1:A:466:ARG:NH2	2.06	0.53
1:A:236:LEU:CD1	1:A:342:LYS:HB3	2.38	0.53
1:B:319:CYS:O	1:B:341:ALA:HA	2.09	0.53
1:E:239:THR:HG23	1:E:240:PRO:N	2.23	0.53
1:F:339:VAL:N	1:F:363:ARG:NH2	2.56	0.53
1:A:499:THR:CG2	1:D:64:PRO:HG2	2.39	0.53
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.89	0.53
1:A:17:PHE:HA	1:A:482:TYR:HD2	1.73	0.53
1:A:258:HIS:HA	1:A:261:ARG:HB2	1.91	0.53
1:F:274:GLY:CA	1:F:314:ILE:HG13	2.39	0.53
1:B:56:ASN:HD22	1:B:84:HIS:CD2	2.27	0.53
1:D:282:ASN:HD21	1:D:284:ASP:HB2	1.74	0.53
1:B:34:THR:HG21	1:B:44:ARG:NH1	2.23	0.53
1:D:29:VAL:HA	1:D:45:VAL:HG21	1.90	0.53
1:D:34:THR:HG21	1:D:44:ARG:NH1	2.23	0.53
1:E:236:LEU:CD1	1:E:342:LYS:HB3	2.38	0.53
1:D:319:CYS:O	1:D:341:ALA:HA	2.09	0.53
1:F:5:ASP:HB2	1:F:333:LYS:HE2	1.90	0.53
1:D:303:GLY:N	1:D:309:ILE:HD11	2.23	0.53
1:D:369:PRO:HG2	1:D:478:ARG:HA	1.89	0.53
1:B:117:VAL:HG23	1:B:485:ALA:HB2	1.91	0.53
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.06	0.53
1:D:447:ASP:O	1:D:451:SER:HB3	2.08	0.53
1:C:447:ASP:O	1:C:451:SER:HB3	2.08	0.53
1:E:447:ASP:O	1:E:451:SER:HB3	2.08	0.53
1:C:112:THR:HG22	1:C:124:GLY:CA	2.32	0.53
1:B:33:LYS:HD3	1:B:41:LYS:HZ3	1.74	0.53
1:A:239:THR:HG23	1:A:240:PRO:N	2.23	0.53
1:D:5:ASP:HB2	1:D:333:LYS:HE2	1.90	0.53
1:C:258:HIS:CD2	1:C:261:ARG:HH11	2.26	0.53
1:A:274:GLY:CA	1:A:314:ILE:HG13	2.39	0.53
1:D:274:GLY:CA	1:D:314:ILE:HG13	2.39	0.53
1:C:274:GLY:CA	1:C:314:ILE:HG13	2.39	0.53
1:C:56:ASN:HD22	1:C:84:HIS:CD2	2.27	0.53
1:C:488:LYS:HB3	4:D:507[B]:NAD:N3A	2.23	0.53
1:F:56:ASN:HD22	1:F:84:HIS:CD2	2.27	0.53
1:D:488:LYS:HB3	4:E:507[B]:NAD:N3A	2.23	0.53
1:F:462:ARG:HE	1:F:466:ARG:NH2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:HG2	1:C:146:ARG:CD	2.33	0.53
1:F:310:TYR:CD1	1:F:311:GLU:N	2.75	0.53
1:D:462:ARG:HE	1:D:466:ARG:NH2	2.06	0.53
1:B:95:TYR:OH	1:B:145:THR:HG22	2.07	0.53
1:A:319:CYS:O	1:A:341:ALA:HA	2.09	0.53
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.74	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:122:PHE:HZ	1:D:385:ILE:HG21	1.72	0.53
1:C:379:THR:O	1:C:382:TYR:HB3	2.09	0.53
1:A:488:LYS:HB3	4:F:508[B]:NAD:N3A	2.23	0.53
3:F:506:AKG:C1	4:F:507:NAD:H5N	2.39	0.53
1:E:19:ARG:NH2	1:E:478:ARG:HD2	2.24	0.53
1:E:282:ASN:HD21	1:E:284:ASP:HB2	1.74	0.53
1:D:310:TYR:CD1	1:D:311:GLU:N	2.75	0.53
1:F:282:ASN:HD21	1:F:284:ASP:HB2	1.74	0.53
1:E:258:HIS:HA	1:E:261:ARG:HB2	1.91	0.53
1:E:360:PHE:CD2	1:E:365:ILE:HD12	2.44	0.53
1:B:258:HIS:HA	1:B:261:ARG:HB2	1.91	0.53
1:D:379:THR:O	1:D:382:TYR:HB3	2.09	0.53
1:B:274:GLY:CA	1:B:314:ILE:HG13	2.39	0.53
1:D:107:LEU:HB3	1:D:126:LYS:CG	2.30	0.53
1:A:9:PHE:CE1	1:A:107:LEU:HD13	2.34	0.53
1:F:19:ARG:NH2	1:F:478:ARG:HD2	2.24	0.53
1:E:40:GLN:HA	1:E:43:ASN:HD22	1.74	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:D:239:THR:HG23	1:D:240:PRO:N	2.23	0.53
1:B:340:LYS:N	1:B:363:ARG:HH22	2.05	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:C:360:PHE:CD2	1:C:365:ILE:HD12	2.44	0.53
1:F:258:HIS:HA	1:F:261:ARG:HB2	1.91	0.53
1:B:360:PHE:CD2	1:B:365:ILE:HD12	2.44	0.53
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.26	0.53
1:E:48:ILE:O	1:E:52:ILE:HG13	2.09	0.53
1:C:162:VAL:HG11	1:D:190:TYR:CE2	2.44	0.53
1:C:29:VAL:HA	1:C:45:VAL:HG21	1.90	0.53
1:C:19:ARG:NH2	1:C:478:ARG:HD2	2.24	0.53
1:F:447:ASP:O	1:F:451:SER:HB3	2.09	0.53
1:C:200:GLY:HA2	1:C:211:ARG:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ALA:HB3	1:B:351:PRO:HG3	1.91	0.53
1:A:379:THR:O	1:A:382:TYR:HB3	2.09	0.53
3:C:506:AKG:C1	4:C:508:NAD:H5N	2.39	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:B:282:ASN:HD21	1:B:284:ASP:HB2	1.74	0.52
1:D:40:GLN:HA	1:D:43:ASN:HD22	1.74	0.52
1:C:46:ARG:HH11	1:C:46:ARG:CG	2.18	0.52
1:C:339:VAL:N	1:C:363:ARG:NH2	2.56	0.52
1:B:418:GLU:HG2	1:B:428:ILE:HG12	1.91	0.52
1:F:418:GLU:HG2	1:F:428:ILE:HG12	1.91	0.52
1:C:418:GLU:HG2	1:C: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:A:201:LYS:NZ	1:A:388:ASN:HD21	2.05	0.52
1:E:9:PHE:CE1	1:E:107:LEU:HD13	2.34	0.52
1:B:107:LEU:HB3	1:B:126:LYS:CG	2.30	0.52
1:F:19:ARG:HD2	1:F:479:THR:HG21	1.89	0.52
1:E:34:THR:HG21	1:E:44:ARG:NH1	2.23	0.52
1:A:334:SER:O	1:A:338:ARG:NH2	2.43	0.52
1:B:334:SER:O	1:B:338:ARG:NH2	2.43	0.52
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.36	0.52
1:C:303:GLY:N	1:C:309:ILE:HD11	2.23	0.52
1:E:117:VAL:HG23	1:E:485:ALA:HB2	1.91	0.52
1:C:258:HIS:HA	1:C:261:ARG:HB2	1.91	0.52
1:D:108:ALA:O	1:D:111:MET:HB2	2.09	0.52
1:C:48:ILE:O	1:C:52:ILE:HG13	2.09	0.52
1:A:56:ASN:HD22	1:A:84:HIS:CD2	2.27	0.52
1:D:87:THR:HG23	1:E:195:HIS:CE1	2.44	0.52
3:D:506:AKG:C1	4:D:508:NAD:H5N	2.39	0.52
1:D:236:LEU:CD1	1:D:342:LYS:HB3	2.38	0.52
1:F:318:ASP:HA	1:F:340:LYS:HG3	1.90	0.52
1:A:318:ASP:HA	1:A:340:LYS:HG3	1.90	0.52
1:C:5:ASP:HB2	1:C:333:LYS:HE2	1.90	0.52
1:A:348:ALA:HB3	1:A:351:PRO:HG3	1.91	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:F:108:ALA:O	1:F:111:MET:HB2	2.09	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:D:56:ASN:HD22	1:D:84:HIS:CD2	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:506:AKG:C1	4:B:508:NAD:H5N	2.39	0.52
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.31	0.52
1:A:108:ALA:O	1:A:111:MET:HB2	2.09	0.52
1:B:462:ARG:HE	1:B:466:ARG:NH2	2.06	0.52
1:D:246:THR:N	1:D:320:ASP:OD1	2.43	0.52
1:E:318:ASP:HA	1:E:340:LYS:HG3	1.90	0.52
1:C:66:ARG:NH1	1:C:70:GLY:HA2	2.25	0.52
1:C:108:ALA:O	1:C:111:MET:HB2	2.09	0.52
1:C:462:ARG:HE	1:C:466:ARG:NH2	2.06	0.52
1:A:246:THR:N	1:A:320:ASP:OD1	2.43	0.52
1:F:200:GLY:HA2	1:F:211:ARG:HD3	1.91	0.52
1:E:33:LYS:HD3	1:E:41:LYS:HZ3	1.74	0.52
1:A:66:ARG:NH1	1:A:70:GLY:HA2	2.25	0.52
1:F:319:CYS:O	1:F:341:ALA:HA	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:A:258:HIS:CD2	1:A:261:ARG:HH11	2.26	0.52
1:E:260:MET:HE1	1:E:288:PRO:HA	1.92	0.52
1:D:48:ILE:O	1:D:52:ILE:HG13	2.09	0.52
1:F:48:ILE:O	1:F:52:ILE:HG13	2.09	0.52
1:B:379:THR:O	1:B:382:TYR:HB3	2.09	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:A:238:MET:HE2	1:A:245:LYS:HE2	1.92	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:E:413:VAL:O	1:E:417:LEU:HG	2.10	0.52
1:A:117:VAL:HG23	1:A:485:ALA:HB2	1.91	0.52
1:E:66:ARG:NH1	1:E:70:GLY:HA2	2.25	0.52
1:A:200:GLY:HA2	1:A:211:ARG:HD3	1.91	0.52
1:A:112:THR:HG22	1:A:124:GLY:CA	2.32	0.52
1:F:413:VAL:O	1:F:417:LEU:HG	2.10	0.52
1:B:66:ARG:NH1	1:B:70:GLY:HA2	2.25	0.52
1:A:44:ARG:NH1	1:A:494:ASN:HD21	2.08	0.52
1:B:29:VAL:HA	1:B:45:VAL:HG21	1.90	0.52
1:A:339:VAL:H	1:A:363:ARG:NH2	2.08	0.52
1:A:51:ILE:HD11	1:D:72:TRP:HB3	1.92	0.52
1:D:418:GLU:HG2	1:D:428:ILE:HG12	1.91	0.52
1:B:108:ALA:O	1:B:111:MET:HB2	2.09	0.52
1:E:274:GLY:CA	1:E:314:ILE:HG13	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:N	1:F:320:ASP:OD1	2.43	0.52
1:B:239:THR:HG23	1:B:240:PRO:N	2.23	0.52
1:B:246:THR:N	1:B:320:ASP:OD1	2.43	0.52
1:C:339:VAL:H	1:C:363:ARG:NH2	2.08	0.52
1:D:413:VAL:O	1:D:417:LEU:HG	2.10	0.52
1:F:117:VAL:HG23	1:F:485:ALA:HB2	1.91	0.52
1: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:48:ILE:O	1:B:52:ILE:HG13	2.09	0.52
1:A:413:VAL:O	1:A:417:LEU:HG	2.10	0.51
1:F:142:GLU:HG2	1:F:146:ARG:CD	2.33	0.51
1:C:44:ARG:NH1	1:C:494:ASN:HD21	2.08	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:E:418:GLU:HG2	1:E:428:ILE:HG12	1.91	0.51
1:F:239:THR:HG23	1:F:240:PRO:N	2.23	0.51
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:E:200:GLY:HA2	1:E:211:ARG:HD3	1.91	0.51
1:C:282:ASN:HD21	1:C:284:ASP:HB2	1.74	0.51
1:A:282:ASN:HD21	1:A:284:ASP:HB2	1.74	0.51
1:B:44:ARG:CZ	1:B:494:ASN:HD21	2.23	0.51
1:C:44:ARG:CZ	1:C:494:ASN:HD21	2.23	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:A:418:GLU:HG2	1:A:428:ILE:HG12	1.91	0.51
1:D:17:PHE:CE1	1:D:486:ILE:HG12	2.46	0.51
1:F:360:PHE:CD2	1:F:365:ILE:HD12	2.44	0.51
1:C:252:PHE:HD2	1:C:295:LYS:HE3	1.76	0.51
1:D:260:MET:HE1	1:D:288:PRO:HA	1.90	0.51
1:F:348:ALA:HB3	1:F:351:PRO:HG3	1.91	0.51
1:E:108:ALA:O	1:E:111:MET:HB2	2.09	0.51
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.71	0.51
1:E:146:ARG:HE	1:E:182:THR:HG22	1.76	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:D:44:ARG:NH1	1:D:494:ASN:HD21	2.08	0.51
1:E:44:ARG:NH1	1:E:494:ASN:HD21	2.08	0.51
1:B:138:ASP:HA	1:B:141:LEU:HD12	1.93	0.51
1:E:246:THR:N	1:E:320:ASP:OD1	2.43	0.51
1:B:19:ARG:NH2	1:B:478:ARG:HD2	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ALA:HB3	1:D:351:PRO:HG3	1.91	0.51
1:E:56:ASN:HD22	1:E:84:HIS:CD2	2.27	0.51
1:B:417:LEU:HD21	1:F:417:LEU:HD11	1.90	0.51
1:A:146:ARG:HE	1:A:182:THR:HG22	1.76	0.51
1:A:346:GLU:HB3	1:A:370:ASP:HB3	1.93	0.51
1:D:334:SER:O	1:D:338:ARG:NH2	2.43	0.51
1:A:252:PHE:HD2	1:A:295:LYS:HE3	1.76	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:C:348:ALA:HB3	1:C:351:PRO:HG3	1.91	0.51
1:A:195:HIS:HE1	1:B:87:THR:HG21	1.72	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:F:346:GLU:HB3	1:F:370:ASP:HB3	1.93	0.51
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.74	0.51
1:C:319:CYS:O	1:C:341:ALA:HA	2.09	0.51
1:A:333:LYS:HB2	1:A:355:GLN:HB3	1.93	0.51
1:E:334:SER:O	1:E:338:ARG:NH2	2.43	0.51
1:D:66:ARG:NH1	1:D:70:GLY:HA2	2.25	0.51
1:E:66:ARG:HG3	1:E:72:TRP:CE2	2.46	0.51
1:C:421:PHE:HE1	1:E:421:PHE:HE1	1.59	0.51
1:D:90:LYS:HD2	1:D:122:PHE:CE1	2.46	0.51
1:C:211:ARG:HG2	1:C:380:VAL:HG12	1.93	0.51
1:D:200:GLY:HA2	1:D:211:ARG:HD3	1.91	0.51
1:E:59:LEU:CD2	1:E:61:LEU:HD11	2.41	0.51
1:B:9:PHE:CE1	1:B:107:LEU:HD13	2.34	0.51
1:E:310:TYR:CD1	1:E:311:GLU:N	2.75	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:F:44:ARG:NH1	1:F:494:ASN:HD21	2.08	0.51
1:F:339:VAL:H	1:F:363:ARG:NH2	2.08	0.51
1:D:339:VAL:H	1:D:363:ARG:NH2	2.08	0.51
1:D:333:LYS:HB2	1:D:355:GLN:HB3	1.93	0.51
1:B:17:PHE:HA	1:B:482:TYR:HD2	1.73	0.51
1:F:211:ARG:HG2	1:F:380:VAL:HG12	1.93	0.51
1:D:489:VAL:O	1:D:493:TYR:HD1	1.94	0.51
1:F:59:LEU:CD2	1:F:61:LEU:HD11	2.41	0.51
1:C:346:GLU:HB3	1:C:370:ASP:HB3	1.93	0.51
1:B:74:VAL:HG11	1:E:54:PRO:HG3	1.92	0.51
1:A:138:ASP:HA	1:A:141:LEU:HD12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ASP:HA	1:D:141:LEU:HD12	1.93	0.51
1:B:421:PHE:CE1	1:F:421:PHE:CE1	2.99	0.51
1:C:413:VAL:O	1:C:417:LEU:HG	2.10	0.51
1:F:90:LYS:HD2	1:F:122:PHE:CE1	2.46	0.51
1:A:87:THR:CG2	1:F:195:HIS:CE1	2.85	0.51
1:E:346:GLU:HB3	1:E:370:ASP:HB3	1.93	0.51
1:F:146:ARG:HE	1:F:182:THR:HG22	1.76	0.51
1:A:44:ARG:CZ	1:A:494:ASN:HD21	2.23	0.51
1:F:316:GLU:CD	1:F:338:ARG:HH11	2.14	0.51
1:D:252:PHE:HD2	1:D:295:LYS:HE3	1.76	0.51
1:B:413:VAL:O	1:B:417:LEU:HG	2.10	0.51
1:B:346:GLU:HB3	1:B:370:ASP:HB3	1.93	0.51
1:E:138:ASP:HA	1:E:141:LEU:HD12	1.93	0.51
1:C:316:GLU:CD	1:C:338:ARG:HH11	2.14	0.51
1:B:303:GLY:N	1:B:309:ILE:HD11	2.23	0.51
1:B:62:SER:HB3	1:E:55:CYS:O	2.11	0.51
1:F:315:LEU:HD11	1:F:330:GLN:HB3	1.93	0.51
1:A:401:TYR:CG	1:B:443:ALA:HB2	2.46	0.51
1:A:210:GLY:O	1:A:214:ALA:HB2	2.11	0.51
1:F:210:GLY:O	1:F:214:ALA:HB2	2.11	0.51
1:A:59:LEU:CD2	1:A:61:LEU:HD11	2.41	0.51
1:B:416:SER:HB3	1:F:430:ILE:CD1	2.41	0.51
1:F:340:LYS:N	1:F:363:ARG:HH22	2.05	0.51
1:F:333:LYS:HB2	1:F:355:GLN:HB3	1.93	0.51
1:B:17:PHE:CE1	1:B:486:ILE:HG12	2.46	0.51
1:C:17:PHE:HA	1:C:482:TYR:HD2	1.73	0.51
1:B:211:ARG:HG2	1:B:380:VAL:HG12	1.93	0.51
1:B:59:LEU:CD2	1:B:61:LEU:HD11	2.41	0.51
4:C:507[B]:NAD:C6N	1:E:459:ARG:HH21	2.24	0.50
1:C:393:SER:HB3	4:C:507[B]:NAD:PA	2.51	0.50
1:E:61:LEU:HD23	1:E:151:GLU:HB3	1.93	0.50
1:E:44:ARG:CZ	1:E:494:ASN:HD21	2.23	0.50
1:A:316:GLU:CD	1:A:338:ARG:HH11	2.14	0.50
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.46	0.50
1:F:17:PHE:CE1	1:F:486:ILE:HG12	2.46	0.50
1:F:252:PHE:HD2	1:F:295:LYS:HE3	1.76	0.50
1:E:315:LEU:HD11	1:E:330:GLN:HB3	1.93	0.50
1:D:59:LEU:CD2	1:D:61:LEU:HD11	2.41	0.50
1:E:489:VAL:O	1:E:493:TYR:HD1	1.94	0.50
1:E:210:GLY:O	1:E:214:ALA:HB2	2.11	0.50
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.93	0.50
1:C:9:PHE:CE1	1:C:107:LEU:HD13	2.34	0.50
1:A:417:LEU:CD1	1:F:417:LEU:HD21	2.40	0.50
1:C:146:ARG:HE	1:C:182:THR:HG22	1.76	0.50
1:B:146:ARG:HE	1:B:182:THR:HG22	1.76	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:B:252:PHE:HD2	1:B:295:LYS:HE3	1.75	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:90:LYS:HD2	1:E:122:PHE:CE1	2.46	0.50
1:B:210:GLY:O	1:B:214:ALA:HB2	2.11	0.50
1:B:489:VAL:O	1:B:493:TYR:HD1	1.94	0.50
1:A:90:LYS:HD2	1:A:122:PHE:CE1	2.46	0.50
1:D:146:ARG:HE	1:D:182:THR:HG22	1.76	0.50
1:D:346:GLU:HB3	1:D:370:ASP:HB3	1.93	0.50
1:D:44:ARG:CZ	1:D:494:ASN:HD21	2.23	0.50
1:D:316:GLU:CD	1:D:338:ARG:HH11	2.15	0.50
1:C:17:PHE:CE1	1:C:486:ILE:HG12	2.46	0.50
1:F:260:MET:HE1	1:F:288:PRO:HA	1.94	0.50
4:B:507[B]:NAD:C6N	1:F:459:ARG:HH21	2.24	0.50
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.31	0.50
1:E:316:GLU:CD	1:E:338:ARG:HH11	2.14	0.50
1:D:66:ARG:HG3	1:D:72:TRP:CE2	2.46	0.50
1:C:66:ARG:HG3	1:C:72:TRP:CE2	2.46	0.50
1:E:252:PHE:HD2	1:E:295:LYS:HE3	1.76	0.50
1:F:443:ALA:HB1	1:F:447:ASP:HB2	1.94	0.50
1:A:489:VAL:O	1:A:493:TYR:HD1	1.94	0.50
1:A:459:ARG:HH21	4:F:508[B]:NAD:C6N	2.24	0.50
1:E:94:ARG:HE	1:E:168:ASN:ND2	2.10	0.50
1:F:66:ARG:HG3	1:F:72:TRP:CE2	2.46	0.50
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:89:CYS:HB3	1:E:125:ALA:HB2	1.93	0.50
1:D:459:ARG:HH21	4:E:507[B]:NAD:C6N	2.24	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:61:LEU:HD23	1:D:151:GLU:HB3	1.93	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:PHE:HA	1:E:482:TYR:HD2	1.73	0.50
1:A:315:LEU:HD11	1:A:330:GLN:HB3	1.93	0.50
1:E:211:ARG:HG2	1:E:380:VAL:HG12	1.92	0.50
1:C:59:LEU:CD2	1:C:61:LEU:HD11	2.41	0.50
1:C:459:ARG:HH21	4:D:507[B]:NAD:C6N	2.24	0.50
1:A:94:ARG:HE	1:A:168:ASN:ND2	2.10	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:C:340:LYS:N	1:C:363:ARG:HH22	2.05	0.50
1:B:445:GLU:O	1:B:449:VAL:HG23	2.12	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:A:14:GLU:O	1:A:17:PHE:HB3	2.12	0.50
1:F:248:ALA:O	1:F:322:LEU:HD12	2.12	0.50
1:B:90:LYS:HD2	1:B:122:PHE:CE1	2.46	0.50
1:F:61:LEU:HD23	1:F:151:GLU:HB3	1.93	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:94:ARG:HE	1:F:168:ASN:ND2	2.10	0.49
1:C:462:ARG:NH2	1:C:466:ARG:HH22	2.00	0.49
1:C:281:TRP:CH2	1:C:283:PRO:HG3	2.47	0.49
1:D:14:GLU:O	1:D:17:PHE:HB3	2.12	0.49
1:C:14:GLU:O	1:C:17:PHE:HB3	2.12	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:A:445:GLU:O	1:A:449:VAL:HG23	2.12	0.49
1:D:210:GLY:O	1:D:214:ALA:HB2	2.11	0.49
1:B:112:THR:HG22	1:B:124:GLY:CA	2.32	0.49
1:F:281:TRP:CH2	1:F:283:PRO:HG3	2.48	0.49
1:A:281:TRP:CH2	1:A: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:A:2:ASP:OD2	1:A:5:ASP:HB3	2.13	0.49
1:E:457:MET:CE	1:E:457:MET:HA	2.42	0.49
1:A:38:GLN:OE1	1:A:40:GLN:HB2	2.12	0.49
1:D:248:ALA:O	1:D:322:LEU:HD12	2.12	0.49
1:C:61:LEU:HD12	1:C:61:LEU:N	2.27	0.49
1:C:210:GLY:O	1:C:214:ALA:HB2	2.11	0.49
1: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
4:A:507[B]:NAD:C6N	1:B:459:ARG:HH21	2.24	0.49

Continued on next page...

Continued from previous page...

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:B:107:LEU:CB	1:B:126:LYS:HG2	2.31	0.49
1:B:462:ARG:NH2	1:B:466:ARG:HH22	2.00	0.49
1:E:93:ILE:HD11	1:E:165:PRO:HB3	1.94	0.49
1:D:93:ILE:HD11	1:D:165:PRO:HB3	1.94	0.49
1:A:87:THR:O	1:A:88:PRO:C	2.50	0.49
1:D:94:ARG:HE	1:D:168:ASN:ND2	2.10	0.49
1:F:94:ARG:CZ	1:F:107:LEU:HD21	2.42	0.49
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.71	0.49
1:B:222:GLY:HA3	1:B:373:LEU:CD2	2.42	0.49
1:E:38:GLN:OE1	1:E:40:GLN:HB2	2.12	0.49
1:D:211:ARG:HG2	1:D:380:VAL:HG12	1.93	0.49
1:E:94:ARG:CZ	1:E:107:LEU:HD21	2.42	0.49
1:B:94:ARG:CZ	1:B: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:D:2:ASP:OD2	1:D:5:ASP:HB3	2.13	0.49
1:F:93:ILE:HD11	1:F:165:PRO:HB3	1.94	0.49
1:A:248:ALA:O	1:A:322:LEU:HD12	2.12	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:B:38:GLN:OE1	1:B:40:GLN:HB2	2.12	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: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:B:99:VAL:HA	1:B:103:GLU:OE1	2.13	0.49
1:A:94:ARG:CZ	1:A:107:LEU:HD21	2.42	0.49
1:B:147:ARG:NH1	1:E:500:PHE:CD1	2.80	0.49
1:B:147:ARG:NH1	1:E:499:THR:OG1	2.43	0.49
1:F:138:ASP:HA	1:F:141:LEU:HD12	1.93	0.49
1:A:66:ARG:HG3	1:A:72:TRP:CE2	2.46	0.49
1:E:2:ASP:OD2	1:E:5:ASP:HB3	2.13	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:B:253:GLY:HA3	4:B:508:NAD:H4B	1.95	0.49
1:C:38:GLN:OE1	1:C:40:GLN:HB2	2.12	0.49
1:E:344:ILE:HD12	1:E:367:VAL:HG22	1.95	0.49
1:F:2:ASP:OD2	1:F:5:ASP:HB3	2.13	0.49
1:E:14:GLU:O	1:E:17:PHE:HB3	2.12	0.49
1:F:14:GLU:O	1:F:17:PHE:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:392:VAL:HG13	1:E:386:LEU:HD21	1.94	0.49
1:F:87:THR:O	1:F:88:PRO:C	2.50	0.49
1:F:222:GLY:HA3	1:F:373:LEU:HD23	1.94	0.49
1:B:222:GLY:HA3	1:B:373:LEU:HD23	1.94	0.49
1:A:64:PRO:HG2	1:D:499:THR:CG2	2.37	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:E:61:LEU:N	1:E:61:LEU:HD12	2.27	0.49
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.93	0.49
1:D:87:THR:O	1:D:88:PRO:C	2.50	0.49
1:D:94:ARG:CZ	1:D:107:LEU:HD21	2.42	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:E:331:LEU:HD12	1:E:352:THR:HG22	1.95	0.49
1:C:248:ALA:O	1:C:322:LEU:HD12	2.12	0.49
1:F:61:LEU:N	1:F:61:LEU:HD12	2.27	0.49
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.13	0.49
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:D:38:GLN:OE1	1:D:40:GLN:HB2	2.12	0.48
1:F:313:SER:CB	1:F:316:GLU:HB2	2.42	0.48
1:B:333:LYS:HB2	1:B:355:GLN:HB3	1.93	0.48
1:A:93:ILE:HD11	1:A:165:PRO:HB3	1.94	0.48
1:A:61:LEU:HD12	1:A:61:LEU:N	2.27	0.48
1:D:391:HIS:C	4:D:507[A]:NAD:H4D	2.33	0.48
1:A:222:GLY:HA3	1:A:373:LEU:HD23	1.94	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:A:303:GLY:N	1:A:309:ILE:HD11	2.23	0.48
1:C:93:ILE:HD11	1:C:165:PRO:HB3	1.94	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:A:61:LEU:HD23	1:A:151:GLU:HB3	1.93	0.48
1:F:445:GLU:O	1:F:449:VAL:HG23	2.12	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
1:C:253:GLY:HA3	4:C:508:NAD:H4B	1.95	0.48
1:A:222:GLY:HA3	1:A:373:LEU:CD2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:TRP:CH2	1:D:283:PRO:HG3	2.48	0.48
1:C:331:LEU:HD12	1:C:352:THR:HG22	1.95	0.48
1:F:331:LEU:HD12	1:F:352:THR:HG22	1.95	0.48
1:C:353:THR:HG22	1:C:355:GLN:H	1.79	0.48
1:A:289:LYS:HG2	1:A:293:ASP:OD1	2.14	0.48
1:E:445:GLU:O	1:E:449:VAL:HG23	2.12	0.48
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.13	0.48
1:D:222:GLY:HA3	1:D:373:LEU:CD2	2.42	0.48
1:C:222:GLY:HA3	1:C:373:LEU:HD23	1.94	0.48
1:A:457:MET:HA	1:A:457:MET:CE	2.42	0.48
1:A:443:ALA:HB1	1:A:447:ASP:HB2	1.94	0.48
1:D:443:ALA:HB1	1:D:447:ASP:HB2	1.94	0.48
1:E:443:ALA:HB1	1:E:447:ASP:HB2	1.94	0.48
1:D:59:LEU:HD23	1:D:61:LEU:HD11	1.96	0.48
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.13	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:94:ARG:HE	1:C:168:ASN:ND2	2.10	0.48
1:B:275:GLU:HA	1:B:275:GLU:OE1	2.14	0.48
1:F:253:GLY:HA3	4:F:507:NAD:H4B	1.95	0.48
1:B:331:LEU:HD12	1:B:352:THR:HG22	1.95	0.48
1:F:353:THR:HG22	1:F:355:GLN:H	1.79	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:D:344:ILE:HD12	1:D:367:VAL:HG22	1.95	0.48
1:B:344:ILE:HD12	1:B:367:VAL:HG22	1.95	0.48
1:F:136:TYR:CD1	1:F:136:TYR:N	2.82	0.48
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.79	0.48
1:E:350:GLY:N	1:E:351:PRO:HD3	2.29	0.48
1:A:59:LEU:HD23	1:A:61:LEU:HD11	1.96	0.48
1:B:59:LEU:HD23	1:B:61:LEU:HD11	1.96	0.48
1:A:150:MET:SD	1:A:186:THR:HG21	2.53	0.48
1:D:275:GLU:HA	1:D:275:GLU:OE1	2.14	0.48
1:D:82:HIS:CG	1:D:112:THR:HG21	2.48	0.48
1:B:281:TRP:CH2	1:B:283:PRO:HG3	2.48	0.48
1:D:340:LYS:N	1:D:363:ARG:HH22	2.05	0.48
1:A:136:TYR:N	1:A:136:TYR:CD1	2.82	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:MET:SD	1:B:186:THR:HG21	2.53	0.48
1:F:369:PRO:CG	1:F:478:ARG:HA	2.44	0.48
1:C:344:ILE:CG2	1:C:367:VAL:HG13	2.44	0.48
1:A:499:THR:OG1	1:D:147:ARG:NH1	2.43	0.48
1:C:428:ILE:HG23	1:D:420:LYS:HZ2	1.78	0.48
1:B:257:LEU:O	1:B:260:MET:HB3	2.14	0.48
1:F:350:GLY:N	1:F:351:PRO:HD3	2.29	0.48
1:D:350:GLY:N	1:D:351:PRO:HD3	2.29	0.48
1:C:59:LEU:HD23	1:C:61:LEU:HD11	1.96	0.48
1:D:462:ARG:NH2	1:D:466:ARG:HH22	2.00	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:A:287:ASP:OD1	1:A:290:GLU:HG3	2.14	0.48
1:B:282:ASN:ND2	1:B:284:ASP:N	2.60	0.48
1:D:331:LEU:HD12	1:D:352:THR:HG22	1.95	0.48
1:B:344:ILE:CG2	1:B:367:VAL:HG13	2.44	0.48
1:A:344:ILE:CG2	1:A:367:VAL:HG13	2.44	0.48
1:D:353:THR:HG22	1:D:355:GLN:H	1.79	0.48
1:B:136:TYR:N	1:B:136:TYR:CD1	2.82	0.48
1:F:17:PHE:HA	1:F:482:TYR:HD2	1.73	0.48
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.96	0.48
1:A:456:THR:HG21	1:F:396:ARG:HE	1.78	0.48
1:A:257:LEU:O	1:A:260:MET:HB3	2.14	0.48
1:D:287:ASP:OD1	1:D:290:GLU:HG3	2.14	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: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:C:275:GLU:HA	1:C:275:GLU:OE1	2.14	0.47
1:A:253:GLY:HA3	4:A:508:NAD:H4B	1.95	0.47
1:E:369:PRO:CG	1:E:478:ARG:HA	2.44	0.47
1:F:282:ASN:ND2	1:F:284:ASP:N	2.60	0.47
1:A:310:TYR:CD1	1:A:311:GLU:N	2.75	0.47
1:E:344:ILE:CG2	1:E:367:VAL:HG13	2.44	0.47
1:D:313:SER:CB	1:D:316:GLU:HB2	2.42	0.47
1:E:333:LYS:HB3	1:E:333:LYS:HE2	1.65	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: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:435:GLU:H	1:C:435:GLU:CD	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TRP:CH2	1:E:499:THR:HG22	2.49	0.47
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.45	0.47
1:A:331:LEU:HD12	1:A:352:THR:HG22	1.95	0.47
1:E:353:THR:HG22	1:E:355:GLN:H	1.79	0.47
1:E:59:LEU:HD23	1:E:61:LEU:HD11	1.96	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:B:333:LYS:HB3	1:B:333:LYS:HE2	1.65	0.47
1:A:369:PRO:CG	1:A:478:ARG:HA	2.44	0.47
1:E:252:PHE:CE1	1:E:291:LEU:HD13	2.49	0.47
1:D:252:PHE:CE1	1:D:291:LEU:HD13	2.49	0.47
1:F:252:PHE:CE1	1:F:291:LEU:HD13	2.49	0.47
1:F:257:LEU:O	1:F:260:MET:HB3	2.14	0.47
1:F:469:MET:O	1:F:471:TYR:N	2.47	0.47
1:F:289:LYS:HG2	1:F:293:ASP:OD1	2.14	0.47
1:E:275:GLU:HA	1:E:275:GLU:OE1	2.14	0.47
1:F:275:GLU:OE1	1:F:275:GLU:HA	2.14	0.47
1:F:344:ILE:CG2	1:F:367:VAL:HG13	2.44	0.47
1:F:457:MET:HA	1:F:457:MET:CE	2.42	0.47
1:C:252:PHE:CE1	1:C:291:LEU:HD13	2.49	0.47
1:D:250:GLN:CD	1:D:315:LEU:HD21	2.35	0.47
1:C:469:MET:O	1:C:471:TYR:N	2.47	0.47
1:E:82:HIS:CG	1:E:112:THR:HG21	2.48	0.47
1:B:33:LYS:HD3	1:B:41:LYS:NZ	2.30	0.47
1:D:136:TYR:N	1:D:136:TYR:CD1	2.82	0.47
1:C:456:THR:HG21	1:D:396:ARG:HE	1.80	0.47
1:A:470:LYS:HE3	1:A: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: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:E:250:GLN:CD	1:E:315:LEU:HD21	2.35	0.47
1:D:470:LYS:HE3	1:D:471:TYR:OH	2.15	0.47
1:C:470:LYS:HE3	1:C:471:TYR:CZ	2.50	0.47
1:E:287:ASP:OD1	1:E:290:GLU:HG3	2.14	0.47
1:C:393:SER:HB3	4:C:507[A]:NAD:O3	2.15	0.47
1:E:253:GLY:HA3	4:E:508:NAD:H4B	1.95	0.47
1:E:381:SER:OG	3:E:506:AKG:O3	2.24	0.47
1:B:282:ASN:C	1:B:282:ASN:ND2	2.68	0.47
1:C:33:LYS:HD3	1:C:41:LYS:NZ	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:PHE:CE2	1:E:185:SER:HB2	2.44	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:A:340:LYS:N	1:A:363:ARG:HH22	2.05	0.47
1:B:313:SER:CB	1:B:316:GLU:HB2	2.42	0.47
1:C:333:LYS:HB3	1:C:333:LYS:HE2	1.65	0.47
1:E:136:TYR:N	1:E:136:TYR:CD1	2.82	0.47
1:C:417:LEU:CD2	1:E:417:LEU:CD1	2.91	0.47
1:A:252:PHE:CE1	1:A:291:LEU:HD13	2.49	0.47
1:D:257:LEU:O	1:D:260:MET:HB3	2.14	0.47
1:E:257:LEU:O	1:E:260:MET:HB3	2.14	0.47
1:F:199:THR:HA	1:F:384:GLN:OE1	2.15	0.47
1:C:350:GLY:N	1:C:351:PRO:HD3	2.29	0.47
1:A:470:LYS:HE3	1:A:471:TYR:CZ	2.50	0.47
1:D:154:LYS:HD2	1:F:189:HIS:CD2	2.50	0.47
1:E:343:ILE:HG12	1:E:366:MET:HE2	1.96	0.47
1:B:470:LYS:HE3	1:B:471:TYR:CZ	2.50	0.47
1:B:470:LYS:HE3	1:B:471:TYR:OH	2.15	0.47
1:E:435:GLU:H	1:E:435:GLU:CD	2.18	0.47
1:E:282:ASN:C	1:E:282:ASN:ND2	2.68	0.47
1:C:220:PHE:HZ	1:C:266:PHE:CD2	2.33	0.47
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.96	0.47
1:C:257:LEU:O	1:C:260:MET:HB3	2.14	0.47
1:C:199:THR:HA	1:C:384:GLN:OE1	2.15	0.47
1:A:350:GLY:N	1:A:351:PRO:HD3	2.29	0.47
1:D:435:GLU:CD	1:D:435:GLU:H	2.18	0.47
1:B:72:TRP:HZ3	1:E:499:THR:CG2	2.21	0.47
1:A:33:LYS:HD3	1:A:41:LYS:NZ	2.30	0.47
1:D:33:LYS:HD3	1:D:41:LYS:NZ	2.30	0.47
1:E:220:PHE:HZ	1:E:266:PHE:CD2	2.33	0.47
1:A:313:SER:CB	1:A:316:GLU:HB2	2.42	0.47
1:A:51:ILE:HA	1:D:74:VAL:CG2	2.45	0.47
1:C:72:TRP:CZ2	1:F:498:VAL:HB	2.49	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:199:THR:HA	1:B:384:GLN:OE1	2.15	0.47
1:E:199:THR:HA	1:E:384:GLN:OE1	2.15	0.47
1:F:59:LEU:HD23	1:F:61:LEU:HD11	1.96	0.47
1:A:469:MET:O	1:A:471:TYR:N	2.47	0.47
1:D:253:GLY:HA3	4:D:508:NAD:H4B	1.95	0.47
1:A:53:LYS:O	1:A:82:HIS:HE1	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:220:PHE:HZ	1:B:266:PHE:CD2	2.33	0.47
1:A:250:GLN:CD	1:A:315:LEU:HD21	2.35	0.47
1:E:469:MET:O	1:E:471:TYR:N	2.47	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:F:53:LYS:O	1:F:82:HIS:HE1	1.98	0.46
1:C:174:ARG:NE	1:C:178:TRP:CH2	2.83	0.46
1:B:174:ARG:NE	1:B:178:TRP:CH2	2.83	0.46
1:F:220:PHE:HZ	1:F:266:PHE:CD2	2.33	0.46
1:F:331:LEU:CD1	1:F:344:ILE:HD13	2.46	0.46
1:E:331:LEU:CD1	1:E:344:ILE:HD13	2.46	0.46
1:A:353:THR:HG22	1:A:355:GLN:H	1.79	0.46
1:E:411:MET:HE3	1:E:415:GLU:HG3	1.97	0.46
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.96	0.46
1:F:250:GLN:CD	1:F:315:LEU:HD21	2.35	0.46
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.50	0.46
1:D:470:LYS:HE3	1:D:471:TYR:CZ	2.50	0.46
1:F:393:SER:HB3	4:F:508[B]:NAD:PA	2.55	0.46
1:D:53:LYS:O	1:D:82:HIS:HE1	1.98	0.46
1:F:282:ASN:C	1:F:282:ASN:ND2	2.68	0.46
1:E:40:GLN:HE21	1:E:40:GLN:HA	1.79	0.46
1:D:457:MET:HA	1:D:457:MET:CE	2.42	0.46
1:D:432:PRO:CB	1:D:436:PHE:HD2	2.28	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:A:489:VAL:HG12	1:A:489:VAL:O	2.15	0.46
1:F:470:LYS:HE3	1:F:471:TYR:CZ	2.50	0.46
1:E:470:LYS:HE3	1:E:471:TYR:CZ	2.50	0.46
1:A:435:GLU:H	1:A:435:GLU:CD	2.18	0.46
1:E:174:ARG:NE	1:E:178:TRP:CH2	2.84	0.46
1:F:33:LYS:HD3	1:F:41:LYS:NZ	2.30	0.46
1:C:331:LEU:CD1	1:C:344:ILE:HD13	2.46	0.46
1:F:331:LEU:HD22	1:F:339:VAL:HG11	1.98	0.46
1:D:369:PRO:CG	1:D:478:ARG:HA	2.44	0.46
1:A:190:TYR:CD2	1:B:162:VAL:CG1	2.99	0.46
1:A:260:MET:HE1	1:A:288:PRO:HA	1.96	0.46
1:A:199:THR:HA	1:A:384:GLN:OE1	2.15	0.46
1:B:469:MET:O	1:B:471:TYR:N	2.47	0.46
1:E:470:LYS:HE3	1:E:471:TYR:OH	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:255:VAL:HG11	4:D:508:NAD:O4D	2.16	0.46
1:A:174:ARG:NE	1:A:178:TRP:CH2	2.84	0.46
1:E:500:PHE:HD1	1:E:500:PHE:O	1.99	0.46
1:C:282:ASN:C	1:C:282:ASN:ND2	2.68	0.46
1:A:500:PHE:HD1	1:A:500:PHE:O	1.99	0.46
1:F:500:PHE:O	1:F:500:PHE:HD1	1.99	0.46
1:D:199:THR:HA	1:D:384:GLN:OE1	2.15	0.46
1:B:489:VAL:HG12	1:B:489:VAL:O	2.15	0.46
1:F:470:LYS:HE3	1:F:471:TYR:OH	2.15	0.46
1:C:470:LYS:HE3	1:C:471:TYR:OH	2.15	0.46
1:A:416:SER:HB3	1:B:430:ILE:HA	1.97	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:A:282:ASN:ND2	1:A:284:ASP:N	2.60	0.46
1:B:33:LYS:HD3	1:B:33:LYS:HA	1.72	0.46
1:A:246:THR:HG22	1:A:320:ASP:H	1.80	0.46
1:F:40:GLN:HA	1:F:40:GLN:HE21	1.79	0.46
1:B:246:THR:HG22	1:B:320:ASP:H	1.80	0.46
1:C:500:PHE:O	1:C:500:PHE:HD1	1.99	0.46
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.96	0.46
1:C:396:ARG:HE	1:E:456:THR:HG21	1.80	0.46
1:C:421:PHE:HE1	1:D:421:PHE:HE1	1.63	0.46
1:F:489:VAL:HG12	1:F:489:VAL:O	2.15	0.46
1:A:84:HIS:C	1:A:86:ARG:N	2.69	0.46
1:D:84:HIS:C	1:D:86:ARG:N	2.69	0.46
1:D:9:PHE:CZ	1:D:328:GLU:HG2	2.51	0.46
1:A:255:VAL:HG11	4:A:508:NAD:O4D	2.16	0.46
1:F:255:VAL:HG11	4:F:507:NAD:O4D	2.16	0.46
1:A:82:HIS:CG	1:A:112:THR:HG21	2.48	0.46
1:B:417:LEU:HD22	1:F:417:LEU:HD13	1.98	0.46
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.71	0.46
1:A:282:ASN:C	1:A:282:ASN:ND2	2.68	0.46
1:E:38:GLN:HB2	1:E:39:GLU:H	1.59	0.46
1:C:238:MET:SD	1:C:342:LYS:HB2	2.56	0.46
1:D:331:LEU:HD22	1:D:339:VAL:HG11	1.98	0.46
1:E:315:LEU:HA	1:E:322:LEU:HD21	1.98	0.46
1:E:393:SER:HB3	4:E:507[B]:NAD:PA	2.55	0.46
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:SD	1:A:342:LYS:HB2	2.56	0.46
1:A:331:LEU:CD1	1:A:344:ILE:HD13	2.46	0.46
1:E:313:SER:CB	1:E:316:GLU:HB2	2.42	0.46
1:C:155:LYS:HD2	1:F:157:PHE:CE1	2.51	0.46
1:A:168:ASN:ND2	1:A:169:MET:H	2.14	0.46
1:C:82:HIS:CG	1:C:112:THR:HG21	2.48	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:B:38:GLN:HB2	1:B:39:GLU:H	1.59	0.46
1:C:40:GLN:HA	1:C:40:GLN:HE21	1.79	0.46
1:E:33:LYS:HD3	1:E:41:LYS:NZ	2.30	0.46
1:E:246:THR:HG22	1:E:320:ASP:H	1.80	0.46
1:B:331:LEU:CD1	1:B:344:ILE:HD13	2.46	0.46
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.96	0.46
1:A:315:LEU:HA	1:A:322:LEU:HD21	1.98	0.46
1:F:90:LYS:HD2	1:F:122:PHE:CD1	2.51	0.46
1:B:90:LYS:HD2	1:B:122:PHE:CD1	2.51	0.46
1:D:90:LYS:HD2	1:D:122:PHE:CD1	2.51	0.46
1:D:168:ASN:ND2	1:D:169:MET:H	2.14	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:D:246:THR:HG22	1:D:320:ASP:H	1.80	0.46
1:F:10:PHE:O	1:F:14:GLU:HB2	2.16	0.46
1:B:498:VAL:HB	1:E:72:TRP:CH2	2.51	0.46
1:B:53:LYS:O	1:B:82:HIS:HE1	1.98	0.46
1:E:282:ASN:ND2	1:E:284:ASP:N	2.60	0.46
1:A:220:PHE:HZ	1:A:266:PHE:CD2	2.33	0.46
1:F:238:MET:SD	1:F:342:LYS:HB2	2.56	0.46
1:D:238:MET:SD	1:D:342:LYS:HB2	2.56	0.46
1:A:500:PHE:CD1	1:D:147:ARG:NH1	2.84	0.46
1:A:10:PHE:O	1:A:14:GLU:HB2	2.16	0.46
1:C:250:GLN:CD	1:C:315:LEU:HD21	2.35	0.46
1:B:61:LEU:HD23	1:B:151:GLU:CB	2.46	0.46
1:C:84:HIS:C	1:C:86:ARG:N	2.69	0.45
1:D:87:THR:CG2	1:E:195:HIS:CE1	2.91	0.45
1:C:255:VAL:HG11	4:C:508:NAD:O4D	2.16	0.45
1:B:255:VAL:HG11	4:B:508:NAD:O4D	2.16	0.45
1:A:282:ASN:HD21	1:A:284:ASP:CB	2.29	0.45
1:D:40:GLN:HE21	1:D:40:GLN:HA	1.79	0.45
1:F:336:ALA:O	1:F:339:VAL:HG13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:PHE:O	1:E:14:GLU:HB2	2.16	0.45
1:D:10:PHE:O	1:D:14:GLU:HB2	2.16	0.45
1:B:500:PHE:HD1	1:B:500:PHE:O	1.99	0.45
1:D:315:LEU:HA	1:D:322:LEU:HD21	1.98	0.45
1:A:61:LEU:HD23	1:A:151:GLU:CB	2.46	0.45
1:D:61:LEU:HD23	1:D:151:GLU:CB	2.46	0.45
1:F:287:ASP:OD1	1:F:290:GLU:HG3	2.14	0.45
1:E:61:LEU:HD23	1:E:151:GLU:CB	2.46	0.45
1:A:9:PHE:CZ	1:A:328:GLU:HG2	2.51	0.45
1:A:409:LEU:HD22	1:F:409:LEU:HD11	1.96	0.45
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.98	0.45
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:C:489:VAL:O	1:C:489:VAL:HG12	2.15	0.45
1:C:61:LEU:HD23	1:C:151:GLU:CB	2.46	0.45
1:E:8:ASN:OD1	1:E:11:LYS:HG3	2.16	0.45
1:F:84:HIS:C	1:F:86:ARG:N	2.69	0.45
1:B:84:HIS:C	1:B:86:ARG:N	2.69	0.45
1:E:168:ASN:ND2	1:E:169:MET:H	2.14	0.45
1:F:174:ARG:NE	1:F:178:TRP:CH2	2.84	0.45
1:C:282:ASN:ND2	1:C:284:ASP:N	2.60	0.45
1:B:331:LEU:HD22	1:B:339:VAL:HG11	1.98	0.45
1:A:336:ALA:O	1:A:339:VAL:HG13	2.16	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:E:386:LEU:HA	1:E:386:LEU:HD12	1.80	0.45
1:C:495:GLU:OE1	1:D:204:SER:OG	2.11	0.45
1:E:230:ALA:O	1:E:231:SER:C	2.55	0.45
1:A:393:SER:HB3	4:A:507[A]:NAD:PA	2.57	0.45
1:C:168:ASN:ND2	1:C:169:MET:H	2.14	0.45
1:A:90:LYS:HD2	1:A:122:PHE:CD1	2.51	0.45
1:F:9:PHE:CZ	1:F:328:GLU:HG2	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:E:336:ALA:O	1:E:339:VAL:HG13	2.16	0.45
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.99	0.45
1:A:379:THR:HG22	1:A:383:PHE:CZ	2.52	0.45
1:D:489:VAL:HG12	1:D:489:VAL:O	2.15	0.45
1:A:321:ILE:HG23	1:A:343:ILE:HG22	1.99	0.45
1:A:8:ASN:OD1	1:A:11:LYS:HG3	2.16	0.45
1:C:8:ASN:OD1	1:C:11:LYS:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ILE:HG23	1:D:343:ILE:HG22	1.99	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:C:282:ASN:HD21	1:C:284:ASP:CB	2.29	0.45
1:A:281:TRP:O	1:A:282:ASN:C	2.55	0.45
1:D:500:PHE:HD1	1:D:500:PHE:O	1.99	0.45
1:D:336:ALA:O	1:D:339:VAL:HG13	2.16	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:379:THR:HG22	1:B:383:PHE:CZ	2.52	0.45
1:F:61:LEU:HD23	1:F:151:GLU:CB	2.46	0.45
1:A:230:ALA:O	1:A:231:SER:C	2.55	0.45
1:D:8:ASN:OD1	1:D:11:LYS:HG3	2.17	0.45
1:B:230:ALA:O	1:B:231:SER:C	2.55	0.45
1:F:230:ALA:O	1:F:231:SER:C	2.55	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:A:154:LYS:HD2	1:E:189:HIS:CD2	2.51	0.45
1:C:362:GLU:C	1:C:364:ASN:H	2.20	0.45
1:A:195:HIS:CE1	1:B:87:THR:CG2	2.90	0.45
1:E:377:GLY:O	1:E:381:SER:HB2	2.17	0.45
1:B:416:SER:HB3	1:F:430:ILE:HD13	1.99	0.45
1:C:370:ASP:HB2	1:C:374:ASN:ND2	2.20	0.45
1:C:281:TRP:O	1:C:282:ASN:C	2.55	0.45
1:C:246:THR:HG22	1:C:320:ASP:H	1.80	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:B:336:ALA:O	1:B:339:VAL:HG13	2.16	0.45
1:E:90:LYS:HD2	1:E:122:PHE:CD1	2.51	0.45
1:F:379:THR:HG22	1:F:383:PHE:CZ	2.52	0.45
1:E:489:VAL:HG12	1:E:489:VAL:O	2.15	0.45
1:C:230:ALA:O	1:C:231:SER:C	2.55	0.45
1:B:8:ASN:OD1	1:B:11:LYS:HG3	2.17	0.45
1:D:230:ALA:O	1:D:231:SER:C	2.55	0.45
1:F:115:CYS:HB3	1:F:120:VAL:O	2.17	0.45
1:E:393:SER:HB3	4:E:507[A]:NAD:O1A	2.17	0.45
1:C:107:LEU:CB	1:C:126:LYS:HG2	2.31	0.45
1:B:9:PHE:CZ	1:B:328:GLU:HG2	2.51	0.45
1:E:282:ASN:H	1:E:307:ALA:HB1	1.82	0.45
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LEU:HD22	1:A:339:VAL:HG11	1.98	0.45
1:C:379:THR:HG22	1:C:383:PHE:CZ	2.52	0.45
1:B:401:TYR:CG	1:F:443:ALA:HB2	2.51	0.45
1:A:377:GLY:O	1:A:381:SER:HB2	2.17	0.45
1:E:115:CYS:HB3	1:E:120:VAL:O	2.17	0.45
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.71	0.45
1:D:10:PHE:HA	1:D:106:ALA:HB2	1.99	0.45
1:C:486:ILE:O	1:C:490:PHE:HB2	2.17	0.45
1:F:230:ALA:O	1:F:234:SER:N	2.49	0.45
1:F:8:ASN:OD1	1:F:11:LYS:HG3	2.16	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:B:64:PRO:HG2	1:E:499:THR:CG2	2.44	0.45
1:F:282:ASN:HD21	1:F:284:ASP:CB	2.29	0.45
1:A:282:ASN:H	1:A:307:ALA:HB1	1.82	0.45
1:A:67:ARG:NH1	1:A:136:TYR:HA	2.32	0.45
1:F:10:PHE:HA	1:F:106:ALA:HB2	1.99	0.45
1:D:115:CYS:HB3	1:D:120:VAL:O	2.17	0.45
1:A:112:THR:HB	1:A:124:GLY:H	1.82	0.44
1:F:112:THR:HB	1:F:124:GLY:H	1.82	0.44
1:D:112:THR:HB	1:D:124:GLY:H	1.82	0.44
1:D:4:GLU:O	1:D:5:ASP:CB	2.65	0.44
1:C:67:ARG:NH1	1:C:136:TYR:HA	2.32	0.44
1:D:417:LEU:CD1	1:E:417:LEU:CD2	2.94	0.44
1:E:321:ILE:HG23	1:E:343:ILE:HG22	1.99	0.44
1:C:362:GLU:C	1:C:364:ASN:N	2.71	0.44
1:E:362:GLU:C	1:E:364:ASN:H	2.20	0.44
1:F:377:GLY:O	1:F:381:SER:HB2	2.17	0.44
1:B:168:ASN:ND2	1:B:169:MET:H	2.14	0.44
1:C:331:LEU:HD22	1:C:339:VAL:HG11	1.98	0.44
1:C:313:SER:CB	1:C:316:GLU:HB2	2.42	0.44
1:B:4:GLU:O	1:B:5:ASP:CB	2.65	0.44
1:A:499:THR:HG23	1:A:501:THR:N	2.33	0.44
1:B:67:ARG:NH1	1:B:136:TYR:HA	2.32	0.44
1:A:486:ILE:O	1:A:490:PHE:HB2	2.17	0.44
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.99	0.44
1:D:486:ILE:O	1:D:490:PHE:HB2	2.18	0.44
1:C:10:PHE:O	1:C:14:GLU:HB2	2.16	0.44
1:B:79:ARG:HD2	1:B:127:ALA:HB2	2.00	0.44
1:F:386:LEU:HD12	1:F:386:LEU:HA	1.80	0.44
1:B:111:MET:HB3	1:B:111:MET:HE2	1.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:HG23	1:C:343:ILE:HG22	1.99	0.44
1:B:232:TYR:CE2	1:B:465:MET:HG2	2.52	0.44
1:B:391:HIS:C	4:B:507[A]:NAD:H4D	2.38	0.44
1:F:282:ASN:H	1:F:307:ALA:HB1	1.82	0.44
1:B:282:ASN:H	1:B:307:ALA:HB1	1.82	0.44
1:C:227:ILE:HA	1:C:233:MET:SD	2.57	0.44
1:F:227:ILE:HG13	1:F:233:MET:SD	2.58	0.44
1:E:263:LEU:HA	1:E:263:LEU:HD23	1.82	0.44
1:C:500:PHE:CD1	1:F:147:ARG:NH1	2.86	0.44
1:F:67:ARG:NH1	1:F:136:TYR:HA	2.32	0.44
1:C:315:LEU:HA	1:C:322:LEU:HD21	1.98	0.44
1:D:111:MET:HB3	1:D:111:MET:HE2	1.72	0.44
1:F:362:GLU:C	1:F:364:ASN:N	2.70	0.44
1:C:115:CYS:HB3	1:C:120:VAL:O	2.17	0.44
1:C:87:THR:HG21	1:D:195:HIS:CE1	2.48	0.44
1:C:391:HIS:C	4:C:507[A]:NAD:H4D	2.38	0.44
1:B:112:THR:HB	1:B:124:GLY:H	1.82	0.44
1:D:282:ASN:H	1:D:307:ALA:HB1	1.82	0.44
1:F:281:TRP:O	1:F:282:ASN:C	2.55	0.44
1:D:227:ILE:HG13	1:D:233:MET:SD	2.58	0.44
1:D:331:LEU:CD1	1:D:344:ILE:HD13	2.46	0.44
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.18	0.44
1:A:4:GLU:O	1:A:5:ASP:CB	2.65	0.44
1:E:4:GLU:O	1:E:5:ASP:CB	2.65	0.44
1:B:355:GLN:HA	1:B:355:GLN:OE1	2.18	0.44
1:F:499:THR:HG23	1:F:501:THR:N	2.33	0.44
1:D:368:ILE:HA	1:D:369:PRO:HD3	1.85	0.44
1:D:67:ARG:NH1	1:D:136:TYR:HA	2.32	0.44
1:F:486:ILE:O	1:F:490:PHE:HB2	2.18	0.44
1:C:62:SER:HB3	1:F:55:CYS:O	2.17	0.44
1:C:432:PRO:CB	1:C:436:PHE:HD2	2.28	0.44
1:E:79:ARG:HD2	1:E:127:ALA:HB2	2.00	0.44
1:C:232:TYR:CE2	1:C:465:MET:HG2	2.52	0.44
1:C:377:GLY:O	1:C:381:SER:HB2	2.17	0.44
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.52	0.44
4:C:508:NAD:N7N	4:C:508:NAD:O2N	2.47	0.44
1:F:168:ASN:ND2	1:F:169:MET:H	2.14	0.44
1:C:185:SER:HB2	1:E:500:PHE:CE2	2.51	0.44
1:A:227:ILE:HG13	1:A:233:MET:SD	2.58	0.44
1:F:263:LEU:HD23	1:F:263:LEU:HA	1.82	0.44
1:B:227:ILE:HG13	1:B:233:MET:SD	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ILE:HA	1:E:233:MET:SD	2.57	0.44
1:B:294:PHE:CE2	1:B:298:HIS:CE1	3.06	0.44
1:A:354:PRO:O	1:A:357:ASP:HB2	2.18	0.44
1:C:67:ARG:HH12	1:C:136:TYR:HA	1.83	0.44
1:E:67:ARG:NH1	1:E:136:TYR:HA	2.32	0.44
1:B:362:GLU:C	1:B:364:ASN:H	2.20	0.44
1:A:362:GLU:C	1:A:364:ASN:N	2.71	0.44
1:E:232:TYR:CE2	1:E:465:MET:HG2	2.52	0.44
1:C:84:HIS:O	1:C:86:ARG:N	2.51	0.44
1:E:112:THR:HB	1:E:124:GLY:H	1.82	0.44
1:B:82:HIS:CG	1:B:112:THR:HG21	2.48	0.44
1:F:37:THR:HG21	1:F:41:LYS:HG3	2.00	0.44
1:B:227:ILE:HA	1:B:233:MET:SD	2.57	0.44
1:C:336:ALA:O	1:C:339:VAL:HG13	2.16	0.44
1:D:227:ILE:HA	1:D:233:MET:SD	2.57	0.44
1:C:4:GLU:O	1:C:5:ASP:CB	2.65	0.44
1:F:354:PRO:O	1:F:357:ASP:HB2	2.18	0.44
1:B:486:ILE:O	1:B:490:PHE:HB2	2.18	0.44
1:D:377:GLY:O	1:D:381:SER:HB2	2.17	0.44
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.52	0.44
1:F:321:ILE:HG23	1:F:343:ILE:HG22	1.99	0.44
1:A:115:CYS:HB3	1:A:120:VAL:O	2.17	0.44
1:D:362:GLU:C	1:D:364:ASN:H	2.20	0.44
1:B:115:CYS:HB3	1:B:120:VAL:O	2.17	0.44
1:A:111:MET:HE2	1:A:111:MET:HB3	1.79	0.44
1:E:473:LEU:HD12	1:E:480:ALA:HB2	2.00	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:A:333:LYS:HB3	1:A:333:LYS:HE2	1.65	0.44
1:F:4:GLU:O	1:F:5:ASP:CB	2.65	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:D:379:THR:HG22	1:D:383:PHE:CZ	2.52	0.44
1:D:235:ILE:H	1:D:235:ILE:HG13	1.69	0.44
1:C:206:GLY:HA2	4:C:507[A]:NAD:H5N	2.00	0.44
1:A:391:HIS:C	4:A:507[A]:NAD:H4D	2.38	0.44
1:C:172:GLY:H	1:C:175:GLU:HG2	1.83	0.44
1:E:219:VAL:HG13	1:E:373:LEU:HD11	2.00	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:67:ARG:HH12	1:A:136:TYR:HA	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HG	1:A:482:TYR:CE1	2.53	0.44
1:D:371:LEU:HG	1:D:482:TYR:CE1	2.53	0.44
1:F:111:MET:HE2	1:F:111:MET:HB3	1.71	0.44
1:E:362:GLU:C	1:E:364:ASN:N	2.71	0.44
1:F:362:GLU:C	1:F:364:ASN:H	2.20	0.44
1:B:377:GLY:O	1:B:381:SER:HB2	2.17	0.44
1:A:227:ILE:HA	1:A:233:MET:SD	2.57	0.44
1:C:294:PHE:CE2	1:C:298:HIS:CE1	3.06	0.44
1:E:354:PRO:O	1:E:357:ASP:HB2	2.18	0.44
1:A:499:THR:OG1	1:D:147:ARG:NH2	2.51	0.44
1:A:406:ASN:HD22	1:A:406:ASN:HA	1.60	0.44
1:C:200:GLY:H	1:C:384:GLN:NE2	2.16	0.44
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:D:281:TRP:O	1:D:282:ASN:C	2.55	0.43
1:B:457:MET:HA	1:B:457:MET:CE	2.42	0.43
1:B:499:THR:HG23	1:B:501:THR:N	2.33	0.43
1:C:371:LEU:HG	1:C:482:TYR:CE1	2.53	0.43
1:D:79:ARG:HD2	1:D:127:ALA:HB2	2.00	0.43
1:A:200:GLY:H	1:A:384:GLN:NE2	2.16	0.43
1:E:172:GLY:H	1:E:175:GLU:HG2	1.83	0.43
1:B:219:VAL:HG13	1:B:373:LEU:HD11	2.00	0.43
1:A:37:THR:HG21	1:A:41:LYS:HG3	2.00	0.43
1:B:25:GLU:OE1	1:B:46:ARG:NE	2.51	0.43
1:C:242:PHE:O	1:C:268:ALA:HA	2.18	0.43
1:F:227:ILE:HA	1:F:233:MET:SD	2.57	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:D:294:PHE:CE2	1:D:298:HIS:CE1	3.06	0.43
1:E:355:GLN:OE1	1:E:355:GLN:HA	2.18	0.43
1:B:354:PRO:O	1:B:357:ASP:HB2	2.18	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:A:79:ARG:HD2	1:A:127:ALA:HB2	2.00	0.43
1:F:79:ARG:HD2	1:F:127:ALA:HB2	2.00	0.43
1:F:200:GLY:H	1:F:384:GLN:NE2	2.16	0.43
1:D:349:ASN:C	1:D:351:PRO:HD3	2.39	0.43
1:C:349:ASN:C	1:C:351:PRO:HD3	2.39	0.43
1:E:230:ALA:O	1:E:234:SER:N	2.49	0.43
1:A:84:HIS:O	1:A:86:ARG:N	2.51	0.43
4:C:507[A]:NAD:N6A	1:E:120:VAL:O	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:HE	1:C:168:ASN:HD22	1.66	0.43
1:F:94:ARG:HE	1:F:168:ASN:HD22	1.66	0.43
1:C:146:ARG:NE	1:C:182:THR:HG22	2.33	0.43
1:B:281:TRP:O	1:B:282:ASN:C	2.55	0.43
1:A:25:GLU:OE1	1:A:46:ARG:NE	2.51	0.43
1:C:37:THR:HG21	1:C:41:LYS:HG3	2.00	0.43
1:D:500:PHE:HE2	1:E:185:SER:CB	2.29	0.43
1:F:25:GLU:OE1	1:F:46:ARG:NE	2.51	0.43
1:E:227:ILE:HG13	1:E:233:MET:SD	2.58	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:C:355:GLN:OE1	1:C:355:GLN:HA	2.18	0.43
1:F:371:LEU:HG	1:F:482:TYR:CE1	2.53	0.43
1:C:79:ARG:HD2	1:C:127:ALA:HB2	2.00	0.43
1:C:401:TYR:CG	1:E:443:ALA:HB2	2.53	0.43
1:D:200:GLY:H	1:D:384:GLN:NE2	2.16	0.43
1:D:362:GLU:C	1:D:364:ASN:N	2.71	0.43
1:C:190:TYR:CE2	1:E:162:VAL:HG11	2.54	0.43
1:B:172:GLY:H	1:B:175:GLU:HG2	1.83	0.43
1:D:391:HIS:CD2	4:D:507[A]:NAD:HO2N	2.12	0.43
1:E:94:ARG:HE	1:E:168:ASN:HD22	1.66	0.43
1:E:146:ARG:NE	1:E:182:THR:HG22	2.33	0.43
1:C:219:VAL:HG13	1:C:373:LEU:HD11	2.00	0.43
1:B:66:ARG:HG3	1:B:72:TRP:CD2	2.54	0.43
1:D:37:THR:HG21	1:D:41:LYS:HG3	2.00	0.43
1:C:227:ILE:HG13	1:C:233:MET:SD	2.58	0.43
1:D:499:THR:HG23	1:D:501:THR:N	2.33	0.43
1:E:90:LYS:HZ3	1:E:164:VAL:HG12	1.83	0.43
1:F:349:ASN:C	1:F:351:PRO:HD3	2.39	0.43
1:C:394:TYR:CE1	1:C:448:ILE:HG13	2.54	0.43
1:B:321:ILE:HG23	1:B:343:ILE:HG22	1.99	0.43
1:F:84:HIS:O	1:F:86:ARG:N	2.51	0.43
1:D:84:HIS:O	1:D:86:ARG:N	2.51	0.43
1:A:94:ARG:HE	1:A:168:ASN:HD22	1.67	0.43
1:F:146:ARG:NE	1:F:182:THR:HG22	2.33	0.43
1:E:499:THR:HG23	1:E:501:THR:N	2.33	0.43
1:A:294:PHE:CE2	1:A:298:HIS:CE1	3.06	0.43
1:D:354:PRO:O	1:D:357:ASP:HB2	2.18	0.43
1:C:473:LEU:HD12	1:C:480:ALA:HB2	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLY:H	1:E:384:GLN:NE2	2.16	0.43
1:A:230:ALA:O	1:A:234:SER:N	2.49	0.43
1:E:394:TYR:CE1	1:E:448:ILE:HG13	2.54	0.43
1:C:112:THR:HB	1:C:124:GLY:H	1.82	0.43
1:D:25:GLU:OE1	1:D:46:ARG:NE	2.52	0.43
1:E:37:THR:HG21	1:E:41:LYS:HG3	2.00	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:B:4:GLU:O	1:B:5:ASP:HB3	2.19	0.43
1:A:499:THR:CB	1:D:64:PRO:HG2	2.49	0.43
1:F:355:GLN:OE1	1:F:355:GLN:HA	2.18	0.43
1:A:190:TYR:CD2	1:B:162:VAL:HG11	2.52	0.43
1:A:394:TYR:CE1	1:A:448:ILE:HG13	2.54	0.43
1:B:57:HIS:HE1	1:E:151:GLU:OE1	2.02	0.43
1:D:57:HIS:CD2	1:D:84:HIS:NE2	2.87	0.43
1:F:275:GLU:C	4:F:507:NAD:C2A	2.87	0.43
1:D:172:GLY:H	1:D:175:GLU:HG2	1.83	0.43
1:F:219:VAL:HG13	1:F:373:LEU:HD11	2.00	0.43
1:F:281:TRP:CG	1:F:310:TYR:HD2	2.36	0.43
1:B:266:PHE:CD1	1:B:266:PHE:N	2.87	0.43
1:A:5:ASP:OD1	1:A:353:THR:HG21	2.19	0.43
1:A:500:PHE:CE2	1:F:185:SER:HB2	2.48	0.43
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.48	0.43
1:E:486:ILE:O	1:E:490:PHE:HB2	2.18	0.43
1:D:67:ARG:HH12	1:D:136:TYR:HA	1.83	0.43
1:E:66:ARG:HG3	1:E:72:TRP:CD2	2.54	0.43
1:A:349:ASN:C	1:A:351:PRO:HD3	2.39	0.43
1:C:111:MET:HB3	1:C:111:MET:HE2	1.70	0.43
1:D:230:ALA:O	1:D:234:SER:N	2.49	0.43
1:F:235:ILE:HG13	1:F:235:ILE:H	1.69	0.43
1:E:84:HIS:O	1:E:86:ARG:N	2.51	0.43
1:D:275:GLU:C	4:D:508:NAD:C2A	2.87	0.43
1:E:219:VAL:O	1:E:223:ILE:HG13	2.19	0.43
1:B:370:ASP:CB	1:B:374:ASN:HD21	2.21	0.43
1:C:266:PHE:N	1:C:266:PHE:CD1	2.87	0.43
1:F:242:PHE:O	1:F:268:ALA:HA	2.18	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:F:67:ARG:HH12	1:F:136:TYR:HA	1.83	0.43
1:B:501:THR:HG22	1:E:66:ARG:H	1.83	0.43
1:B:396:ARG:HE	1:F:456:THR:HG21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:ASN:C	1:E:351:PRO:HD3	2.39	0.43
1:A:362:GLU:C	1:A:364:ASN:H	2.20	0.43
1:F:394:TYR:CE1	1:F:448:ILE:HG13	2.54	0.43
1:D:394:TYR:CE1	1:D:448:ILE:HG13	2.54	0.43
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.83	0.43
1:B:393:SER:HB3	4:B:507[B]:NAD:PA	2.57	0.43
1:F:57:HIS:CD2	1:F:84:HIS:NE2	2.87	0.43
4:E:508:NAD:N7N	4:E:508:NAD:O2N	2.47	0.43
1:E:25:GLU:OE1	1:E:46:ARG:NE	2.51	0.43
1:B:238:MET:SD	1:B:342:LYS:HB3	2.59	0.43
1:C:499:THR:CG2	1:F:64:PRO:HG2	2.44	0.43
1:F:294:PHE:CE2	1:F:298:HIS:CE1	3.06	0.43
1:D:2:ASP:O	1:D:3:ARG:C	2.58	0.43
1:A:408:HIS:HB3	1:B:436:PHE:HB2	2.01	0.43
1:D:162:VAL:HG11	1:E:190:TYR:CE2	2.53	0.43
1:A:86:ARG:CZ	4:F:508[A]:NAD:C4N	2.97	0.43
1:D:169:MET:HE1	1:D:327:SER:HA	2.01	0.43
1:C:275:GLU:C	4:C:508:NAD:C2A	2.87	0.43
1:E:275:GLU:C	4:E:508:NAD:C2A	2.87	0.43
1:C:370:ASP:CB	1:C:374:ASN:HD21	2.21	0.43
1:E:23:ILE:HD12	1:E:479:THR:OG1	2.19	0.43
1:A:146:ARG:NE	1:A:182:THR:HG22	2.34	0.43
1:F:238:MET:SD	1:F:342:LYS:HB3	2.59	0.43
1:B:242:PHE:CD1	1:B:263:LEU:HD22	2.54	0.43
1:E:238:MET:SD	1:E:342:LYS:HB3	2.59	0.43
1:D:242:PHE:CD1	1:D:263:LEU:HD22	2.54	0.43
1:B:5:ASP:OD1	1:B:353:THR:HG21	2.19	0.43
1:F:2:ASP:O	1:F:3:ARG:C	2.57	0.43
1:D:473:LEU:HD12	1:D:480:ALA:HB2	2.00	0.43
1:C:23:ILE:HD12	1:C:479:THR:OG1	2.19	0.43
1:B:200:GLY:H	1:B:384:GLN:NE2	2.16	0.43
1:B:230:ALA:O	1:B:234:SER:N	2.49	0.43
4:C:507[A]:NAD:C4N	1:E:86:ARG:CZ	2.97	0.42
1:B:57:HIS:CD2	1:B:84:HIS:NE2	2.87	0.42
1:E:186:THR:HG22	1:E:187:ILE:N	2.34	0.42
1:B:169:MET:HE1	1:B:327:SER:HA	2.00	0.42
1:A:275:GLU:C	4:A:508:NAD:C2A	2.87	0.42
4:F:507:NAD:O2N	4:F:507:NAD:N7N	2.47	0.42
1:A:219:VAL:O	1:A:223:ILE:HG13	2.19	0.42
1:E:281:TRP:CG	1:E:310:TYR:HD2	2.36	0.42
1:C:281:TRP:CG	1:C:310:TYR:HD2	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:HB2	1:C:242:PHE:HE2	1.84	0.42
1:F:66:ARG:HG3	1:F:72:TRP:CD2	2.54	0.42
1:C:5:ASP:HB2	1:C:333:LYS:NZ	2.34	0.42
1:E:5:ASP:HB2	1:E:333:LYS:NZ	2.34	0.42
1:D:66:ARG:HG3	1:D:72:TRP:CD2	2.54	0.42
1:D:23:ILE:HD12	1:D:479:THR:OG1	2.19	0.42
1:A:23:ILE:HD12	1:A:479:THR:OG1	2.19	0.42
1:B:432:PRO:CB	1:B:436:PHE:HD2	2.28	0.42
1:F:219:VAL:O	1:F:223:ILE:HG13	2.19	0.42
1:C:219:VAL:O	1:C:223:ILE:HG13	2.19	0.42
1:B:37:THR:HG21	1:B:41:LYS:HG3	2.00	0.42
1:B:40:GLN:HE21	1:B:40:GLN:HA	1.79	0.42
1:C:25:GLU:OE1	1:C:46:ARG:NE	2.51	0.42
1:E:33:LYS:HA	1:E:41:LYS:HZ1	1.84	0.42
1:C:238:MET:SD	1:C:342:LYS:HB3	2.59	0.42
1:A:242:PHE:CD1	1:A:263:LEU:HD22	2.54	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:C:4:GLU:O	1:C:5:ASP:HB3	2.19	0.42
1:F:5:ASP:HB2	1:F:333:LYS:NZ	2.34	0.42
1:B:371:LEU:HG	1:B:482:TYR:CE1	2.53	0.42
1:A:185:SER:HB2	1:B:500:PHE:CE2	2.51	0.42
1:C:86:ARG:NH2	4:D:507[A]:NAD:C5N	2.83	0.42
1:B:84:HIS:O	1:B:86:ARG:N	2.51	0.42
1:B:275:GLU:C	4:B:508:NAD:C2A	2.87	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:D:38:GLN:HB2	1:D:39:GLU:H	1.59	0.42
1:A:224:GLU:HB2	1:A:242:PHE:HE2	1.84	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:E:242:PHE:CD1	1:E:263:LEU:HD22	2.54	0.42
1:B:421:PHE:CZ	1:F:421:PHE:HD1	2.37	0.42
1:B:23:ILE:CD1	1:B:473:LEU:HD21	2.47	0.42
1:C:157:PHE:CE1	1:F:155:LYS:HD2	2.55	0.42
1:C:406:ASN:HA	1:C:406:ASN:HD22	1.60	0.42
1:A:401:TYR:CE2	1:B:443:ALA:N	2.87	0.42
4:B:507[A]:NAD:C5N	1:F:86:ARG:NH2	2.83	0.42
1:B:186:THR:HG22	1:B:187:ILE:N	2.35	0.42
1:A:219:VAL:HG13	1:A:373:LEU:HD11	2.00	0.42
1:D:146:ARG:NE	1:D:182:THR:HG22	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:TRP:CG	1:D:310:TYR:HD2	2.36	0.42
1:C:282:ASN:H	1:C:307:ALA:HB1	1.82	0.42
1:D:29:VAL:CA	1:D:45:VAL:HG21	2.50	0.42
1:C:33:LYS:HA	1:C:33:LYS:HD3	1.72	0.42
1:C:29:VAL:CA	1:C:45:VAL:HG21	2.50	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:F:242:PHE:HB2	1:F:266:PHE:O	2.20	0.42
1:B:242:PHE:O	1:B:268:ALA:HA	2.18	0.42
1:E:266:PHE:CD1	1:E:266:PHE:N	2.87	0.42
1:A:4:GLU:O	1:A:5:ASP:HB3	2.19	0.42
1:E:5:ASP:OD1	1:E:353:THR:HG21	2.19	0.42
1:F:4:GLU:O	1:F:5:ASP:HB3	2.19	0.42
1:B:23:ILE:HD12	1:B:479:THR:OG1	2.19	0.42
1:F:406:ASN:HD22	1:F:406:ASN:HA	1.60	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:C:57:HIS:CD2	1:C:84:HIS:NE2	2.87	0.42
4:B:507[A]:NAD:C4N	1:F:86:ARG:CZ	2.97	0.42
1:E:57:HIS:CD2	1:E:84:HIS:NE2	2.87	0.42
1:D:86:ARG:NH2	4:E:507[A]:NAD:C5N	2.82	0.42
1:B:281:TRP:CG	1:B:310:TYR:HD2	2.36	0.42
1:C:242:PHE:CD1	1:C:263:LEU:HD22	2.54	0.42
1:A:66:ARG:HG3	1:A:72:TRP:CD2	2.54	0.42
1:E:242:PHE:HB2	1:E:266:PHE:O	2.20	0.42
1:D:224:GLU:HB2	1:D:242:PHE:HE2	1.84	0.42
1:B:5:ASP:HB2	1:B:333:LYS:NZ	2.34	0.42
1:C:66:ARG:HG3	1:C:72:TRP:CD2	2.54	0.42
1:B:349:ASN:C	1:B:351:PRO:HD3	2.39	0.42
1:A:386:LEU:HD21	1:F:392:VAL:HG13	2.00	0.42
1:B:2:ASP:O	1:B:3:ARG:C	2.58	0.42
1:F:158:ILE:HG13	1:F:165:PRO:CD	2.50	0.42
1:A:110:LEU:O	1:A:114:LYS:HB2	2.20	0.42
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.83	0.42
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.91	0.42
1:A:57:HIS:CD2	1:A:84:HIS:NE2	2.87	0.42
1:E:393:SER:CB	4:E:507[A]:NAD:PA	3.07	0.42
1:F:186:THR:HG22	1:F:187:ILE:N	2.35	0.42
1:E:370:ASP:HB2	1:E:374:ASN:ND2	2.20	0.42
1:F:172:GLY:H	1:F:175:GLU:HG2	1.83	0.42
1:A:242:PHE:O	1:A:268:ALA:HA	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:5:ASP:OD1	1:F:353:THR:HG21	2.19	0.42
1:B:473:LEU:HD12	1:B:480:ALA:HB2	2.00	0.42
1:B:158:ILE:HG13	1:B:165:PRO:CD	2.50	0.42
1:D:158:ILE:HG13	1:D:165:PRO:CD	2.50	0.42
1:A:274:GLY:N	1:A:314:ILE:HG13	2.35	0.42
1:B:274:GLY:N	1:B:314:ILE:HG13	2.35	0.42
1:D:86:ARG:CZ	4:E:507[A]:NAD:C4N	2.97	0.42
1:F:23:ILE:HD12	1:F:479:THR:OG1	2.19	0.42
1:B:219:VAL:O	1:B:223:ILE:HG13	2.19	0.42
1:F:282:ASN:HD21	1:F:284:ASP:H	1.66	0.42
1:E:42:ARG:O	1:E:46:ARG:N	2.53	0.42
1:F:32:LEU:CD1	1:F:44:ARG:HH11	2.33	0.42
1:E:224:GLU:HB2	1:E:242:PHE:HE2	1.84	0.42
1:D:428:ILE:H	1:D:428:ILE:HD13	1.84	0.42
1:A:432:PRO:CB	1:A:436:PHE:HD2	2.28	0.42
1:A:158:ILE:HG13	1:A:165:PRO:CD	2.50	0.42
1:B:411:MET:HE3	1:B:415:GLU:HG3	2.01	0.42
1:A:443:ALA:HB2	1:F:401:TYR:CG	2.55	0.42
1:F:274:GLY:N	1:F:314:ILE:HG13	2.35	0.42
1:C:235:ILE:HG13	1:C:235:ILE:H	1.69	0.42
1:C:120:VAL:O	4:D:507[A]:NAD:N6A	2.49	0.42
1:C:86:ARG:CZ	4:D:507[A]:NAD:C4N	2.97	0.42
4:A:507[A]:NAD:C5N	1:B:86:ARG:NH2	2.83	0.42
1:A:29:VAL:HG22	1:A:42:ARG:HA	2.02	0.42
1:D:32:LEU:CD1	1:D:44:ARG:HH11	2.33	0.42
1:C:32:LEU:CD1	1:C:44:ARG:HH11	2.33	0.42
1:E:32:LEU:CD1	1:E:44:ARG:HH11	2.33	0.42
1:F:224:GLU:HB2	1:F:242:PHE:HE2	1.84	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: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:406:ASN:HB3	1:B:440:ILE:HD11	2.02	0.42
1:F:110:LEU:HA	1:F:110:LEU:HD23	1.87	0.42
1:D:450:HIS:CE1	5:D:514:HOH:O	2.72	0.42
1:C:186:THR:HG22	1:C:187:ILE:N	2.34	0.42
1:D:186:THR:HG22	1:D:187:ILE:N	2.35	0.42
1:A:33:LYS:HA	1:A:33:LYS:HD3	1.72	0.42
1:D:32:LEU:HD11	1:D:44:ARG:HH11	1.85	0.42

Continued on next page...

Continued from previous page...

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:C:38:GLN:HB2	1:C:39:GLU:H	1.59	0.42
1:E:33:LYS:HD3	1:E:33:LYS:HA	1.72	0.42
1:F:29:VAL:HG22	1:F:42:ARG:HA	2.02	0.42
1:E:321:ILE:HG23	1:E:343:ILE:CG2	2.50	0.42
1:F:321:ILE:HG23	1:F:343:ILE:CG2	2.50	0.42
1:F:110:LEU:O	1:F:114:LYS:HB2	2.20	0.42
4:A:507[A]:NAD:C4N	1:B:86:ARG:CZ	2.97	0.41
1:F:169:MET:CE	1:F:327:SER:HA	2.51	0.41
1:A:370:ASP:CB	1:A:374:ASN:HD21	2.21	0.41
1:B:32:LEU:CD1	1:B:44:ARG:HH11	2.33	0.41
1:F:42:ARG:O	1:F:46:ARG:N	2.53	0.41
1:D:266:PHE:N	1:D:266:PHE:CD1	2.87	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:E:158:ILE:HG13	1:E:165:PRO:CD	2.50	0.41
1:A:406:ASN:HB3	1:A:440:ILE:HD11	2.02	0.41
1:D:406:ASN:HB3	1:D:440:ILE:HD11	2.02	0.41
1:D:321:ILE:HG23	1:D:343:ILE:CG2	2.50	0.41
1:A:186:THR:HG22	1:A:187:ILE:N	2.35	0.41
1:D:276:SER:N	4:D:508:NAD:C2A	2.84	0.41
1:A:32:LEU:CD1	1:A:44:ARG:HH11	2.33	0.41
1:A:147:ARG:NH1	1:D:500:PHE:CD1	2.88	0.41
1:D:294:PHE:CD2	1:D:298:HIS:ND1	2.88	0.41
1:B:5:ASP:CB	1:B:333:LYS:HE2	2.51	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:C:401:TYR:CD2	1:E:443:ALA:HB2	2.55	0.41
1:D:110:LEU:O	1:D:114:LYS:HB2	2.20	0.41
1:A:86:ARG:NH2	4:F:508[A]:NAD:C5N	2.83	0.41
1:E:393:SER:HB3	4:E:507[A]:NAD:O3	2.20	0.41
1:D:169:MET:CE	1:D:327:SER:HA	2.51	0.41
1:E:276:SER:N	4:E:508:NAD:C2A	2.84	0.41
1:E:169:MET:CE	1:E:327:SER:HA	2.51	0.41
1:B:94:ARG:HE	1:B:168:ASN:HD22	1.67	0.41
1:D:219:VAL:O	1:D:223:ILE:HG13	2.19	0.41
1:D:219:VAL:HG13	1:D:373:LEU:HD11	2.00	0.41
1:A:32:LEU:HD11	1:A:44:ARG:HH11	1.85	0.41
1:D:32:LEU:CD1	1:D:44:ARG:NH1	2.83	0.41
1:A:239:THR:HG23	1:A:240:PRO:O	2.20	0.41
1:D:242:PHE:HB2	1:D:266:PHE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ALA:N	1:D:337:PRO:CD	2.83	0.41
1:E:336:ALA:N	1:E:337:PRO:CD	2.83	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:4:GLU:O	1:E:5:ASP:HB3	2.19	0.41
1:A:498:VAL:HB	1:D:72:TRP:CZ2	2.55	0.41
1:A:428:ILE:HG23	1:F:420:LYS:HZ2	1.85	0.41
1:D:274:GLY:N	1:D:314:ILE:HG13	2.35	0.41
1:C:274:GLY:N	1:C:314:ILE:HG13	2.35	0.41
1:A:321:ILE:HG23	1:A:343:ILE:CG2	2.50	0.41
1:A:321:ILE:HA	1:A:343:ILE:O	2.20	0.41
1:D:13:VAL:HA	1:D:16:PHE:CD1	2.55	0.41
1:D:286:ILE:HD12	1:D:286:ILE:N	2.35	0.41
1:A:276:SER:N	4:A:508:NAD:C2A	2.84	0.41
1:A:111:MET:HE1	1:A:378:VAL:CG1	2.50	0.41
1:F:276:SER:N	4:F:507:NAD:C2A	2.84	0.41
1:C:175:GLU:HA	1:C:178:TRP:CE3	2.56	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: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: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:D:432:PRO:HB3	1:D:436:PHE:CD2	2.48	0.41
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.48	0.41
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.87	0.41
1:B:13:VAL:HA	1:B:16:PHE:CD1	2.55	0.41
1:C:13:VAL:HA	1:C:16:PHE:CD1	2.55	0.41
1:B:204:SER:OG	1:F:495:GLU:OE1	2.18	0.41
4:C:507[A]:NAD:C5N	1:E:86:ARG:NH2	2.83	0.41
1:B:32:LEU:CD1	1:B:44:ARG:NH1	2.84	0.41
1:A:246:THR:CG2	1:A:319:CYS:HA	2.51	0.41
1:F:246:THR:CG2	1:F:319:CYS:HA	2.51	0.41
1:E:331:LEU:HD13	1:E:344:ILE:HD13	2.03	0.41
1:A:336:ALA:N	1:A:337:PRO:CD	2.83	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:F:406:ASN:HB3	1:F:440:ILE:HD11	2.02	0.41
1:E:321:ILE:HA	1:E:343:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ALA:O	1:C:234:SER:N	2.49	0.41
1:B:321:ILE:HG23	1:B:343:ILE:CG2	2.50	0.41
1:E:286:ILE:HD12	1:E:286:ILE:N	2.35	0.41
1:C:169:MET:CE	1:C:327:SER:HA	2.51	0.41
1:D:29:VAL:HG22	1:D:42:ARG:HA	2.02	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: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: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: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:E:406:ASN:HB3	1:E:440:ILE:HD11	2.02	0.41
1:C:321:ILE:HA	1:C:343:ILE:O	2.20	0.41
1:E:13:VAL:HA	1:E:16:PHE:CD1	2.55	0.41
3:D:506:AKG:O2	4:D:508:NAD:C6N	2.68	0.41
3:F:506:AKG:O2	4:F:507:NAD:C6N	2.68	0.41
1:F:175:GLU:HA	1:F:178:TRP:CE3	2.56	0.41
1:D:42:ARG:O	1:D:46:ARG:N	2.53	0.41
1:C:32:LEU:CD1	1:C:44:ARG:NH1	2.84	0.41
1:E:32:LEU:HD11	1:E:44:ARG:HH11	1.85	0.41
1:F:33:LYS:HA	1:F:41:LYS:HZ3	1.85	0.41
1:F:331:LEU:HD13	1:F:344:ILE:HD13	2.03	0.41
1:D:331:LEU:HD13	1:D:344:ILE:HD13	2.03	0.41
1:E:344:ILE:HB	1:E:367:VAL:HA	2.03	0.41
1:F:294:PHE:CD2	1:F:298:HIS:ND1	2.88	0.41
1:C:2:ASP:O	1:C:3:ARG:C	2.58	0.41
1:F:333:LYS:HE2	1:F:333:LYS:HB3	1.65	0.41
1:B:421:PHE:CZ	1:F:421:PHE:CD1	3.09	0.41
1:A:495:GLU:HB2	1:F:205:GLN:HE21	1.86	0.41
1:B:155:LYS:HD2	1:E:157:PHE:CE1	2.56	0.41
1:B:401:TYR:CD1	1:F:443:ALA:HB2	2.56	0.41
1:E:274:GLY:N	1:E:314:ILE:HG13	2.35	0.41
1:A:386:LEU:HA	1:A:386:LEU:HD12	1.80	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:C:110:LEU:O	1:C:114:LYS:HB2	2.20	0.41
1:A:15:GLY:O	1:A:18:ASP:N	2.54	0.41
1:E:110:LEU:O	1:E:114:LYS:HB2	2.20	0.41
1:F:302:LEU:HD23	1:F:302:LEU:HA	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:O	1:B:114:LYS:HB2	2.20	0.41
4:B:507[A]:NAD:N6A	1:F:120:VAL:O	2.49	0.41
3:C:506:AKG:O2	4:C:508:NAD:C6N	2.68	0.41
1:F:23:ILE:CD1	1:F:473:LEU:HD21	2.47	0.41
1:D:370:ASP:HB2	1:D:374:ASN:ND2	2.20	0.41
1:E:32:LEU:CD1	1:E:44:ARG:NH1	2.83	0.41
1:A:238:MET:SD	1:A:342:LYS:HB3	2.59	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:C:344:ILE:HB	1:C:367:VAL:HA	2.03	0.41
1:A:294:PHE:CD2	1:A:298:HIS:ND1	2.88	0.41
1:B:294:PHE:CD2	1:B:298:HIS:ND1	2.88	0.41
1:A:5:ASP:HB2	1:A:333:LYS:CE	2.50	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:C:360:PHE:HB3	1:C:365:ILE:HB	2.03	0.41
1:C:15:GLY:O	1:C:18:ASP:N	2.54	0.41
1:A:87:THR:HG21	1:F:195:HIS:CE1	2.51	0.41
1:E:86:ARG:HD2	1:E:86:ARG:HA	1.85	0.41
1:B:57:HIS:CE1	1:E:151:GLU:OE1	2.74	0.41
1:D:94:ARG:HE	1:D:168:ASN:HD22	1.67	0.41
1:C:276:SER:N	4:C:508:NAD:C2A	2.84	0.41
1:F:413:VAL:O	1:F:416:SER:HB2	2.21	0.41
1:B:42:ARG:O	1:B:46:ARG:N	2.53	0.41
1:A:32:LEU:CD1	1:A:44:ARG:NH1	2.84	0.41
1:B:32:LEU:HD11	1:B:44:ARG:HH11	1.85	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:29:VAL:CA	1:E:45:VAL:HG21	2.50	0.41
1:A:227:ILE:HD11	1:A:245:LYS:HG2	2.03	0.41
1:A:238:MET:HE3	1:A:320:ASP:HB3	2.03	0.41
1:E:239:THR:HG23	1:E:240:PRO:O	2.20	0.41
1:E:224:GLU:HB2	1:E:242:PHE:CE2	2.56	0.41
1:C:498:VAL:HB	1:F:72:TRP:CZ2	2.55	0.41
1:D:298:HIS:O	1:D:299:GLY:C	2.60	0.41
1:C:417:LEU:CD1	1:D:417:LEU:CD2	2.96	0.41
1:A:409:LEU:HD12	1:B:436:PHE:HZ	1.83	0.41
1:C:158:ILE:HG13	1:C:165:PRO:CD	2.50	0.41
1:C:93:ILE:HA	1:C:127:ALA:HB3	2.03	0.41
1:A:360:PHE:HB3	1:A:365:ILE:HB	2.03	0.41
1:D:360:PHE:O	1:D:365:ILE:N	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ILE:HA	1:D:343:ILE:O	2.20	0.41
1:F:321:ILE:HA	1:F:343:ILE:O	2.20	0.41
1:A:13:VAL:HA	1:A:16:PHE:CD1	2.55	0.41
1:B:15:GLY:O	1:B:18:ASP:N	2.54	0.41
1:C:286:ILE:N	1:C:286:ILE:HD12	2.35	0.41
1:B:286:ILE:N	1:B:286:ILE:HD12	2.36	0.41
3:B:506:AKG:O2	4:B:508:NAD:C6N	2.68	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
1:D:26:ASP:HA	1:D:42:ARG:HH12	1.86	0.41
1:C:32:LEU:HD11	1:C:44:ARG:HH11	1.85	0.41
1:E:29:VAL:HG22	1:E:42:ARG:HA	2.02	0.41
1:D:224:GLU:HB2	1:D:242:PHE:CE2	2.56	0.41
1:D:344:ILE:HB	1:D:367:VAL:HA	2.03	0.41
1:C:298:HIS:O	1:C:299:GLY:C	2.59	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:C:413:VAL:O	1:C:416:SER:HB2	2.21	0.41
1:C:55:CYS:O	1:F:62:SER:HB3	2.21	0.41
1:F:360:PHE:HB3	1:F:365:ILE:HB	2.03	0.41
1:D:273:VAL:HG21	1:D:291:LEU:HD11	2.03	0.41
1:B:90:LYS:O	1:B:111:MET:HE2	2.21	0.41
1:F:15:GLY:O	1:F:18:ASP:N	2.54	0.41
1:D:15:GLY:O	1:D:18:ASP:N	2.54	0.41
1:D:175:GLU:HA	1:D:178:TRP:CE3	2.56	0.40
1:B:29:VAL:HG22	1:B:42:ARG:HA	2.02	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:499:THR:CB	1:F:64:PRO:HG2	2.51	0.40
1:B:298:HIS:O	1:B:299:GLY:C	2.60	0.40
1:D:113:TYR:HB2	1:D:371:LEU:HD21	2.02	0.40
1:E:432:PRO:CB	1:E:436:PHE:HD2	2.28	0.40
1:D:165:PRO:HD2	1:D:197:CYS:O	2.21	0.40
1:F:93:ILE:HA	1:F:127:ALA:HB3	2.04	0.40
1:D:360:PHE:HB3	1:D:365:ILE:HB	2.03	0.40
1:F:385:ILE:CG2	1:F:386:LEU:N	2.85	0.40
1:B:385:ILE:CG2	1:B:386:LEU:N	2.85	0.40
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.69	0.40
1:B:321:ILE:HA	1:B:343:ILE:O	2.20	0.40
1:F:286:ILE:HD12	1:F:286:ILE:N	2.36	0.40
1:C:361:LEU:HD23	1:C:361:LEU:HA	1.97	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:GLY:O	1:E:18:ASP:N	2.54	0.40
1:B:276:SER:N	4:B:508:NAD:C2A	2.84	0.40
1:B:238:MET:HE2	1:B:245:LYS:HE2	2.03	0.40
1:E:227:ILE:HD11	1:E:245:LYS:HG2	2.03	0.40
1:C:54:PRO:HG3	1:F:74:VAL:HG11	2.02	0.40
1:C:457:MET:CE	1:C:457:MET:HA	2.42	0.40
1:A:113:TYR:HB2	1:A:371:LEU:HD21	2.02	0.40
1:A:205:GLN:HE21	1:B:495:GLU:HB2	1.86	0.40
1:E:273:VAL:HG21	1:E:291:LEU:HD11	2.03	0.40
1:B:360:PHE:HB3	1:B:365:ILE:HB	2.03	0.40
1:E:360:PHE:HB3	1:E:365:ILE:HB	2.03	0.40
1:C:406:ASN:HB3	1:C:440:ILE:HD11	2.02	0.40
1:B:167:PRO:HG3	1:B:176:MET:CG	2.51	0.40
1:C:167:PRO:HG3	1:C:176:MET:CG	2.51	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:370:ASP:CB	1:E:374:ASN:HD21	2.21	0.40
1:F:346:GLU:OE2	1:F:369:PRO:HA	2.22	0.40
1:A:26:ASP:HA	1:A:42:ARG:HH12	1.86	0.40
1:B:29:VAL:CA	1:B:45:VAL:HG21	2.50	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:B:336:ALA:N	1:B:337:PRO:CD	2.83	0.40
1:D:333:LYS:HB3	1:D:333:LYS:HE2	1.65	0.40
1:C:23:ILE:CD1	1:C:473:LEU:HD21	2.47	0.40
1:A:409:LEU:HD21	1:B:409:LEU:CD2	2.51	0.40
1:E:113:TYR:HB2	1:E:371:LEU:HD21	2.02	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:E:469:MET:O	1:E:470:LYS:C	2.60	0.40
1:C:321:ILE:HG23	1:C:343:ILE:CG2	2.50	0.40
1:B:413:VAL:O	1:B:416:SER:HB2	2.21	0.40
1:E:175:GLU:HA	1:E:178:TRP:CE3	2.56	0.40
1:E:346:GLU:OE2	1:E:369:PRO:HA	2.22	0.40
1:A:224:GLU:HB2	1:A:242:PHE:CE2	2.56	0.40
1:F:24:VAL:O	1:F:25:GLU:C	2.60	0.40
1:E:246:THR:CG2	1:E:319:CYS:HA	2.51	0.40
1:C:417:LEU:HD21	1:E:417:LEU:HD12	2.01	0.40
1:A:23:ILE:CD1	1:A:473:LEU:HD21	2.47	0.40
1:D:411:MET:HE3	1:D:415:GLU:HG3	2.02	0.40
1:B:165:PRO:HD2	1:B:197:CYS:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:VAL:HG21	1:A:291:LEU:HD11	2.03	0.40
1:F:273:VAL:HG21	1:F:291:LEU:HD11	2.03	0.40
1:E:110:LEU:HA	1:E:110:LEU:HD23	1.87	0.40
1:A:286:ILE:HD12	1:A:286:ILE:N	2.36	0.40
1:A:169:MET:CE	1:A:327:SER:HA	2.51	0.40
1:F:26:ASP:HA	1:F:42:ARG:HH12	1.86	0.40
1:E:331:LEU:HA	1:E:335:ASN:HD21	1.87	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:239:THR:HG23	1:C:240:PRO:O	2.20	0.40
1:E:413:VAL:O	1:E:416:SER:HB2	2.21	0.40
1:C:110:LEU:HD23	1:C:110:LEU:HA	1.87	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 23
1	B	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3 23
1	C	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3 23
1	D	499/501 (100%)	417 (84%)	59 (12%)	23 (5%)	3 23

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	20
1	B	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	C	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	D	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	E	417/417 (100%)	359 (86%)	58 (14%)	4	20
1	F	417/417 (100%)	359 (86%)	58 (14%)	4	20
All	All	2502/2502 (100%)	2154 (86%)	348 (14%)	4	20

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	A	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	A	506	-	3,9,9	1.06	0	4,11,11	3.18	3 (75%)
4	NAD	A	507[A]	-	38,48,48	2.28	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	A	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	A	508	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
2	PO4	B	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	B	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	B	504	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
2	PO4	B	505	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
3	AKG	B	506	-	3,9,9	1.05	0	4,11,11	3.17	3 (75%)
4	NAD	B	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	B	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	B	508	-	38,48,48	2.22	12 (31%)	47,73,73	2.78	15 (31%)
2	PO4	C	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	C	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	C	504	-	4,4,4	1.68	1 (25%)	6,6,6	0.29	0
2	PO4	C	505	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
3	AKG	C	506	-	3,9,9	1.07	0	4,11,11	3.18	3 (75%)
4	NAD	C	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	C	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	C	508	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
2	PO4	D	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	D	503	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
2	PO4	D	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	D	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	D	506	-	3,9,9	1.04	0	4,11,11	3.18	3 (75%)
4	NAD	D	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	D	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	D	508	-	38,48,48	2.24	12 (31%)	47,73,73	2.79	16 (34%)
2	PO4	E	502	-	4,4,4	1.12	1 (25%)	6,6,6	0.29	0
2	PO4	E	503	-	4,4,4	1.14	1 (25%)	6,6,6	0.29	0
2	PO4	E	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	E	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	E	506	-	3,9,9	1.08	0	4,11,11	3.18	3 (75%)
4	NAD	E	507[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.76	16 (34%)
4	NAD	E	507[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)
4	NAD	E	508	-	38,48,48	2.24	12 (31%)	47,73,73	2.79	15 (31%)
2	PO4	F	502	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	503	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	504	-	4,4,4	1.13	1 (25%)	6,6,6	0.29	0
2	PO4	F	505	-	4,4,4	1.67	1 (25%)	6,6,6	0.29	0
3	AKG	F	506	-	3,9,9	1.08	0	4,11,11	3.19	3 (75%)
4	NAD	F	507	-	38,48,48	2.23	12 (31%)	47,73,73	2.78	16 (34%)
4	NAD	F	508[A]	-	38,48,48	2.27	11 (28%)	47,73,73	2.77	16 (34%)
4	NAD	F	508[B]	-	38,48,48	2.47	11 (28%)	47,73,73	2.35	16 (34%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	507[B]	NAD	C2N-C3N	-4.30	1.32	1.39
4	B	507[B]	NAD	C2N-C3N	-4.29	1.32	1.39
4	E	507[B]	NAD	C2N-C3N	-4.27	1.32	1.39
4	F	508[B]	NAD	C2N-C3N	-4.27	1.32	1.39
4	C	507[B]	NAD	C2N-C3N	-4.25	1.32	1.39
4	D	507[B]	NAD	C2N-C3N	-4.23	1.32	1.39
4	E	508	NAD	C2N-C3N	-3.66	1.33	1.39
4	D	508	NAD	C2N-C3N	-3.66	1.33	1.39
4	F	507	NAD	C2N-C3N	-3.64	1.33	1.39
4	C	508	NAD	C2N-C3N	-3.64	1.33	1.39
4	A	508	NAD	C2N-C3N	-3.64	1.33	1.39
4	B	508	NAD	C2N-C3N	-3.61	1.33	1.39
4	A	507[A]	NAD	C2N-C3N	-3.44	1.33	1.39
4	F	508[A]	NAD	C2N-C3N	-3.44	1.33	1.39
4	C	507[A]	NAD	C2N-C3N	-3.43	1.33	1.39
4	E	507[A]	NAD	C2N-C3N	-3.43	1.33	1.39
4	B	507[A]	NAD	C2N-C3N	-3.42	1.33	1.39
4	D	507[A]	NAD	C2N-C3N	-3.40	1.33	1.39
4	E	507[A]	NAD	PN-O1N	-3.13	1.39	1.51
4	C	507[A]	NAD	PN-O1N	-3.13	1.39	1.51
4	A	507[A]	NAD	PN-O1N	-3.12	1.39	1.51
4	F	508[A]	NAD	PN-O1N	-3.12	1.39	1.51
4	B	507[A]	NAD	PN-O1N	-3.12	1.39	1.51
4	D	507[A]	NAD	PN-O1N	-3.11	1.39	1.51
4	E	507[A]	NAD	PA-O5B	-2.87	1.45	1.59
4	D	507[A]	NAD	PA-O5B	-2.87	1.45	1.59
4	A	507[A]	NAD	PA-O5B	-2.87	1.45	1.59
4	F	508[A]	NAD	PA-O5B	-2.87	1.45	1.59
4	C	507[A]	NAD	PA-O5B	-2.86	1.45	1.59
4	B	507[A]	NAD	PA-O5B	-2.86	1.45	1.59
4	D	507[B]	NAD	PA-O5B	-2.71	1.46	1.59
4	F	508[B]	NAD	PA-O5B	-2.71	1.46	1.59
4	B	507[B]	NAD	PA-O5B	-2.70	1.46	1.59
4	E	507[B]	NAD	PA-O5B	-2.70	1.46	1.59
4	C	507[B]	NAD	PA-O5B	-2.70	1.46	1.59
4	A	507[B]	NAD	PA-O5B	-2.70	1.46	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	508	NAD	PA-O5B	-2.54	1.47	1.59
4	C	508	NAD	PA-O5B	-2.54	1.47	1.59
4	B	508	NAD	PA-O5B	-2.53	1.47	1.59
4	A	508	NAD	PA-O5B	-2.53	1.47	1.59
4	F	507	NAD	PA-O5B	-2.52	1.47	1.59
4	E	508	NAD	PA-O5B	-2.51	1.47	1.59
4	E	507[B]	NAD	PN-O1N	-2.45	1.42	1.51
4	D	507[B]	NAD	PN-O1N	-2.44	1.42	1.51
4	F	508[B]	NAD	PN-O1N	-2.44	1.42	1.51
4	C	507[B]	NAD	PN-O1N	-2.44	1.42	1.51
4	A	507[B]	NAD	PN-O1N	-2.44	1.42	1.51
4	B	507[B]	NAD	PN-O1N	-2.42	1.42	1.51
4	E	508	NAD	C3D-C4D	-2.07	1.47	1.53
4	D	508	NAD	C3D-C4D	-2.06	1.47	1.53
4	F	507	NAD	C3D-C4D	-2.06	1.47	1.53
4	A	507[A]	NAD	C6A-N6A	-2.06	1.28	1.34
4	A	508	NAD	C3D-C4D	-2.06	1.47	1.53
4	C	508	NAD	C3D-C4D	-2.06	1.47	1.53
4	E	507[A]	NAD	C6A-N6A	-2.05	1.28	1.34
4	B	508	NAD	C3D-C4D	-2.05	1.47	1.53
4	D	507[A]	NAD	C6A-N6A	-2.04	1.28	1.34
4	F	508[A]	NAD	C6A-N6A	-2.04	1.28	1.34
4	B	507[A]	NAD	C6A-N6A	-2.04	1.28	1.34
4	C	507[A]	NAD	C6A-N6A	-2.04	1.28	1.34
4	C	507[B]	NAD	C6N-N1N	2.03	1.40	1.35
4	E	507[B]	NAD	C6N-N1N	2.04	1.40	1.35
4	A	507[A]	NAD	C6N-N1N	2.04	1.40	1.35
4	D	507[A]	NAD	C6N-N1N	2.05	1.41	1.35
4	F	508[A]	NAD	C6N-N1N	2.05	1.41	1.35
4	C	507[A]	NAD	C6N-N1N	2.05	1.41	1.35
4	B	507[A]	NAD	C6N-N1N	2.06	1.41	1.35
4	B	507[B]	NAD	C6N-N1N	2.06	1.41	1.35
4	D	507[B]	NAD	C6N-N1N	2.06	1.41	1.35
4	E	507[A]	NAD	C6N-N1N	2.06	1.41	1.35
4	F	508[B]	NAD	C6N-N1N	2.06	1.41	1.35
4	A	507[B]	NAD	C6N-N1N	2.07	1.41	1.35
4	B	508	NAD	C3B-C4B	2.11	1.58	1.53
4	C	508	NAD	C3B-C4B	2.11	1.58	1.53
4	A	508	NAD	C3B-C4B	2.12	1.58	1.53
4	E	508	NAD	C3B-C4B	2.13	1.58	1.53
4	E	507[B]	NAD	O4B-C1B	2.13	1.43	1.41
4	D	508	NAD	C3B-C4B	2.13	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	507	NAD	C3B-C4B	2.13	1.58	1.53
4	C	507[B]	NAD	O4B-C1B	2.15	1.43	1.41
4	B	507[B]	NAD	O4B-C1B	2.15	1.43	1.41
4	A	507[B]	NAD	O4B-C1B	2.16	1.43	1.41
2	E	502	PO4	P-O4	2.17	1.61	1.53
2	F	503	PO4	P-O4	2.17	1.61	1.53
2	D	503	PO4	P-O4	2.17	1.61	1.53
2	A	503	PO4	P-O4	2.18	1.61	1.53
4	F	508[B]	NAD	O4B-C1B	2.18	1.44	1.41
2	B	505	PO4	P-O4	2.18	1.61	1.53
2	B	502	PO4	P-O4	2.18	1.61	1.53
2	C	502	PO4	P-O4	2.18	1.61	1.53
2	C	503	PO4	P-O4	2.18	1.61	1.53
2	D	504	PO4	P-O4	2.18	1.61	1.53
2	D	502	PO4	P-O4	2.19	1.61	1.53
2	A	504	PO4	P-O4	2.19	1.61	1.53
2	C	505	PO4	P-O4	2.19	1.61	1.53
2	E	504	PO4	P-O4	2.19	1.61	1.53
2	A	502	PO4	P-O4	2.19	1.61	1.53
2	F	502	PO4	P-O4	2.19	1.61	1.53
2	B	503	PO4	P-O4	2.19	1.61	1.53
4	D	507[B]	NAD	O4B-C1B	2.20	1.44	1.41
2	E	503	PO4	P-O4	2.20	1.61	1.53
2	F	504	PO4	P-O4	2.20	1.61	1.53
4	F	507	NAD	C5N-C4N	2.27	1.43	1.38
4	C	508	NAD	C5N-C4N	2.27	1.43	1.38
4	E	508	NAD	C5N-C4N	2.28	1.43	1.38
4	A	508	NAD	C5N-C4N	2.29	1.43	1.38
4	D	508	NAD	C5N-C4N	2.29	1.43	1.38
4	B	508	NAD	C5N-C4N	2.31	1.43	1.38
4	B	507[A]	NAD	O2D-C2D	2.40	1.48	1.43
4	D	507[A]	NAD	O2D-C2D	2.40	1.48	1.43
4	C	507[A]	NAD	O2D-C2D	2.42	1.48	1.43
4	E	507[A]	NAD	O2D-C2D	2.42	1.48	1.43
4	F	508[A]	NAD	O2D-C2D	2.42	1.48	1.43
4	A	507[A]	NAD	O2D-C2D	2.44	1.48	1.43
4	C	507[B]	NAD	C5N-C4N	2.64	1.44	1.38
4	B	507[B]	NAD	C5N-C4N	2.64	1.44	1.38
4	F	508[B]	NAD	C5N-C4N	2.65	1.44	1.38
4	D	507[B]	NAD	C5N-C4N	2.66	1.44	1.38
4	E	507[B]	NAD	C5N-C4N	2.67	1.44	1.38
4	A	507[B]	NAD	C5N-C4N	2.68	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	507	NAD	C6N-N1N	2.76	1.42	1.35
4	E	508	NAD	C6N-N1N	2.76	1.42	1.35
4	B	508	NAD	C6N-N1N	2.78	1.42	1.35
4	A	508	NAD	C6N-N1N	2.79	1.42	1.35
4	D	508	NAD	C6N-N1N	2.80	1.43	1.35
4	C	508	NAD	C6N-N1N	2.80	1.43	1.35
4	D	508	NAD	C2A-N3A	2.99	1.37	1.32
4	A	508	NAD	C2A-N3A	3.01	1.37	1.32
4	C	508	NAD	C2A-N3A	3.02	1.37	1.32
4	E	508	NAD	C2A-N3A	3.02	1.37	1.32
4	B	508	NAD	C7N-N7N	3.03	1.39	1.33
4	F	507	NAD	C2A-N3A	3.04	1.37	1.32
4	B	508	NAD	C2A-N3A	3.04	1.37	1.32
4	C	508	NAD	C7N-N7N	3.04	1.39	1.33
4	A	508	NAD	C7N-N7N	3.05	1.39	1.33
4	F	507	NAD	C7N-N7N	3.06	1.39	1.33
4	B	508	NAD	C3N-C7N	3.07	1.55	1.50
4	E	508	NAD	C7N-N7N	3.07	1.39	1.33
4	C	508	NAD	C3N-C7N	3.08	1.55	1.50
4	D	508	NAD	C7N-N7N	3.08	1.39	1.33
4	F	507	NAD	C3N-C7N	3.11	1.55	1.50
4	A	508	NAD	C3N-C7N	3.11	1.55	1.50
4	D	508	NAD	C3N-C7N	3.13	1.55	1.50
2	D	505	PO4	P-O4	3.14	1.64	1.53
2	F	505	PO4	P-O4	3.15	1.64	1.53
2	A	505	PO4	P-O4	3.15	1.64	1.53
4	E	508	NAD	C3N-C7N	3.15	1.55	1.50
2	B	504	PO4	P-O4	3.15	1.64	1.53
2	E	505	PO4	P-O4	3.16	1.64	1.53
2	C	504	PO4	P-O4	3.16	1.64	1.53
4	D	507[A]	NAD	C4A-N3A	4.06	1.41	1.35
4	A	507[A]	NAD	C4A-N3A	4.08	1.41	1.35
4	B	507[A]	NAD	C4A-N3A	4.09	1.41	1.35
4	F	508[A]	NAD	C4A-N3A	4.09	1.41	1.35
4	C	507[A]	NAD	C4A-N3A	4.09	1.41	1.35
4	E	507[A]	NAD	C4A-N3A	4.12	1.41	1.35
4	B	507[B]	NAD	C4A-N3A	4.43	1.42	1.35
4	C	507[B]	NAD	C4A-N3A	4.46	1.42	1.35
4	F	508[B]	NAD	C4A-N3A	4.47	1.42	1.35
4	A	507[B]	NAD	C4A-N3A	4.49	1.42	1.35
4	D	507[B]	NAD	C4A-N3A	4.52	1.42	1.35
4	E	507[A]	NAD	C3N-C7N	4.52	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	507[A]	NAD	C3N-C7N	4.53	1.57	1.50
4	C	507[A]	NAD	C3N-C7N	4.53	1.57	1.50
4	F	508[A]	NAD	C3N-C7N	4.55	1.57	1.50
4	E	507[B]	NAD	C4A-N3A	4.55	1.42	1.35
4	D	507[A]	NAD	C3N-C7N	4.57	1.57	1.50
4	A	507[A]	NAD	C3N-C7N	4.59	1.57	1.50
4	E	507[A]	NAD	C2A-N3A	4.69	1.40	1.32
4	D	507[A]	NAD	C2A-N3A	4.70	1.40	1.32
4	C	507[A]	NAD	C2A-N3A	4.70	1.40	1.32
4	B	507[A]	NAD	C2A-N3A	4.73	1.40	1.32
4	F	508[A]	NAD	C2A-N3A	4.73	1.40	1.32
4	A	507[A]	NAD	C2A-N3A	4.73	1.40	1.32
4	B	507[A]	NAD	C7N-N7N	4.99	1.43	1.33
4	E	507[A]	NAD	C7N-N7N	4.99	1.43	1.33
4	D	507[A]	NAD	C7N-N7N	5.00	1.43	1.33
4	F	508[A]	NAD	C7N-N7N	5.00	1.43	1.33
4	D	508	NAD	PA-O1A	5.01	1.69	1.51
4	A	507[A]	NAD	C7N-N7N	5.02	1.43	1.33
4	C	508	NAD	PA-O1A	5.02	1.69	1.51
4	A	508	NAD	PA-O1A	5.02	1.69	1.51
4	B	508	NAD	PA-O1A	5.03	1.69	1.51
4	E	508	NAD	PA-O1A	5.04	1.69	1.51
4	F	507	NAD	PA-O1A	5.05	1.69	1.51
4	C	507[A]	NAD	C7N-N7N	5.05	1.43	1.33
4	A	507[B]	NAD	C2A-N3A	5.05	1.41	1.32
4	D	507[B]	NAD	C2A-N3A	5.09	1.41	1.32
4	E	507[B]	NAD	C2A-N3A	5.09	1.41	1.32
4	C	507[B]	NAD	C2A-N3A	5.10	1.41	1.32
4	F	508[B]	NAD	C2A-N3A	5.11	1.41	1.32
4	A	507[B]	NAD	C3N-C7N	5.13	1.58	1.50
4	B	507[B]	NAD	C2A-N3A	5.15	1.41	1.32
4	B	507[B]	NAD	C3N-C7N	5.17	1.58	1.50
4	E	507[B]	NAD	C3N-C7N	5.17	1.58	1.50
4	C	507[B]	NAD	C3N-C7N	5.17	1.58	1.50
4	F	508[B]	NAD	C3N-C7N	5.18	1.58	1.50
4	D	507[B]	NAD	C3N-C7N	5.20	1.58	1.50
4	C	508	NAD	C4A-N3A	5.53	1.43	1.35
4	B	508	NAD	C4A-N3A	5.54	1.43	1.35
4	A	508	NAD	C4A-N3A	5.58	1.43	1.35
4	E	508	NAD	C4A-N3A	5.58	1.43	1.35
4	F	507	NAD	C4A-N3A	5.61	1.43	1.35
4	D	508	NAD	C4A-N3A	5.63	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	507[B]	NAD	PA-O1A	5.90	1.72	1.51
4	B	507[B]	NAD	PA-O1A	5.91	1.72	1.51
4	F	508[B]	NAD	PA-O1A	5.91	1.72	1.51
4	E	507[B]	NAD	PA-O1A	5.91	1.72	1.51
4	A	507[B]	NAD	PA-O1A	5.91	1.72	1.51
4	D	507[B]	NAD	PA-O1A	5.92	1.72	1.51
4	B	508	NAD	O4B-C1B	5.93	1.48	1.41
4	F	507	NAD	O4B-C1B	5.95	1.48	1.41
4	A	508	NAD	O4B-C1B	5.96	1.48	1.41
4	D	508	NAD	O4B-C1B	5.97	1.48	1.41
4	C	508	NAD	O4B-C1B	5.99	1.48	1.41
4	E	508	NAD	O4B-C1B	6.01	1.48	1.41
4	D	507[A]	NAD	PA-O1A	6.02	1.73	1.51
4	A	507[A]	NAD	PA-O1A	6.04	1.73	1.51
4	F	508[A]	NAD	PA-O1A	6.04	1.73	1.51
4	C	507[A]	NAD	PA-O1A	6.05	1.73	1.51
4	B	507[A]	NAD	PA-O1A	6.05	1.73	1.51
4	E	507[A]	NAD	PA-O1A	6.06	1.73	1.51
4	D	507[B]	NAD	C7N-N7N	6.55	1.46	1.33
4	C	507[B]	NAD	C7N-N7N	6.56	1.46	1.33
4	A	507[B]	NAD	C7N-N7N	6.56	1.46	1.33
4	F	508[B]	NAD	C7N-N7N	6.56	1.46	1.33
4	B	507[B]	NAD	C7N-N7N	6.57	1.46	1.33
4	E	507[B]	NAD	C7N-N7N	6.60	1.46	1.33

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	507	NAD	N3A-C2A-N1A	-11.36	120.20	128.89
4	D	508	NAD	N3A-C2A-N1A	-11.35	120.20	128.89
4	C	508	NAD	N3A-C2A-N1A	-11.35	120.21	128.89
4	A	508	NAD	N3A-C2A-N1A	-11.34	120.21	128.89
4	B	508	NAD	N3A-C2A-N1A	-11.34	120.22	128.89
4	E	508	NAD	N3A-C2A-N1A	-11.33	120.22	128.89
4	B	507[A]	NAD	N3A-C2A-N1A	-10.14	121.13	128.89
4	C	507[A]	NAD	N3A-C2A-N1A	-10.12	121.15	128.89
4	F	508[A]	NAD	N3A-C2A-N1A	-10.06	121.19	128.89
4	D	507[A]	NAD	N3A-C2A-N1A	-10.04	121.21	128.89
4	E	507[A]	NAD	N3A-C2A-N1A	-10.03	121.21	128.89
4	A	507[A]	NAD	N3A-C2A-N1A	-10.02	121.22	128.89
4	C	507[B]	NAD	N3A-C2A-N1A	-9.21	121.85	128.89
4	B	507[B]	NAD	N3A-C2A-N1A	-9.20	121.85	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	508[B]	NAD	N3A-C2A-N1A	-9.19	121.86	128.89
4	A	507[B]	NAD	N3A-C2A-N1A	-9.19	121.86	128.89
4	E	507[B]	NAD	N3A-C2A-N1A	-9.17	121.87	128.89
4	D	507[B]	NAD	N3A-C2A-N1A	-9.15	121.89	128.89
4	C	507[A]	NAD	C4B-O4B-C1B	-4.81	104.43	109.72
4	B	508	NAD	O3-PA-O5B	-4.80	90.20	102.94
4	E	508	NAD	O3-PA-O5B	-4.79	90.22	102.94
4	F	507	NAD	O3-PA-O5B	-4.79	90.23	102.94
4	D	508	NAD	O3-PA-O5B	-4.79	90.24	102.94
4	F	508[A]	NAD	C4B-O4B-C1B	-4.78	104.46	109.72
4	A	508	NAD	O3-PA-O5B	-4.78	90.25	102.94
4	D	507[A]	NAD	C4B-O4B-C1B	-4.78	104.46	109.72
4	C	508	NAD	O3-PA-O5B	-4.78	90.25	102.94
4	B	507[A]	NAD	C4B-O4B-C1B	-4.78	104.47	109.72
4	E	507[A]	NAD	C4B-O4B-C1B	-4.77	104.48	109.72
4	A	507[A]	NAD	C4B-O4B-C1B	-4.75	104.50	109.72
4	D	508	NAD	O4B-C1B-N9A	-4.41	98.86	108.10
4	E	508	NAD	O4B-C1B-N9A	-4.40	98.88	108.10
4	C	508	NAD	O4B-C1B-N9A	-4.39	98.91	108.10
4	C	508	NAD	C5N-C6N-N1N	-4.39	112.88	120.47
4	A	508	NAD	O4B-C1B-N9A	-4.38	98.92	108.10
4	B	508	NAD	O4B-C1B-N9A	-4.38	98.92	108.10
4	F	507	NAD	O4B-C1B-N9A	-4.38	98.93	108.10
4	E	508	NAD	C5N-C6N-N1N	-4.38	112.90	120.47
4	A	508	NAD	C5N-C6N-N1N	-4.38	112.90	120.47
4	F	507	NAD	C5N-C6N-N1N	-4.37	112.91	120.47
4	D	508	NAD	C5N-C6N-N1N	-4.37	112.91	120.47
4	B	508	NAD	C5N-C6N-N1N	-4.36	112.93	120.47
4	A	507[B]	NAD	C5N-C6N-N1N	-4.27	113.09	120.47
4	F	508[B]	NAD	C5N-C6N-N1N	-4.26	113.10	120.47
4	C	507[B]	NAD	C5N-C6N-N1N	-4.26	113.11	120.47
4	E	507[B]	NAD	C5N-C6N-N1N	-4.25	113.12	120.47
4	D	507[B]	NAD	C5N-C6N-N1N	-4.23	113.14	120.47
4	B	507[B]	NAD	C5N-C6N-N1N	-4.23	113.15	120.47
4	A	507[A]	NAD	C3N-C7N-N7N	-4.18	113.24	117.82
4	D	507[B]	NAD	C5N-C4N-C3N	-4.18	115.08	120.33
4	A	507[B]	NAD	C5N-C4N-C3N	-4.17	115.09	120.33
4	F	508[B]	NAD	C5N-C4N-C3N	-4.15	115.12	120.33
4	F	508[A]	NAD	C3N-C7N-N7N	-4.15	113.28	117.82
4	B	507[A]	NAD	C3N-C7N-N7N	-4.14	113.28	117.82
4	C	507[B]	NAD	C5N-C4N-C3N	-4.14	115.13	120.33
4	C	507[A]	NAD	C3N-C7N-N7N	-4.14	113.29	117.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507[B]	NAD	C5N-C4N-C3N	-4.14	115.13	120.33
4	D	507[A]	NAD	C3N-C7N-N7N	-4.14	113.29	117.82
4	C	507[A]	NAD	C5N-C6N-N1N	-4.12	113.34	120.47
4	E	507[B]	NAD	C5N-C4N-C3N	-4.12	115.15	120.33
4	E	507[A]	NAD	C5N-C6N-N1N	-4.12	113.35	120.47
4	A	507[A]	NAD	C5N-C6N-N1N	-4.11	113.35	120.47
4	F	508[A]	NAD	C5N-C6N-N1N	-4.11	113.37	120.47
4	E	507[A]	NAD	C3N-C7N-N7N	-4.10	113.33	117.82
4	D	507[A]	NAD	C5N-C6N-N1N	-4.08	113.41	120.47
4	B	507[A]	NAD	C5N-C6N-N1N	-4.08	113.42	120.47
4	A	507[A]	NAD	C5N-C4N-C3N	-4.07	115.22	120.33
4	C	507[A]	NAD	C5N-C4N-C3N	-4.07	115.22	120.33
4	F	508[A]	NAD	C5N-C4N-C3N	-4.06	115.23	120.33
4	D	507[A]	NAD	C5N-C4N-C3N	-4.04	115.25	120.33
4	B	507[A]	NAD	C5N-C4N-C3N	-4.03	115.27	120.33
4	E	507[A]	NAD	C5N-C4N-C3N	-4.02	115.28	120.33
4	F	508[A]	NAD	O4B-C1B-N9A	-3.96	99.81	108.10
4	D	507[A]	NAD	O4B-C1B-N9A	-3.96	99.82	108.10
4	C	507[A]	NAD	O4B-C1B-N9A	-3.95	99.83	108.10
4	E	507[A]	NAD	O4B-C1B-N9A	-3.95	99.83	108.10
4	A	507[A]	NAD	O4B-C1B-N9A	-3.95	99.84	108.10
4	B	507[A]	NAD	O4B-C1B-N9A	-3.95	99.84	108.10
4	E	508	NAD	C5N-C4N-C3N	-3.57	115.84	120.33
4	A	508	NAD	C5N-C4N-C3N	-3.55	115.87	120.33
4	B	508	NAD	C5N-C4N-C3N	-3.54	115.89	120.33
4	F	507	NAD	C5N-C4N-C3N	-3.53	115.90	120.33
4	D	508	NAD	C5N-C4N-C3N	-3.53	115.90	120.33
4	C	508	NAD	C5N-C4N-C3N	-3.51	115.92	120.33
4	D	507[B]	NAD	C3N-C7N-N7N	-3.48	114.01	117.82
4	B	507[B]	NAD	C3N-C7N-N7N	-3.48	114.01	117.82
4	C	507[B]	NAD	C3N-C7N-N7N	-3.46	114.03	117.82
4	F	508[B]	NAD	C3N-C7N-N7N	-3.45	114.04	117.82
4	E	508	NAD	C4B-O4B-C1B	-3.45	105.93	109.72
4	E	507[B]	NAD	C3N-C7N-N7N	-3.45	114.05	117.82
4	A	507[B]	NAD	C3N-C7N-N7N	-3.45	114.05	117.82
4	C	508	NAD	C4B-O4B-C1B	-3.44	105.94	109.72
4	D	508	NAD	C4B-O4B-C1B	-3.44	105.94	109.72
4	A	508	NAD	C4B-O4B-C1B	-3.42	105.96	109.72
4	B	508	NAD	C4B-O4B-C1B	-3.42	105.96	109.72
4	F	507	NAD	C4B-O4B-C1B	-3.37	106.02	109.72
4	E	507[B]	NAD	O4B-C1B-N9A	-3.28	101.24	108.10
4	C	507[B]	NAD	O4B-C1B-N9A	-3.27	101.25	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	508[B]	NAD	O4B-C1B-N9A	-3.26	101.27	108.10
4	D	507[B]	NAD	O4B-C1B-N9A	-3.26	101.27	108.10
4	A	507[B]	NAD	O4B-C1B-N9A	-3.25	101.28	108.10
4	B	507[B]	NAD	O4B-C1B-N9A	-3.25	101.30	108.10
4	B	507[A]	NAD	C1B-N9A-C4A	-2.53	123.13	126.94
4	E	507[A]	NAD	C1B-N9A-C4A	-2.52	123.14	126.94
4	F	508[A]	NAD	C1B-N9A-C4A	-2.52	123.14	126.94
4	C	507[A]	NAD	C1B-N9A-C4A	-2.50	123.17	126.94
4	D	507[A]	NAD	C1B-N9A-C4A	-2.50	123.17	126.94
4	A	507[A]	NAD	C1B-N9A-C4A	-2.49	123.19	126.94
4	C	507[B]	NAD	O3-PA-O5B	-2.48	96.37	102.94
4	B	507[B]	NAD	O3-PA-O5B	-2.48	96.37	102.94
4	F	508[B]	NAD	O3-PA-O5B	-2.47	96.38	102.94
4	A	507[B]	NAD	O3-PA-O5B	-2.47	96.38	102.94
4	C	508	NAD	O7N-C7N-C3N	-2.47	116.89	119.59
4	E	507[B]	NAD	O3-PA-O5B	-2.47	96.39	102.94
4	D	507[B]	NAD	O3-PA-O5B	-2.46	96.40	102.94
4	B	508	NAD	O7N-C7N-C3N	-2.44	116.92	119.59
4	A	508	NAD	O7N-C7N-C3N	-2.44	116.93	119.59
4	D	508	NAD	O7N-C7N-C3N	-2.43	116.93	119.59
4	F	507	NAD	O7N-C7N-C3N	-2.42	116.95	119.59
4	A	507[A]	NAD	C3N-C2N-N1N	-2.42	117.58	120.36
4	E	508	NAD	O7N-C7N-C3N	-2.41	116.95	119.59
4	D	507[A]	NAD	C3N-C2N-N1N	-2.41	117.59	120.36
4	C	507[A]	NAD	C3N-C2N-N1N	-2.40	117.60	120.36
4	B	507[A]	NAD	C3N-C2N-N1N	-2.38	117.62	120.36
4	F	508[A]	NAD	C3N-C2N-N1N	-2.37	117.63	120.36
4	E	507[A]	NAD	C3N-C2N-N1N	-2.34	117.66	120.36
4	F	507	NAD	C4D-O4D-C1D	-2.04	107.48	109.72
4	C	508	NAD	C4D-O4D-C1D	-2.02	107.49	109.72
4	D	508	NAD	C4D-O4D-C1D	-2.00	107.52	109.72
4	A	508	NAD	C4D-O4D-C1D	-2.00	107.52	109.72
4	B	508	NAD	O2N-PN-O1N	2.01	123.44	112.53
4	E	508	NAD	O2N-PN-O1N	2.01	123.44	112.53
4	C	508	NAD	O2N-PN-O1N	2.02	123.45	112.53
4	A	508	NAD	O2N-PN-O1N	2.02	123.46	112.53
4	F	507	NAD	O2N-PN-O1N	2.02	123.46	112.53
4	D	508	NAD	O2N-PN-O1N	2.02	123.47	112.53
4	C	507[A]	NAD	O5B-C5B-C4B	2.05	116.68	109.12
4	A	507[A]	NAD	O5B-C5B-C4B	2.06	116.70	109.12
4	F	508[A]	NAD	O5B-C5B-C4B	2.06	116.71	109.12
4	F	507	NAD	N6A-C6A-N1A	2.06	123.62	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507[A]	NAD	O5B-C5B-C4B	2.06	116.73	109.12
4	E	507[A]	NAD	O5B-C5B-C4B	2.07	116.74	109.12
4	D	507[A]	NAD	O5B-C5B-C4B	2.07	116.76	109.12
4	C	508	NAD	N6A-C6A-N1A	2.08	123.66	119.20
4	B	507[B]	NAD	O2B-C2B-C3B	2.08	118.59	111.83
4	E	507[B]	NAD	O2B-C2B-C3B	2.09	118.61	111.83
4	A	508	NAD	N6A-C6A-N1A	2.09	123.68	119.20
4	D	507[B]	NAD	O2B-C2B-C3B	2.09	118.62	111.83
4	B	508	NAD	N6A-C6A-N1A	2.09	123.69	119.20
4	F	508[B]	NAD	O2B-C2B-C3B	2.09	118.63	111.83
4	C	507[B]	NAD	O2B-C2B-C3B	2.10	118.65	111.83
4	D	508	NAD	N6A-C6A-N1A	2.10	123.71	119.20
4	E	508	NAD	N6A-C6A-N1A	2.10	123.72	119.20
4	A	507[B]	NAD	O2B-C2B-C3B	2.11	118.69	111.83
4	C	507[B]	NAD	C2D-C3D-C4D	2.13	106.99	102.61
4	D	507[B]	NAD	C2D-C3D-C4D	2.14	107.00	102.61
4	A	507[B]	NAD	O7N-C7N-N7N	2.14	125.60	122.59
4	F	508[B]	NAD	C2D-C3D-C4D	2.14	107.00	102.61
4	E	507[B]	NAD	C2D-C3D-C4D	2.14	107.01	102.61
4	E	507[B]	NAD	O7N-C7N-N7N	2.14	125.61	122.59
4	C	507[B]	NAD	O7N-C7N-N7N	2.15	125.62	122.59
4	B	507[B]	NAD	O4D-C1D-N1N	2.15	110.49	108.13
4	D	507[B]	NAD	O4D-C1D-N1N	2.15	110.49	108.13
4	A	507[B]	NAD	C2D-C3D-C4D	2.15	107.03	102.61
4	B	507[B]	NAD	C2D-C3D-C4D	2.15	107.04	102.61
4	F	508[B]	NAD	O7N-C7N-N7N	2.16	125.64	122.59
4	F	508[B]	NAD	O4D-C1D-N1N	2.16	110.51	108.13
4	B	508	NAD	O7N-C7N-N7N	2.17	125.66	122.59
4	C	507[B]	NAD	O4D-C1D-N1N	2.18	110.52	108.13
4	E	507[B]	NAD	O4D-C1D-N1N	2.18	110.53	108.13
4	B	507[B]	NAD	O7N-C7N-N7N	2.18	125.67	122.59
4	A	507[B]	NAD	O4D-C1D-N1N	2.19	110.54	108.13
4	A	508	NAD	O7N-C7N-N7N	2.19	125.68	122.59
4	F	507	NAD	O7N-C7N-N7N	2.20	125.69	122.59
4	C	508	NAD	O7N-C7N-N7N	2.20	125.69	122.59
4	E	508	NAD	O7N-C7N-N7N	2.20	125.69	122.59
4	D	507[B]	NAD	O7N-C7N-N7N	2.20	125.69	122.59
4	D	508	NAD	O7N-C7N-N7N	2.21	125.70	122.59
4	C	507[B]	NAD	O2N-PN-O1N	2.22	124.56	112.53
4	D	507[B]	NAD	O2N-PN-O1N	2.22	124.57	112.53
4	F	508[B]	NAD	O2N-PN-O1N	2.22	124.58	112.53
4	A	507[B]	NAD	O2N-PN-O1N	2.22	124.58	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	507[B]	NAD	O2N-PN-O1N	2.23	124.59	112.53
4	B	507[B]	NAD	O2N-PN-O1N	2.23	124.62	112.53
4	C	507[B]	NAD	C2B-C3B-C4B	2.32	107.38	102.61
4	F	508[B]	NAD	C2B-C3B-C4B	2.33	107.39	102.61
4	B	507[B]	NAD	C2B-C3B-C4B	2.33	107.39	102.61
4	E	507[B]	NAD	C2B-C3B-C4B	2.33	107.39	102.61
4	A	507[B]	NAD	C2B-C3B-C4B	2.33	107.40	102.61
4	D	507[B]	NAD	C2B-C3B-C4B	2.34	107.42	102.61
3	D	506	AKG	C4-C3-C2	2.38	118.99	112.98
3	B	506	AKG	C4-C3-C2	2.38	118.99	112.98
3	A	506	AKG	C4-C3-C2	2.39	119.01	112.98
3	F	506	AKG	C4-C3-C2	2.39	119.03	112.98
3	E	506	AKG	C4-C3-C2	2.39	119.03	112.98
3	C	506	AKG	C4-C3-C2	2.40	119.05	112.98
4	D	507[B]	NAD	PN-O3-PA	2.55	139.88	132.73
4	E	507[B]	NAD	PN-O3-PA	2.55	139.90	132.73
4	F	508[B]	NAD	PN-O3-PA	2.56	139.91	132.73
4	A	507[B]	NAD	PN-O3-PA	2.56	139.93	132.73
4	C	507[B]	NAD	PN-O3-PA	2.56	139.93	132.73
4	B	507[B]	NAD	PN-O3-PA	2.57	139.94	132.73
4	F	507	NAD	O4D-C1D-N1N	2.70	111.10	108.13
4	D	508	NAD	O4D-C1D-N1N	2.70	111.10	108.13
4	C	508	NAD	O4D-C1D-N1N	2.70	111.10	108.13
4	B	508	NAD	O4D-C1D-N1N	2.73	111.13	108.13
4	A	508	NAD	O4D-C1D-N1N	2.73	111.13	108.13
4	E	508	NAD	O4D-C1D-N1N	2.77	111.17	108.13
4	C	507[A]	NAD	O7N-C7N-N7N	2.94	126.74	122.59
4	E	507[A]	NAD	O7N-C7N-N7N	2.97	126.78	122.59
4	D	507[A]	NAD	O7N-C7N-N7N	2.98	126.79	122.59
4	F	508[A]	NAD	O7N-C7N-N7N	2.98	126.79	122.59
4	B	507[A]	NAD	O7N-C7N-N7N	2.99	126.80	122.59
4	A	507[A]	NAD	O7N-C7N-N7N	3.00	126.82	122.59
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	3.14	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	3.15	124.20	119.44
4	A	507[A]	NAD	C6N-C5N-C4N	3.15	124.20	119.44
3	D	506	AKG	C3-C4-C5	3.18	118.58	112.75
3	B	506	AKG	C3-C4-C5	3.19	118.60	112.75
4	E	507[B]	NAD	C6N-C5N-C4N	3.20	124.28	119.44
3	A	506	AKG	C3-C4-C5	3.21	118.63	112.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	506	AKG	C3-C4-C5	3.22	118.64	112.75
4	B	507[B]	NAD	C6N-C5N-C4N	3.22	124.31	119.44
3	C	506	AKG	C3-C4-C5	3.23	118.66	112.75
3	F	506	AKG	C3-C4-C5	3.23	118.66	112.75
4	C	507[B]	NAD	C6N-C5N-C4N	3.23	124.33	119.44
4	F	508[B]	NAD	C6N-C5N-C4N	3.24	124.34	119.44
4	A	507[A]	NAD	C2D-C3D-C4D	3.24	109.27	102.61
4	C	507[A]	NAD	C2D-C3D-C4D	3.24	109.28	102.61
4	E	507[A]	NAD	C2D-C3D-C4D	3.25	109.29	102.61
4	A	507[B]	NAD	C6N-C5N-C4N	3.25	124.36	119.44
4	F	508[A]	NAD	C2D-C3D-C4D	3.26	109.30	102.61
4	D	507[B]	NAD	C6N-C5N-C4N	3.26	124.36	119.44
4	B	507[A]	NAD	C2D-C3D-C4D	3.26	109.31	102.61
4	D	507[A]	NAD	C2D-C3D-C4D	3.26	109.32	102.61
4	B	508	NAD	C4A-C5A-N7A	3.37	112.58	109.48
4	A	508	NAD	C4A-C5A-N7A	3.42	112.62	109.48
4	F	507	NAD	C4A-C5A-N7A	3.42	112.62	109.48
4	D	508	NAD	C4A-C5A-N7A	3.42	112.63	109.48
4	C	508	NAD	C4A-C5A-N7A	3.45	112.65	109.48
4	E	508	NAD	C4A-C5A-N7A	3.45	112.66	109.48
4	D	508	NAD	C6N-C5N-C4N	3.79	125.16	119.44
4	B	508	NAD	C6N-C5N-C4N	3.79	125.17	119.44
4	F	507	NAD	C6N-C5N-C4N	3.79	125.18	119.44
4	A	508	NAD	C6N-C5N-C4N	3.81	125.20	119.44
4	C	508	NAD	C6N-C5N-C4N	3.82	125.22	119.44
4	E	508	NAD	C6N-C5N-C4N	3.82	125.22	119.44
4	B	507[B]	NAD	C2N-C3N-C4N	4.00	122.74	118.29
4	A	507[B]	NAD	C2N-C3N-C4N	4.01	122.76	118.29
4	C	507[B]	NAD	C2N-C3N-C4N	4.02	122.76	118.29
4	F	508[B]	NAD	C2N-C3N-C4N	4.02	122.76	118.29
4	D	507[B]	NAD	C2N-C3N-C4N	4.02	122.77	118.29
4	E	507[B]	NAD	C2N-C3N-C4N	4.03	122.77	118.29
4	C	508	NAD	C2N-C3N-C4N	4.09	122.85	118.29
4	B	508	NAD	C2N-C3N-C4N	4.11	122.87	118.29
4	A	508	NAD	C2N-C3N-C4N	4.13	122.89	118.29
4	F	507	NAD	C2N-C3N-C4N	4.16	122.92	118.29
4	D	508	NAD	C2N-C3N-C4N	4.16	122.92	118.29
4	E	508	NAD	C2N-C3N-C4N	4.17	122.94	118.29
4	A	507[A]	NAD	PN-O3-PA	4.21	144.56	132.73
4	E	507[A]	NAD	PN-O3-PA	4.22	144.58	132.73
4	C	507[A]	NAD	PN-O3-PA	4.22	144.59	132.73
4	F	508[A]	NAD	PN-O3-PA	4.23	144.60	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	507[A]	NAD	PN-O3-PA	4.23	144.62	132.73
4	B	507[A]	NAD	PN-O3-PA	4.24	144.63	132.73
3	C	506	AKG	O5-C2-C3	4.60	128.98	120.28
4	D	507[B]	NAD	C2A-N1A-C6A	4.61	127.00	118.77
3	B	506	AKG	O5-C2-C3	4.61	129.00	120.28
3	A	506	AKG	O5-C2-C3	4.62	129.01	120.28
3	E	506	AKG	O5-C2-C3	4.62	129.01	120.28
4	A	507[B]	NAD	C2A-N1A-C6A	4.62	127.02	118.77
4	C	507[B]	NAD	C2A-N1A-C6A	4.62	127.03	118.77
4	F	508[B]	NAD	C2A-N1A-C6A	4.62	127.03	118.77
4	E	507[B]	NAD	C2A-N1A-C6A	4.62	127.03	118.77
3	F	506	AKG	O5-C2-C3	4.63	129.03	120.28
4	B	507[B]	NAD	C2A-N1A-C6A	4.65	127.07	118.77
3	D	506	AKG	O5-C2-C3	4.65	129.06	120.28
4	E	507[A]	NAD	C2N-C3N-C4N	4.73	123.56	118.29
4	B	507[A]	NAD	C2N-C3N-C4N	4.75	123.58	118.29
4	F	508[A]	NAD	C2N-C3N-C4N	4.77	123.60	118.29
4	D	507[A]	NAD	C2A-N1A-C6A	4.78	127.30	118.77
4	A	507[A]	NAD	C2A-N1A-C6A	4.78	127.31	118.77
4	F	508[A]	NAD	C2A-N1A-C6A	4.78	127.31	118.77
4	C	507[A]	NAD	C2N-C3N-C4N	4.78	123.61	118.29
4	C	507[A]	NAD	C2A-N1A-C6A	4.79	127.33	118.77
4	E	507[A]	NAD	C2A-N1A-C6A	4.79	127.33	118.77
4	A	507[A]	NAD	C2N-C3N-C4N	4.80	123.63	118.29
4	D	507[A]	NAD	C2N-C3N-C4N	4.80	123.63	118.29
4	B	507[A]	NAD	C2A-N1A-C6A	4.80	127.35	118.77
4	C	507[A]	NAD	C2B-C1B-N9A	5.07	122.04	114.29
4	E	507[A]	NAD	C2B-C1B-N9A	5.08	122.05	114.29
4	B	507[A]	NAD	C2B-C1B-N9A	5.09	122.06	114.29
4	D	507[A]	NAD	C2B-C1B-N9A	5.09	122.06	114.29
4	F	508[A]	NAD	C2B-C1B-N9A	5.09	122.06	114.29
4	A	507[A]	NAD	C2B-C1B-N9A	5.10	122.08	114.29
4	F	507	NAD	C2A-N1A-C6A	5.95	129.40	118.77
4	B	508	NAD	C2A-N1A-C6A	5.96	129.42	118.77
4	C	508	NAD	C2A-N1A-C6A	5.96	129.42	118.77
4	A	508	NAD	C2A-N1A-C6A	5.97	129.43	118.77
4	E	508	NAD	C2A-N1A-C6A	5.97	129.44	118.77
4	D	508	NAD	C2A-N1A-C6A	5.98	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.