



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:41 PM GMT

PDB ID : 1LDN  
Title : STRUCTURE OF A TERNARY COMPLEX OF AN ALLOSTERIC LACTATE DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 2.5 ANGSTROMS RESOLUTION  
Authors : Wigley, D.B.; Gamblin, S.J.; Turkenburg, J.P.; Dodson, E.J.; Piontek, K.; Muirhead, H.; Holbrook, J.J.  
Deposited on : 1991-11-19  
Resolution : 2.50 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](mailto: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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

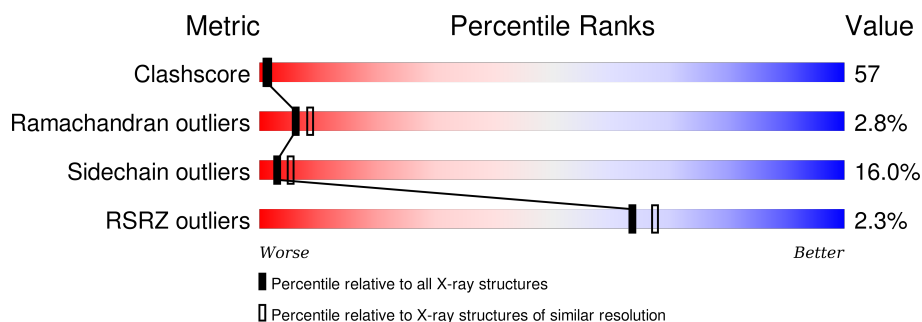
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	316	<div> <div>4%</div> <div>24% 53% 18%</div> <div>.</div> </div>
1	B	316	<div> <div>2%</div> <div>32% 48% 15% 5%</div> <div>.</div> </div>
1	C	316	<div> <div>3%</div> <div>37% 42% 17%</div> <div>.</div> </div>
1	D	316	<div> <div>2%</div> <div>31% 47% 17%</div> <div>.</div> </div>
1	E	316	<div> <div>2%</div> <div>29% 53% 16%</div> <div>.</div> </div>
1	F	316	<div> <div>3%</div> <div>34% 46% 15% 6%</div> <div>.</div> </div>
1	G	316	<div> <div>%</div> <div>30% 49% 18%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	H	316	

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	FBP	B	353[D]	-	-	-	X
2	FBP	E	353[E]	-	-	-	X
2	FBP	E	353[G]	-	-	-	X
3	OXM	A	351	-	-	X	-
3	OXM	B	351	-	-	X	-
3	OXM	C	351	-	-	X	-
3	OXM	E	351	-	-	X	-

## 2 Entry composition

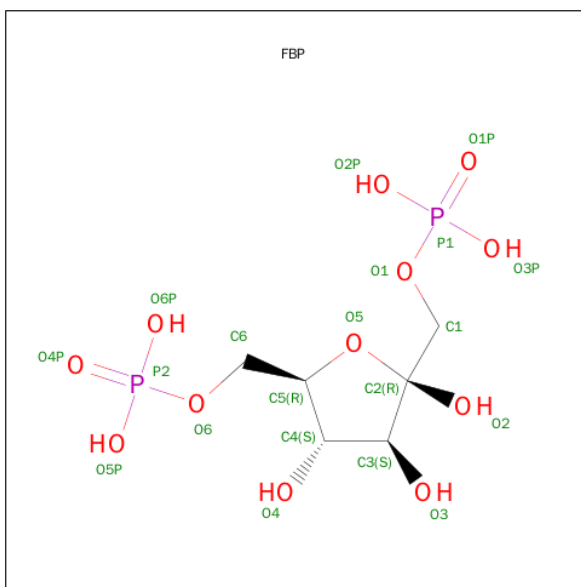
There are 5 unique types of molecules in this entry. The entry contains 20716 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE.

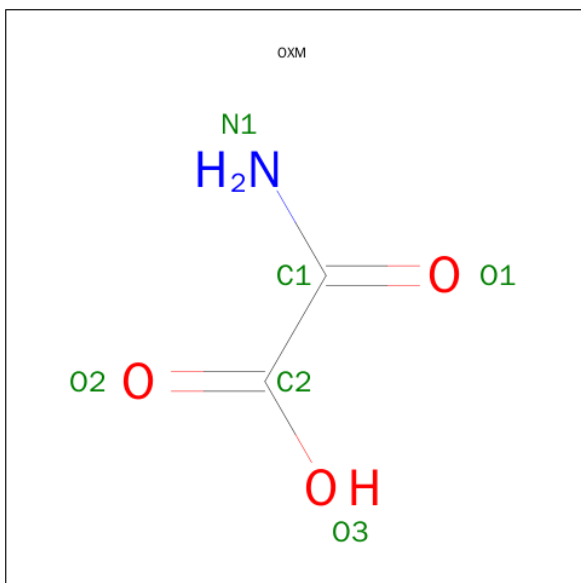
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	B	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	C	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	D	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	E	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	F	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	G	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			
1	H	316	Total	C	N	O	S	0	0	0
			2448	1561	423	456	8			

- Molecule 2 is SUGAR (FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



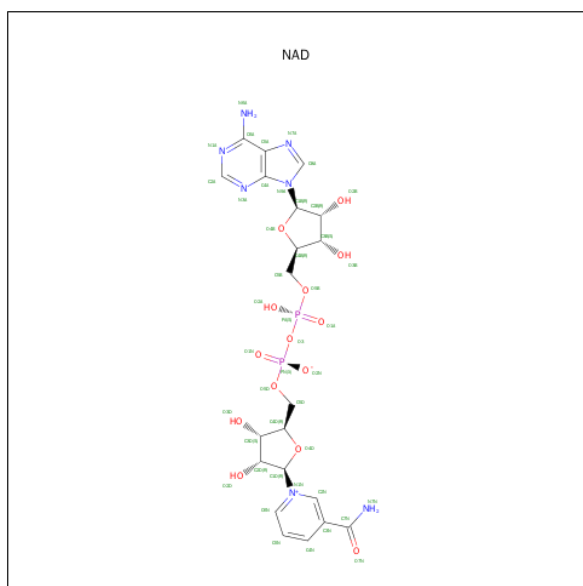
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	1
			40	12	24	4		
2	B	1	Total	C	O	P	0	1
			40	12	24	4		
2	E	1	Total	C	O	P	0	1
			40	12	24	4		
2	F	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula:  $C_2H_3NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		
3	E	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		
3	G	1	Total	C	N	O	0	0
			6	2	1	3		
3	H	1	Total	C	N	O	0	0
			6	2	1	3		

- 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	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

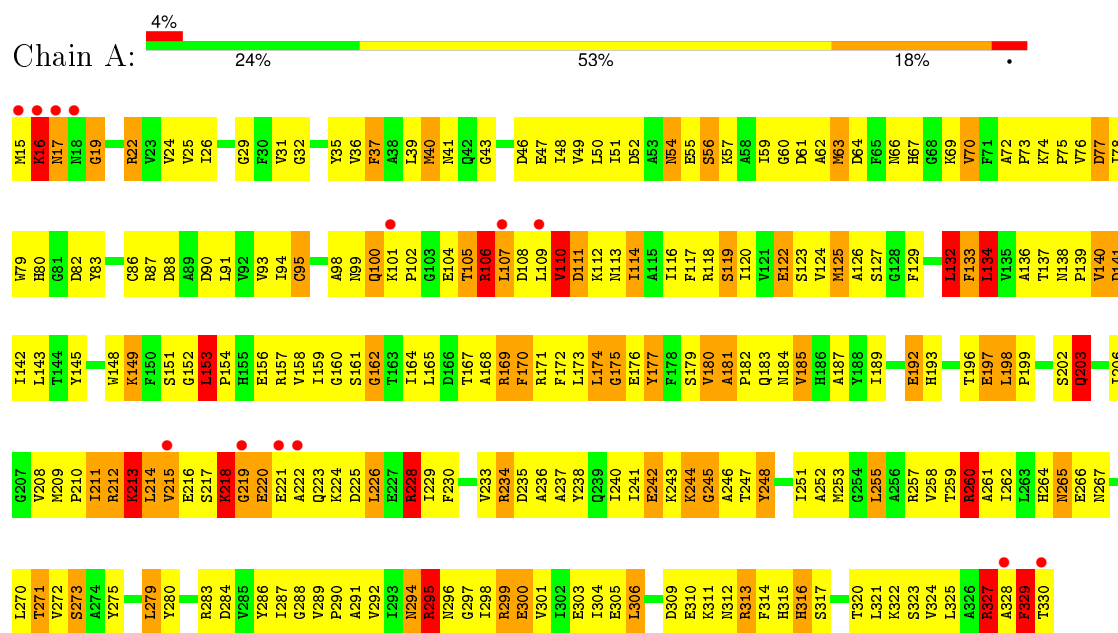
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	72	Total	O	0	0
			72	72		
5	C	69	Total	O	0	0
			69	69		
5	D	74	Total	O	0	0
			74	74		
5	E	70	Total	O	0	0
			70	70		
5	F	72	Total	O	0	0
			72	72		
5	G	70	Total	O	0	0
			70	70		
5	H	73	Total	O	0	0
			73	73		

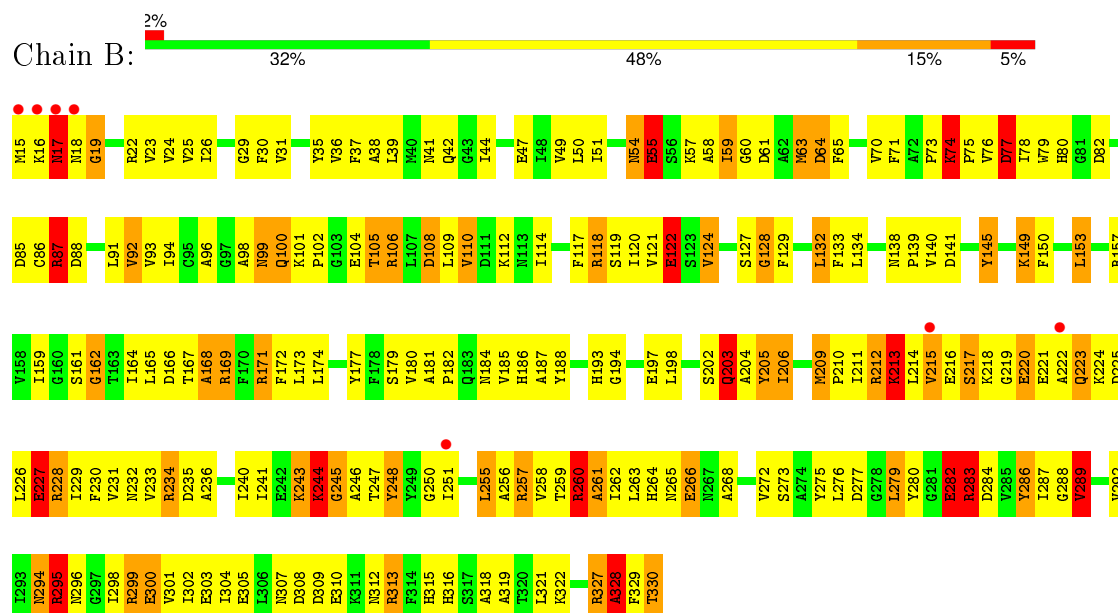
### 3 Residue-property plots

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.

#### • Molecule 1: L-LACTATE DEHYDROGENASE

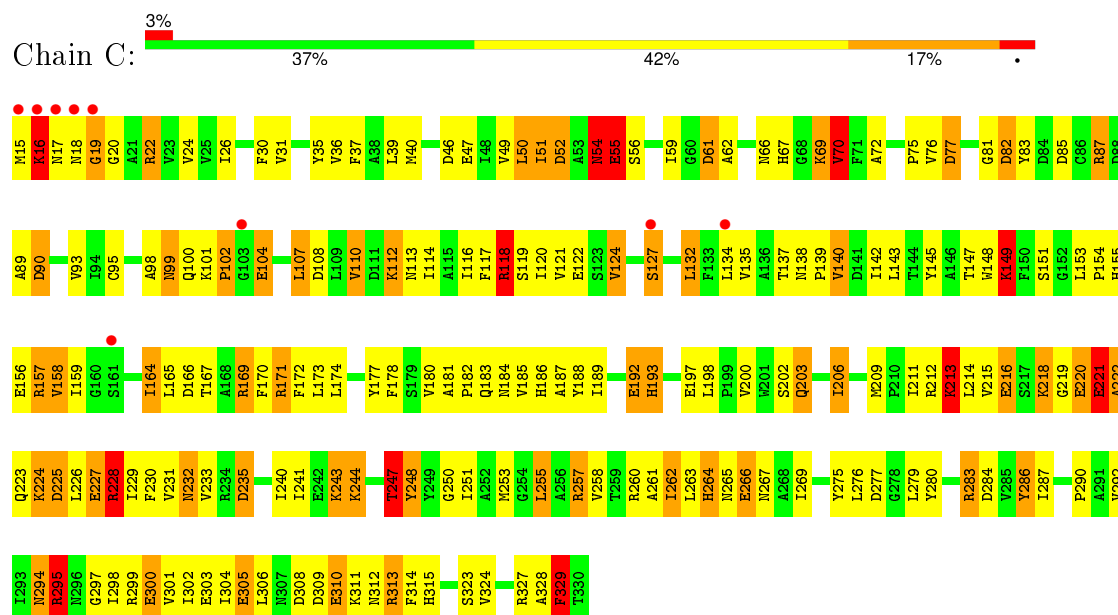


#### • Molecule 1: L-LACTATE DEHYDROGENASE

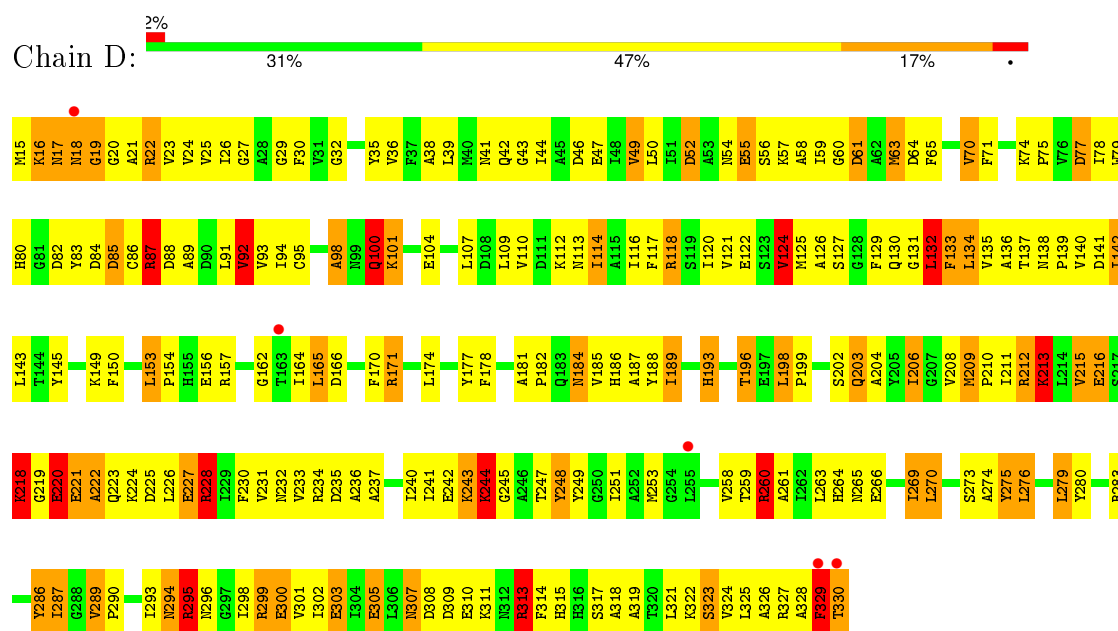




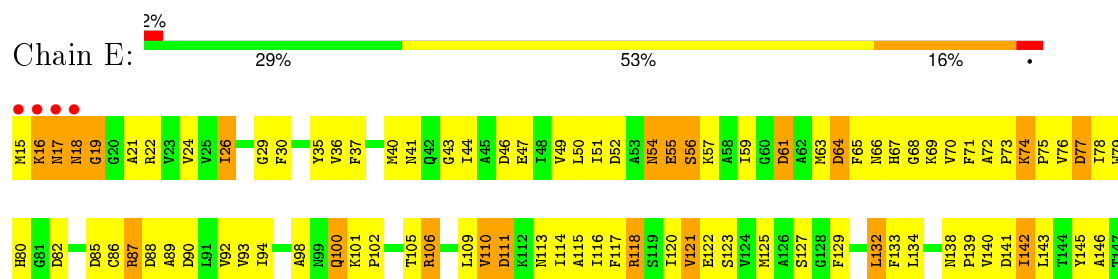
• Molecule 1: L-LACTATE DEHYDROGENASE

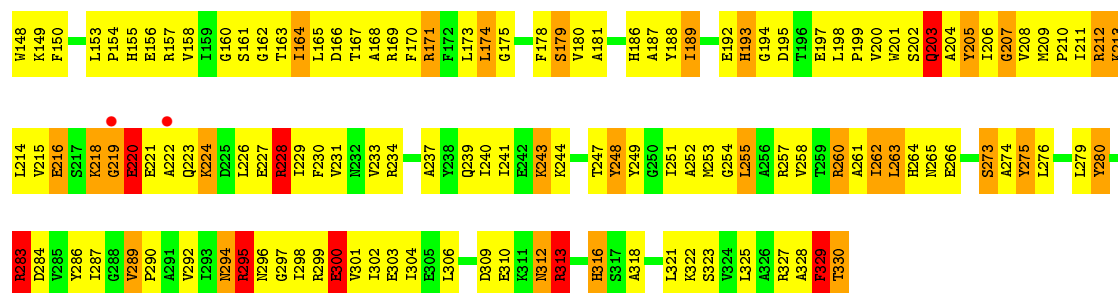


• Molecule 1: L-LACTATE DEHYDROGENASE

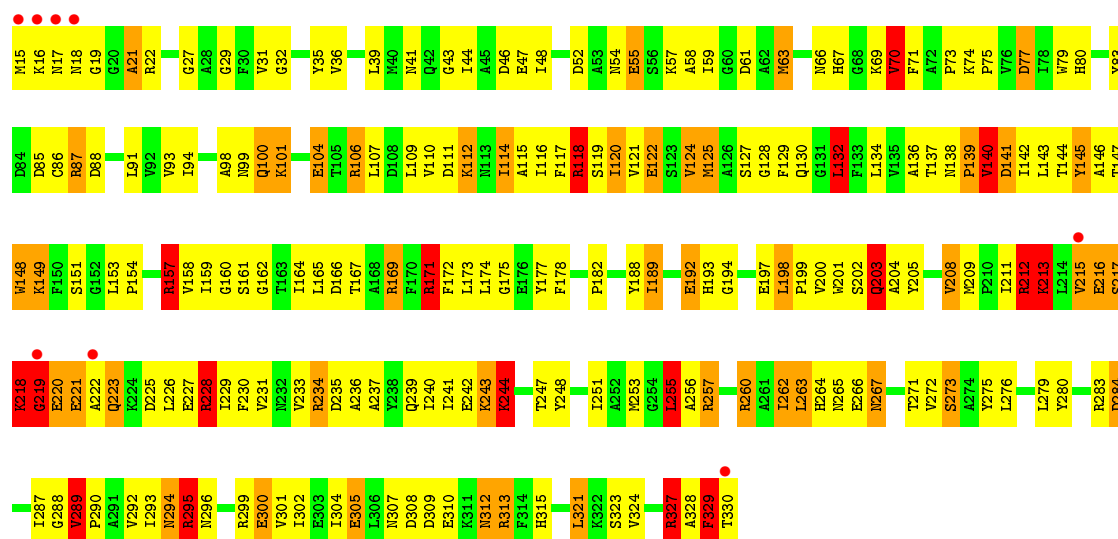


• Molecule 1: L-LACTATE DEHYDROGENASE

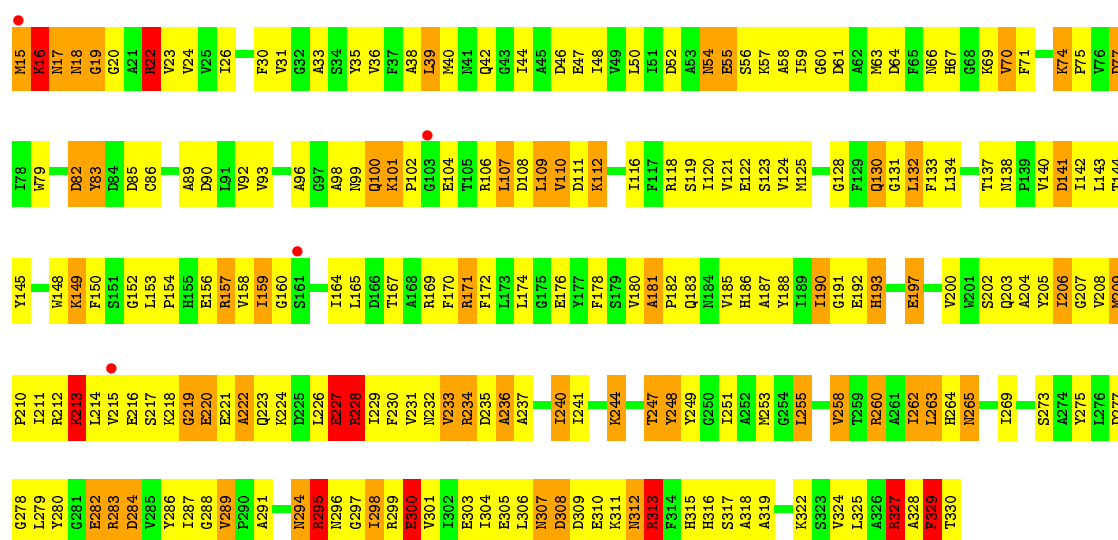




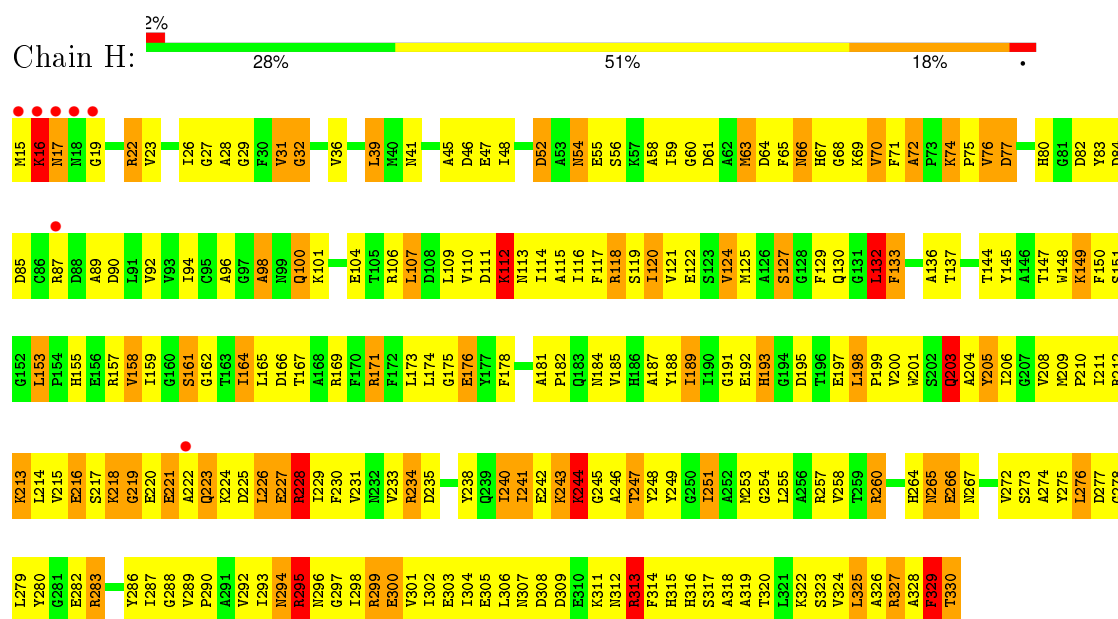
• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.90Å 118.20Å 135.50Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 29.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 68.0 (29.59-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.81 (at 2.51Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.157 , (Not available) 0.146 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 140.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 62506 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OXM, FBP, 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	0.85	0/2496	2.02	79/3384 (2.3%)
1	B	0.85	0/2496	2.05	74/3384 (2.2%)
1	C	0.82	0/2496	2.02	73/3384 (2.2%)
1	D	0.83	0/2496	2.01	83/3384 (2.5%)
1	E	0.83	0/2496	2.14	68/3384 (2.0%)
1	F	0.83	0/2496	2.17	89/3384 (2.6%)
1	G	0.83	0/2496	1.97	72/3384 (2.1%)
1	H	0.84	0/2496	2.15	80/3384 (2.4%)
All	All	0.83	0/19968	2.07	618/27072 (2.3%)

There are no bond length outliers.

All (618) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	171	ARG	CD-NE-CZ	40.03	179.65	123.60
1	B	327	ARG	CD-NE-CZ	32.41	168.97	123.60
1	H	228	ARG	CD-NE-CZ	24.99	158.59	123.60
1	F	327	ARG	CD-NE-CZ	24.62	158.07	123.60
1	F	228	ARG	CD-NE-CZ	22.54	155.15	123.60
1	F	234	ARG	NE-CZ-NH1	22.29	131.45	120.30
1	E	283	ARG	NE-CZ-NH1	20.19	130.40	120.30
1	E	327	ARG	NE-CZ-NH1	-19.20	110.70	120.30
1	C	212	ARG	NE-CZ-NH1	17.43	129.02	120.30
1	F	234	ARG	NE-CZ-NH2	-17.07	111.76	120.30
1	C	212	ARG	CD-NE-CZ	16.91	147.27	123.60
1	D	234	ARG	NE-CZ-NH1	16.39	128.50	120.30
1	H	87	ARG	NE-CZ-NH2	-16.33	112.14	120.30
1	H	157	ARG	NE-CZ-NH1	-16.07	112.27	120.30
1	H	87	ARG	NE-CZ-NH1	15.63	128.12	120.30
1	F	157	ARG	NE-CZ-NH1	-15.26	112.67	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	ARG	NE-CZ-NH2	-15.11	112.75	120.30
1	F	283	ARG	NE-CZ-NH2	14.92	127.76	120.30
1	A	157	ARG	NE-CZ-NH2	14.51	127.56	120.30
1	D	212	ARG	NE-CZ-NH1	14.17	127.38	120.30
1	D	171	ARG	NE-CZ-NH1	14.03	127.31	120.30
1	H	295	ARG	NE-CZ-NH1	13.95	127.28	120.30
1	H	132	LEU	CA-CB-CG	13.67	146.74	115.30
1	C	295	ARG	CD-NE-CZ	13.61	142.66	123.60
1	C	257	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	H	260	ARG	NE-CZ-NH1	-13.05	113.77	120.30
1	E	22	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	A	157	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	F	283	ARG	NE-CZ-NH1	-12.72	113.94	120.30
1	F	234	ARG	CD-NE-CZ	12.65	141.31	123.60
1	B	132	LEU	CA-CB-CG	12.32	143.63	115.30
1	F	106	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	D	171	ARG	CD-NE-CZ	11.88	140.24	123.60
1	G	277	ASP	CB-CG-OD2	-11.87	107.61	118.30
1	H	329	PHE	C-N-CA	11.74	151.06	121.70
1	A	234	ARG	NE-CZ-NH1	-11.71	114.45	120.30
1	E	327	ARG	NE-CZ-NH2	11.45	126.02	120.30
1	H	171	ARG	CD-NE-CZ	11.43	139.60	123.60
1	D	87	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	H	313	ARG	NE-CZ-NH1	-11.37	114.62	120.30
1	D	212	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	E	295	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	G	22	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	D	87	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	C	305	GLU	CA-CB-CG	10.94	137.47	113.40
1	E	283	ARG	CD-NE-CZ	10.82	138.74	123.60
1	H	106	ARG	NE-CZ-NH1	-10.77	114.92	120.30
1	D	260	ARG	NE-CZ-NH1	-10.69	114.95	120.30
1	G	295	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	B	99	ASN	CA-CB-CG	10.49	136.49	113.40
1	F	313	ARG	NE-CZ-NH1	-10.47	115.07	120.30
1	A	212	ARG	CD-NE-CZ	10.41	138.18	123.60
1	G	277	ASP	CB-CG-OD1	10.38	127.65	118.30
1	G	99	ASN	CA-CB-CG	10.36	136.18	113.40
1	C	87	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	F	118	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	C	98	ALA	C-N-CA	10.18	147.16	121.70
1	D	313	ARG	NE-CZ-NH1	-10.13	115.23	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	327	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	E	82	ASP	CA-CB-CG	10.09	135.59	113.40
1	B	169	ARG	NE-CZ-NH1	-10.05	115.28	120.30
1	B	153	LEU	CA-CB-CG	10.00	138.29	115.30
1	G	329	PHE	C-N-CA	9.99	146.68	121.70
1	B	87	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	A	299	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	A	327	ARG	CA-CB-CG	9.94	135.26	113.40
1	E	106	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	F	299	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	E	22	ARG	CD-NE-CZ	-9.73	109.98	123.60
1	G	295	ARG	CD-NE-CZ	9.72	137.21	123.60
1	A	106	ARG	CD-NE-CZ	9.71	137.19	123.60
1	G	283	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	212	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	C	283	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	G	327	ARG	CD-NE-CZ	9.36	136.70	123.60
1	D	212	ARG	CD-NE-CZ	9.32	136.64	123.60
1	D	153	LEU	CA-CB-CG	9.31	136.72	115.30
1	B	329	PHE	C-N-CA	9.26	144.84	121.70
1	B	257	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	D	234	ARG	CD-NE-CZ	9.17	136.44	123.60
1	E	228	ARG	CD-NE-CZ	9.16	136.42	123.60
1	D	329	PHE	CB-CG-CD1	-9.14	114.40	120.80
1	G	260	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	B	244	LYS	CA-CB-CG	9.13	133.49	113.40
1	A	88	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	C	52	ASP	CB-CG-OD1	-9.12	110.10	118.30
1	C	169	ARG	NE-CZ-NH1	-9.05	115.78	120.30
1	F	295	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	H	157	ARG	CD-NE-CZ	-8.95	111.06	123.60
1	G	313	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	H	212	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	H	64	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	B	308	ASP	CB-CG-OD1	-8.85	110.33	118.30
1	A	169	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	G	228	ARG	CD-NE-CZ	8.83	135.96	123.60
1	G	61	ASP	CB-CG-OD1	8.76	126.19	118.30
1	G	283	ARG	CD-NE-CZ	8.74	135.84	123.60
1	D	329	PHE	C-N-CA	8.72	143.50	121.70
1	A	329	PHE	C-N-CA	8.70	143.44	121.70
1	H	329	PHE	CB-CG-CD1	-8.66	114.73	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	ARG	NE-CZ-NH1	-8.62	115.99	120.30
1	C	104	GLU	OE1-CD-OE2	8.59	133.61	123.30
1	E	64	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	F	87	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	315	HIS	CA-CB-CG	-8.58	99.02	113.60
1	B	188	TYR	CA-CB-CG	8.57	129.69	113.40
1	G	157	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	C	295	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	H	283	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	G	260	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	E	212	ARG	CD-NE-CZ	8.50	135.50	123.60
1	F	100	GLN	N-CA-CB	8.48	125.87	110.60
1	C	212	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	H	329	PHE	CA-CB-CG	-8.46	93.59	113.90
1	G	171	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	C	82	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	181	ALA	CB-CA-C	8.37	122.66	110.10
1	E	186	HIS	CA-CB-CG	-8.37	99.37	113.60
1	G	308	ASP	CB-CG-OD2	8.33	125.80	118.30
1	G	22	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	F	118	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	22	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	E	228	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	F	228	ARG	CG-CD-NE	8.24	129.10	111.80
1	C	55	GLU	OE1-CD-OE2	8.21	133.16	123.30
1	H	283	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	C	87	ARG	CD-NE-CZ	8.20	135.08	123.60
1	A	125	MET	CA-CB-CG	8.20	127.23	113.30
1	C	228	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	E	82	ASP	CB-CG-OD1	8.18	125.66	118.30
1	H	234	ARG	CD-NE-CZ	8.16	135.03	123.60
1	A	228	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	E	260	ARG	NE-CZ-NH1	-8.00	116.30	120.30
1	F	141	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	D	52	ASP	CB-CG-OD1	7.97	125.47	118.30
1	H	98	ALA	C-N-CA	7.95	141.58	121.70
1	D	64	ASP	CB-CG-OD1	7.93	125.44	118.30
1	F	203	GLN	CA-CB-CG	7.85	130.67	113.40
1	E	205	TYR	CB-CG-CD2	7.81	125.69	121.00
1	D	286	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	E	195	ASP	CB-CG-OD2	7.78	125.30	118.30
1	B	106	ARG	CD-NE-CZ	-7.74	112.77	123.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ALA	C-N-CA	-7.72	102.39	121.70
1	F	153	LEU	CA-CB-CG	7.71	133.04	115.30
1	C	61	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	E	260	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	64	ASP	CB-CG-OD1	7.65	125.18	118.30
1	B	82	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	295	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	157	ARG	NE-CZ-NH2	7.63	124.12	120.30
1	C	206	ILE	N-CA-C	-7.60	90.47	111.00
1	C	225	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	G	181	ALA	CB-CA-C	7.58	121.47	110.10
1	H	22	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	227	GLU	CB-CG-CD	7.48	134.39	114.20
1	G	300	GLU	O-C-N	7.47	134.66	122.70
1	A	82	ASP	CA-CB-CG	7.46	129.80	113.40
1	E	188	TYR	CA-CB-CG	7.45	127.56	113.40
1	A	299	ARG	NH1-CZ-NH2	7.45	127.59	119.40
1	C	157	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	F	327	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	G	330	THR	N-CA-CB	7.42	124.39	110.30
1	F	104	GLU	CA-CB-CG	7.42	129.71	113.40
1	B	234	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	F	70	VAL	N-CA-CB	7.41	127.81	111.50
1	A	329	PHE	CB-CG-CD1	-7.41	115.61	120.80
1	F	260	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	A	309	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	E	327	ARG	CA-CB-CG	7.33	129.53	113.40
1	H	234	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	G	141	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	D	55	GLU	OE1-CD-OE2	7.31	132.07	123.30
1	C	253	MET	CA-CB-CG	7.28	125.67	113.30
1	A	141	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	F	171	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	G	17	ASN	CA-CB-CG	-7.20	97.56	113.40
1	F	289	VAL	CB-CA-C	7.19	125.06	111.40
1	B	212	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	E	207	GLY	N-CA-C	-7.18	95.15	113.10
1	H	157	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	F	63	MET	CA-CB-CG	7.12	125.41	113.30
1	B	230	PHE	CB-CG-CD1	-7.11	115.83	120.80
1	C	329	PHE	C-N-CA	7.10	139.46	121.70
1	F	169	ARG	NE-CZ-NH2	-7.08	116.76	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	104	GLU	OE1-CD-OE2	7.07	131.78	123.30
1	E	299	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	B	282	GLU	CA-CB-CG	7.03	128.87	113.40
1	H	283	ARG	CD-NE-CZ	7.03	133.44	123.60
1	B	286	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	234	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	H	100	GLN	N-CA-CB	6.99	123.19	110.60
1	C	222	ALA	N-CA-C	-6.98	92.16	111.00
1	D	156	GLU	CA-CB-CG	6.98	128.75	113.40
1	E	100	GLN	CA-C-O	6.98	134.75	120.10
1	D	329	PHE	CA-CB-CG	-6.97	97.17	113.90
1	F	228	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	G	122	GLU	OE1-CD-OE2	6.93	131.61	123.30
1	E	189	ILE	N-CA-CB	6.92	126.72	110.80
1	H	89	ALA	CB-CA-C	6.92	120.48	110.10
1	G	222	ALA	CB-CA-C	6.92	120.47	110.10
1	E	87	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	64	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	D	98	ALA	C-N-CA	6.89	138.93	121.70
1	C	225	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	90	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	235	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	F	171	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	226	LEU	CB-CA-C	6.85	123.21	110.20
1	E	280	TYR	CA-CB-CG	6.85	126.41	113.40
1	F	88	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	G	212	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	84	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	B	17	ASN	CA-CB-CG	-6.82	98.41	113.40
1	D	82	ASP	CA-CB-CG	6.82	128.40	113.40
1	A	260	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	G	193	HIS	N-CA-CB	6.79	122.82	110.60
1	C	277	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	F	313	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	F	203	GLN	N-CA-CB	-6.75	98.45	110.60
1	C	118	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	D	295	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	242	GLU	OE1-CD-OE2	6.75	131.39	123.30
1	B	169	ARG	CD-NE-CZ	-6.72	114.19	123.60
1	B	64	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	192	GLU	CG-CD-OE2	-6.71	104.88	118.30
1	C	286	TYR	CB-CG-CD1	-6.71	116.97	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	PHE	CA-C-O	6.71	134.20	120.10
1	H	277	ASP	CB-CG-OD1	6.70	124.33	118.30
1	H	203	GLN	CA-CB-CG	6.69	128.11	113.40
1	H	299	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	G	234	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	F	295	ARG	CD-NE-CZ	6.67	132.94	123.60
1	F	305	GLU	CA-CB-CG	6.64	128.01	113.40
1	G	82	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	H	313	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	H	195	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	D	63	MET	O-C-N	6.60	133.25	122.70
1	B	289	VAL	N-CA-CB	-6.59	96.99	111.50
1	C	16	LYS	CA-C-N	-6.57	102.74	117.20
1	D	135	VAL	CB-CA-C	6.54	123.83	111.40
1	A	108	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	295	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	E	90	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	270	LEU	CA-CB-CG	6.52	130.29	115.30
1	E	329	PHE	C-N-CA	6.51	137.97	121.70
1	H	313	ARG	CG-CD-NE	-6.50	98.15	111.80
1	H	235	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	186	HIS	CA-CB-CG	-6.49	102.56	113.60
1	E	193	HIS	N-CA-CB	6.49	122.29	110.60
1	A	299	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	118	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	186	HIS	CA-CB-CG	-6.48	102.58	113.60
1	F	140	VAL	CA-CB-CG1	6.46	120.59	110.90
1	H	84	ASP	CB-CA-C	6.46	123.32	110.40
1	D	100	GLN	CA-C-O	6.46	133.66	120.10
1	F	83	TYR	CB-CG-CD2	6.44	124.86	121.00
1	A	252	ALA	CB-CA-C	6.44	119.75	110.10
1	E	249	TYR	CB-CG-CD2	6.43	124.86	121.00
1	F	267	ASN	CB-CA-C	6.43	123.25	110.40
1	H	221	GLU	O-C-N	6.41	132.96	122.70
1	H	276	LEU	CB-CG-CD2	-6.41	100.10	111.00
1	A	329	PHE	CA-CB-CG	-6.41	98.52	113.90
1	E	115	ALA	CB-CA-C	6.41	119.71	110.10
1	G	122	GLU	CA-CB-CG	-6.40	99.32	113.40
1	C	221	GLU	CA-C-N	-6.39	103.13	117.20
1	B	108	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	242	GLU	CG-CD-OE1	-6.39	105.53	118.30
1	H	226	LEU	CB-CA-C	6.37	122.31	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	LYS	CA-C-O	6.36	133.46	120.10
1	H	300	GLU	CA-CB-CG	6.36	127.38	113.40
1	F	21	ALA	CB-CA-C	6.35	119.63	110.10
1	B	77	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	G	16	LYS	CA-C-N	-6.35	103.22	117.20
1	D	308	ASP	CB-CG-OD2	6.35	124.01	118.30
1	F	169	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	G	289	VAL	CB-CA-C	6.34	123.44	111.40
1	B	145	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	G	282	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	G	118	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	185	VAL	CA-C-O	-6.31	106.84	120.10
1	B	329	PHE	CA-C-O	6.31	133.35	120.10
1	F	192	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	G	96	ALA	N-CA-CB	6.29	118.91	110.10
1	G	212	ARG	CA-CB-CG	6.29	127.23	113.40
1	F	99	ASN	CA-CB-CG	6.28	127.21	113.40
1	F	122	GLU	CB-CA-C	-6.24	97.92	110.40
1	F	171	ARG	CD-NE-CZ	6.23	132.32	123.60
1	A	106	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	C	50	LEU	CA-CB-CG	6.23	129.62	115.30
1	B	122	GLU	OE1-CD-OE2	6.22	130.77	123.30
1	F	132	LEU	CA-CB-CG	6.22	129.60	115.30
1	D	215	VAL	CA-CB-CG2	6.20	120.20	110.90
1	H	277	ASP	CA-C-O	6.19	133.10	120.10
1	H	273	SER	N-CA-CB	6.19	119.78	110.50
1	D	88	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	C	308	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	175	GLY	N-CA-C	-6.17	97.68	113.10
1	D	276	LEU	CA-CB-CG	6.17	129.48	115.30
1	G	107	LEU	CB-CA-C	6.17	121.91	110.20
1	H	277	ASP	CB-CA-C	6.17	122.73	110.40
1	E	260	ARG	CA-CB-CG	6.16	126.96	113.40
1	A	225	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	F	244	LYS	CA-CB-CG	6.16	126.95	113.40
1	G	176	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	F	215	VAL	O-C-N	6.16	132.55	122.70
1	H	22	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	228	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	D	228	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	316	HIS	CA-CB-CG	-6.14	103.17	113.60
1	C	257	ARG	NE-CZ-NH2	6.14	123.37	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PHE	CA-CB-CG	6.14	128.63	113.90
1	A	98	ALA	CA-C-O	6.13	132.98	120.10
1	B	313	ARG	O-C-N	6.13	132.51	122.70
1	B	266	GLU	CA-CB-CG	6.13	126.89	113.40
1	D	25	VAL	O-C-N	6.13	132.51	122.70
1	E	106	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	C	52	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	303	GLU	O-C-N	6.12	132.49	122.70
1	D	85	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	305	GLU	OE1-CD-OE2	6.08	130.59	123.30
1	B	232	ASN	O-C-N	6.08	132.42	122.70
1	H	221	GLU	N-CA-C	-6.07	94.60	111.00
1	B	168	ALA	CB-CA-C	6.07	119.21	110.10
1	E	88	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	G	16	LYS	CA-C-O	6.06	132.83	120.10
1	H	228	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	230	PHE	CA-CB-CG	-6.05	99.37	113.90
1	D	244	LYS	CA-CB-CG	6.05	126.70	113.40
1	B	228	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	314	PHE	CB-CG-CD1	-6.04	116.57	120.80
1	C	102	PRO	N-CA-C	-6.02	96.44	112.10
1	B	261	ALA	CB-CA-C	6.02	119.13	110.10
1	B	329	PHE	CA-CB-CG	-6.02	99.45	113.90
1	D	141	ASP	CB-CG-OD1	6.02	123.71	118.30
1	B	236	ALA	N-CA-CB	5.99	118.48	110.10
1	D	132	LEU	CA-CB-CG	5.99	129.06	115.30
1	E	100	GLN	CA-CB-CG	5.98	126.56	113.40
1	F	309	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	157	ARG	CD-NE-CZ	-5.96	115.25	123.60
1	A	181	ALA	N-CA-CB	-5.96	101.76	110.10
1	E	192	GLU	CG-CD-OE1	5.96	130.22	118.30
1	A	77	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	132	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	128	GLY	N-CA-C	-5.95	98.23	113.10
1	C	228	ARG	CD-NE-CZ	5.95	131.92	123.60
1	D	100	GLN	CA-CB-CG	5.94	126.47	113.40
1	D	299	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	G	15	MET	O-C-N	5.94	132.21	122.70
1	E	313	ARG	CD-NE-CZ	5.94	131.91	123.60
1	B	203	GLN	N-CA-CB	-5.93	99.92	110.60
1	F	145	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	C	108	ASP	CB-CG-OD2	-5.93	112.96	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	LEU	O-C-N	5.93	132.19	122.70
1	C	264	HIS	CA-CB-CG	-5.93	103.53	113.60
1	A	133	PHE	N-CA-CB	5.92	121.26	110.60
1	D	124	VAL	CA-CB-CG1	5.92	119.78	110.90
1	B	245	GLY	N-CA-C	5.92	127.89	113.10
1	G	83	TYR	CA-CB-CG	-5.92	102.16	113.40
1	C	192	GLU	CB-CG-CD	5.91	130.15	114.20
1	D	220	GLU	C-N-CA	5.91	136.46	121.70
1	H	87	ARG	CD-NE-CZ	5.90	131.86	123.60
1	A	220	GLU	C-N-CA	5.90	136.44	121.70
1	F	327	ARG	CA-CB-CG	5.89	126.36	113.40
1	B	85	ASP	CA-CB-CG	5.88	126.33	113.40
1	C	118	ARG	CD-NE-CZ	5.86	131.81	123.60
1	F	255	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	192	GLU	CG-CD-OE1	5.86	130.01	118.30
1	G	63	MET	O-C-N	5.85	132.06	122.70
1	C	232	ASN	O-C-N	5.85	132.06	122.70
1	E	309	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	H	39	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	310	GLU	CA-CB-CG	5.83	126.24	113.40
1	B	88	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	B	328	ALA	CA-C-O	-5.82	107.87	120.10
1	E	156	GLU	CA-CB-CG	5.82	126.20	113.40
1	D	269	ILE	CB-CA-C	5.82	123.23	111.60
1	G	55	GLU	CG-CD-OE2	-5.82	106.67	118.30
1	F	260	ARG	O-C-N	5.81	131.99	122.70
1	G	228	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	E	300	GLU	CB-CA-C	-5.79	98.81	110.40
1	B	283	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	H	31	VAL	CB-CA-C	5.79	122.41	111.40
1	A	271	THR	N-CA-CB	5.79	121.30	110.30
1	D	87	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	283	ARG	CA-CB-CG	5.78	126.12	113.40
1	G	248	TYR	CA-CB-CG	5.77	124.37	113.40
1	A	309	ASP	CA-CB-CG	-5.77	100.70	113.40
1	B	205	TYR	CA-CB-CG	-5.77	102.43	113.40
1	H	171	ARG	CA-CB-CG	-5.77	100.70	113.40
1	H	212	ARG	NH1-CZ-NH2	-5.77	113.05	119.40
1	H	240	ILE	O-C-N	5.76	131.92	122.70
1	B	212	ARG	CA-CB-CG	5.76	126.07	113.40
1	C	283	ARG	CD-NE-CZ	-5.76	115.54	123.60
1	H	107	LEU	CB-CA-C	5.76	121.14	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	212	ARG	CD-NE-CZ	5.75	131.66	123.60
1	G	258	VAL	CA-CB-CG2	5.75	119.53	110.90
1	C	227	GLU	CB-CG-CD	5.75	129.73	114.20
1	D	249	TYR	CB-CG-CD2	5.75	124.45	121.00
1	G	150	PHE	CA-CB-CG	5.75	127.70	113.90
1	H	300	GLU	CB-CA-C	-5.75	98.90	110.40
1	D	232	ASN	CB-CG-OD1	-5.75	110.11	121.60
1	G	122	GLU	O-C-N	5.74	131.88	122.70
1	G	99	ASN	CB-CA-C	5.72	121.85	110.40
1	D	79	TRP	CA-CB-CG	5.72	124.57	113.70
1	F	283	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	B	171	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	134	LEU	CB-CA-C	5.71	121.05	110.20
1	B	77	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	64	ASP	CB-CA-C	5.70	121.79	110.40
1	B	283	ARG	CG-CD-NE	5.69	123.76	111.80
1	D	193	HIS	N-CA-CB	5.69	120.85	110.60
1	G	282	GLU	CB-CA-C	-5.69	99.02	110.40
1	C	54	ASN	O-C-N	5.69	131.80	122.70
1	H	244	LYS	CA-CB-CG	5.69	125.92	113.40
1	D	206	ILE	N-CA-C	-5.68	95.65	111.00
1	E	316	HIS	CA-CB-CG	-5.68	103.94	113.60
1	A	238	TYR	CB-CG-CD1	5.68	124.41	121.00
1	B	260	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	F	321	LEU	CB-CA-C	5.67	120.97	110.20
1	H	158	VAL	N-CA-CB	5.67	123.97	111.50
1	F	100	GLN	CB-CA-C	-5.66	99.08	110.40
1	B	22	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	150	PHE	O-C-N	5.66	131.75	122.70
1	B	55	GLU	CG-CD-OE2	-5.65	107.00	118.30
1	A	203	GLN	N-CA-CB	-5.65	100.43	110.60
1	G	236	ALA	CB-CA-C	5.65	118.58	110.10
1	G	171	ARG	NH1-CZ-NH2	5.65	125.61	119.40
1	G	282	GLU	CA-CB-CG	5.65	125.82	113.40
1	B	227	GLU	CA-CB-CG	5.64	125.81	113.40
1	F	106	ARG	CA-CB-CG	5.63	125.80	113.40
1	D	325	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	232	ASN	OD1-CG-ND2	5.63	134.85	121.90
1	A	214	LEU	CA-CB-CG	5.62	128.22	115.30
1	F	300	GLU	CG-CD-OE1	-5.60	107.09	118.30
1	B	206	ILE	N-CA-C	-5.60	95.88	111.00
1	B	85	ASP	CB-CG-OD1	5.59	123.33	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	171	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	206	ILE	O-C-N	5.58	132.69	123.20
1	C	104	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	H	255	LEU	CB-CA-C	5.58	120.80	110.20
1	A	16	LYS	CA-C-N	-5.58	104.93	117.20
1	A	177	TYR	CA-CB-CG	5.57	123.99	113.40
1	B	329	PHE	CA-C-N	-5.57	104.94	117.20
1	E	312	ASN	CA-CB-CG	-5.56	101.17	113.40
1	A	197	GLU	CA-CB-CG	5.56	125.63	113.40
1	F	125	MET	CG-SD-CE	5.55	109.09	100.20
1	F	70	VAL	O-C-N	5.55	131.57	122.70
1	G	284	ASP	N-CA-CB	-5.54	100.62	110.60
1	H	297	GLY	CA-C-O	-5.54	110.64	120.60
1	A	22	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	H	63	MET	N-CA-CB	5.53	120.56	110.60
1	C	169	ARG	NH1-CZ-NH2	5.52	125.48	119.40
1	C	227	GLU	CA-CB-CG	5.52	125.55	113.40
1	A	245	GLY	N-CA-C	5.52	126.90	113.10
1	F	257	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	74	LYS	N-CA-CB	-5.51	100.68	110.60
1	D	92	VAL	CB-CA-C	5.51	121.86	111.40
1	G	55	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	D	184	ASN	CA-CB-CG	5.50	125.50	113.40
1	D	188	TYR	CA-CB-CG	5.50	123.84	113.40
1	F	189	ILE	N-CA-C	-5.50	96.16	111.00
1	H	106	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	E	55	GLU	CA-CB-CG	5.49	125.47	113.40
1	D	234	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	C	132	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	88	ASP	CB-CG-OD2	5.48	123.23	118.30
1	G	283	ARG	O-C-N	5.48	131.46	122.70
1	C	266	GLU	N-CA-C	5.48	125.79	111.00
1	D	286	TYR	CB-CG-CD1	5.48	124.29	121.00
1	F	284	ASP	CB-CG-OD1	-5.47	113.37	118.30
1	H	266	GLU	N-CA-C	5.47	125.78	111.00
1	H	98	ALA	CA-C-O	5.47	131.58	120.10
1	C	193	HIS	N-CA-CB	5.46	120.44	110.60
1	E	37	PHE	CB-CA-C	5.46	121.33	110.40
1	D	249	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	D	101	LYS	CB-CA-C	5.46	121.32	110.40
1	D	242	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	F	287	ILE	CB-CA-C	5.45	122.50	111.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ARG	CD-NE-CZ	5.45	131.23	123.60
1	C	70	VAL	N-CA-CB	5.45	123.48	111.50
1	D	188	TYR	CB-CA-C	-5.44	99.52	110.40
1	E	255	LEU	CA-CB-CG	5.43	127.80	115.30
1	H	153	LEU	CA-CB-CG	5.43	127.78	115.30
1	F	99	ASN	N-CA-CB	-5.42	100.84	110.60
1	B	87	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	C	113	ASN	CA-C-N	5.42	129.12	117.20
1	A	313	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	H	242	GLU	OE1-CD-OE2	5.41	129.80	123.30
1	F	329	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	C	149	LYS	CA-CB-CG	5.41	125.30	113.40
1	C	228	ARG	CG-CD-NE	5.40	123.14	111.80
1	A	279	LEU	CA-CB-CG	-5.39	102.89	115.30
1	D	104	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	F	101	LYS	O-C-N	5.39	131.35	121.10
1	A	215	VAL	O-C-N	5.38	131.32	122.70
1	B	169	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	149	LYS	CB-CA-C	-5.38	99.63	110.40
1	C	158	VAL	O-C-N	5.38	131.30	122.70
1	D	171	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	289	VAL	N-CA-CB	-5.37	99.68	111.50
1	G	222	ALA	N-CA-C	-5.37	96.49	111.00
1	F	289	VAL	N-CA-CB	-5.37	99.69	111.50
1	F	220	GLU	CA-C-O	5.36	131.35	120.10
1	H	133	PHE	N-CA-CB	5.36	120.24	110.60
1	E	260	ARG	CD-NE-CZ	-5.36	116.10	123.60
1	H	313	ARG	CD-NE-CZ	-5.36	116.10	123.60
1	F	221	GLU	CG-CD-OE1	-5.35	107.59	118.30
1	F	276	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	25	VAL	O-C-N	5.35	131.25	122.70
1	G	30	PHE	O-C-N	5.34	131.25	122.70
1	F	260	ARG	CD-NE-CZ	-5.34	116.12	123.60
1	C	22	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	122	GLU	CA-C-O	5.34	131.31	120.10
1	E	212	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	E	205	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	G	193	HIS	N-CA-C	-5.34	96.59	111.00
1	F	253	MET	CB-CA-C	5.33	121.07	110.40
1	A	327	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	E	328	ALA	C-N-CA	-5.32	108.39	121.70
1	G	108	ASP	CB-CG-OD2	-5.32	113.51	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	LYS	C-N-CA	5.32	133.46	122.30
1	A	82	ASP	CB-CA-C	5.30	121.00	110.40
1	G	191	GLY	N-CA-C	-5.30	99.86	113.10
1	E	300	GLU	CA-CB-CG	5.30	125.05	113.40
1	D	16	LYS	CA-C-N	-5.29	105.57	117.20
1	C	218	LYS	CA-C-N	-5.28	105.65	116.20
1	E	203	GLN	CA-CB-CG	5.28	125.01	113.40
1	E	275	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	D	232	ASN	CA-CB-CG	-5.27	101.81	113.40
1	G	33	ALA	O-C-N	5.26	131.12	122.70
1	A	185	VAL	O-C-N	5.26	131.11	122.70
1	B	157	ARG	CD-NE-CZ	5.25	130.95	123.60
1	C	253	MET	N-CA-CB	5.24	120.03	110.60
1	D	222	ALA	N-CA-C	-5.24	96.85	111.00
1	A	270	LEU	CB-CA-C	5.24	120.16	110.20
1	D	245	GLY	N-CA-C	5.23	126.18	113.10
1	H	16	LYS	CA-C-N	-5.22	105.71	117.20
1	H	31	VAL	CA-C-N	5.21	126.62	116.20
1	E	220	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	D	61	ASP	CB-CG-OD1	5.19	122.97	118.30
1	H	276	LEU	N-CA-CB	-5.19	100.02	110.40
1	E	76	VAL	CB-CA-C	5.19	121.26	111.40
1	F	98	ALA	C-N-CA	5.19	134.67	121.70
1	G	123	SER	N-CA-CB	-5.19	102.72	110.50
1	H	193	HIS	N-CA-CB	5.19	119.94	110.60
1	F	208	VAL	O-C-N	5.19	131.00	122.70
1	A	279	LEU	CA-C-O	-5.18	109.22	120.10
1	E	312	ASN	OD1-CG-ND2	5.18	133.82	121.90
1	A	193	HIS	N-CA-CB	5.17	119.91	110.60
1	A	220	GLU	CG-CD-OE1	5.17	128.64	118.30
1	D	307	ASN	CB-CA-C	5.17	120.73	110.40
1	E	61	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	133	PHE	CA-CB-CG	5.16	126.29	113.90
1	C	247	THR	CA-CB-CG2	5.16	119.63	112.40
1	F	157	ARG	CD-NE-CZ	-5.16	116.37	123.60
1	E	90	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	212	ARG	O-C-N	5.16	130.95	122.70
1	G	123	SER	CB-CA-C	5.15	119.89	110.10
1	B	286	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	E	82	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	E	102	PRO	N-CA-C	-5.15	98.71	112.10
1	F	295	ARG	NH1-CZ-NH2	-5.15	113.74	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	B	134	LEU	CB-CA-C	5.15	119.98	110.20
1	B	212	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	A	37	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	F	292	VAL	CA-CB-CG2	5.14	118.61	110.90
1	D	49	VAL	CA-CB-CG2	5.13	118.60	110.90
1	H	72	ALA	N-CA-CB	5.13	117.29	110.10
1	D	329	PHE	CB-CG-CD2	5.13	124.39	120.80
1	F	55	GLU	CA-CB-CG	5.13	124.69	113.40
1	C	55	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	B	299	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	F	260	ARG	CG-CD-NE	-5.12	101.05	111.80
1	H	260	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	D	215	VAL	CB-CA-C	5.11	121.11	111.40
1	G	227	GLU	CG-CD-OE2	5.11	128.52	118.30
1	A	153	LEU	N-CA-C	-5.11	97.21	111.00
1	C	62	ALA	CB-CA-C	5.11	117.76	110.10
1	E	133	PHE	CA-CB-CG	5.11	126.15	113.90
1	F	85	ASP	CB-CG-OD1	5.11	122.89	118.30
1	H	32	GLY	N-CA-C	5.11	125.86	113.10
1	C	52	ASP	O-C-N	5.10	130.87	122.70
1	F	219	GLY	N-CA-C	5.10	125.85	113.10
1	D	64	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	F	329	PHE	CA-CB-CG	-5.10	101.66	113.90
1	A	174	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	220	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	H	52	ASP	CB-CG-OD1	5.09	122.88	118.30
1	H	16	LYS	N-CA-C	-5.09	97.27	111.00
1	E	263	LEU	CB-CA-C	5.08	119.86	110.20
1	H	206	ILE	N-CA-C	-5.08	97.28	111.00
1	E	201	TRP	O-C-N	5.08	130.83	122.70
1	H	176	GLU	CG-CD-OE1	5.08	128.45	118.30
1	G	307	ASN	CB-CA-C	5.07	120.54	110.40
1	A	279	LEU	CA-C-N	5.07	128.35	117.20
1	B	181	ALA	CB-CA-C	5.07	117.70	110.10
1	F	221	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	F	307	ASN	CA-CB-CG	5.07	124.54	113.40
1	G	295	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	C	329	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	D	305	GLU	CG-CD-OE1	-5.05	108.20	118.30
1	F	120	ILE	O-C-N	5.05	130.78	122.70
1	G	206	ILE	N-CA-C	-5.05	97.38	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	171	ARG	O-C-N	5.05	130.77	122.70
1	H	188	TYR	CB-CA-C	-5.04	100.32	110.40
1	E	234	ARG	CD-NE-CZ	5.03	130.65	123.60
1	F	88	ASP	O-C-N	5.03	130.75	122.70
1	F	271	THR	N-CA-CB	5.03	119.85	110.30
1	H	76	VAL	CB-CA-C	5.03	120.95	111.40
1	C	295	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
1	A	286	TYR	N-CA-C	-5.02	97.44	111.00
1	C	99	ASN	CA-CB-CG	5.02	124.45	113.40
1	H	188	TYR	CB-CG-CD2	5.02	124.01	121.00
1	B	295	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	G	17	ASN	CA-C-N	-5.01	106.18	117.20
1	E	297	GLY	N-CA-C	-5.01	100.58	113.10
1	B	295	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	2448	0	2432	346	0
1	B	2448	0	2433	311	0
1	C	2448	0	2432	313	2
1	D	2448	0	2433	308	0
1	E	2448	0	2433	310	0
1	F	2448	0	2433	297	0
1	G	2448	0	2432	298	0
1	H	2448	0	2432	320	0
2	A	40	0	20	0	0
2	B	40	0	20	0	0
2	E	40	0	20	0	0
2	F	40	0	20	0	0
3	A	6	0	2	2	0
3	B	6	0	2	2	0
3	C	6	0	2	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	2	1	0
3	E	6	0	2	2	0
3	F	6	0	2	1	0
3	G	6	0	2	1	0
3	H	6	0	2	0	0
4	A	44	0	26	7	0
4	B	44	0	26	9	0
4	C	44	0	26	3	0
4	D	44	0	26	6	0
4	E	44	0	26	9	0
4	F	44	0	26	6	0
4	G	44	0	26	9	0
4	H	44	0	26	4	0
5	A	72	0	0	34	0
5	B	72	0	0	27	2
5	C	69	0	0	23	0
5	D	74	0	0	20	0
5	E	70	0	0	29	0
5	F	72	0	0	23	0
5	G	70	0	0	22	0
5	H	73	0	0	22	0
All	All	20716	0	19764	2265	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (2265) 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:E:279:LEU:HB2	5:E:398:HOH:O	1.34	1.26
1:A:15:MET:HB2	1:A:19:GLY:CA	1.69	1.21
5:E:421:HOH:O	1:H:70:VAL:HG22	1.35	1.21
1:D:215:VAL:HG23	5:D:405:HOH:O	1.42	1.18
1:D:215:VAL:HB	1:D:222:ALA:CB	1.71	1.17
1:F:204:ALA:HB1	1:F:211:ILE:HD12	1.28	1.15
1:D:101:LYS:HD2	5:D:423:HOH:O	1.47	1.13
1:E:15:MET:HB2	1:E:19:GLY:N	1.64	1.12
1:H:215:VAL:HB	1:H:222:ALA:CB	1.80	1.11
1:A:15:MET:HB2	1:A:19:GLY:HA3	1.28	1.11
1:H:215:VAL:HB	1:H:222:ALA:HB1	1.17	1.11
1:B:209:MET:HG2	1:B:214:LEU:HD21	1.28	1.11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:HB	1:B:222:ALA:HB1	1.24	1.11
1:D:221:GLU:HA	5:D:425:HOH:O	1.47	1.10
1:F:212:ARG:HH12	1:F:226:LEU:HB2	1.07	1.10
1:G:209:MET:HG2	1:G:214:LEU:HD21	1.20	1.09
1:G:265:ASN:HB3	1:H:15:MET:HA	1.32	1.09
1:E:215:VAL:HA	1:E:218:LYS:HD2	1.30	1.09
1:D:22:ARG:HG2	1:D:89:ALA:HA	1.30	1.08
1:B:149:LYS:HA	1:B:149:LYS:HE2	1.36	1.08
1:G:16:LYS:N	1:G:16:LYS:HD2	1.62	1.08
1:B:153:LEU:O	5:B:384:HOH:O	1.72	1.07
1:A:206:ILE:HD11	1:A:211:ILE:HD11	1.14	1.07
1:E:118:ARG:HH11	1:E:118:ARG:HB3	1.02	1.07
1:F:198:LEU:HB3	1:F:313:ARG:HD3	1.37	1.07
1:A:100:GLN:HB2	1:A:105:THR:O	1.54	1.06
1:F:146:ALA:HA	1:F:329:PHE:HZ	1.16	1.06
1:G:112:LYS:HA	1:G:112:LYS:HE2	1.37	1.05
1:H:114:ILE:HG21	1:H:330:THR:HA	1.35	1.05
1:H:112:LYS:O	1:H:115:ALA:HB3	1.56	1.05
1:H:118:ARG:HG2	1:H:150:PHE:CE2	1.91	1.05
1:H:210:PRO:HG2	1:H:213:LYS:HD3	1.14	1.05
1:G:215:VAL:HB	1:G:222:ALA:HB1	1.08	1.05
1:G:213:LYS:HZ3	1:G:213:LYS:HB2	1.21	1.05
1:G:265:ASN:CB	1:H:15:MET:HA	1.85	1.04
1:D:15:MET:N	5:D:359:HOH:O	1.87	1.04
1:F:212:ARG:HH12	1:F:226:LEU:CB	1.68	1.04
1:H:209:MET:HG3	1:H:214:LEU:HD21	1.39	1.04
1:F:265:ASN:HD22	1:F:295:ARG:HB2	1.23	1.04
1:B:118:ARG:HH11	1:B:118:ARG:HB3	0.90	1.04
1:E:215:VAL:HB	1:E:222:ALA:HB1	1.37	1.03
1:D:215:VAL:HG21	1:D:226:LEU:HD11	1.37	1.03
4:G:352:NAD:H2D	5:G:452:HOH:O	1.56	1.03
1:C:221:GLU:OE1	1:C:224:LYS:HG2	1.59	1.03
1:G:221:GLU:HA	5:G:501:HOH:O	1.57	1.02
1:C:221:GLU:HG2	1:C:223:GLN:HB2	1.40	1.02
1:F:212:ARG:HH11	1:F:226:LEU:HD12	1.23	1.02
1:A:295:ARG:HD2	1:B:15:MET:CG	1.90	1.02
1:A:182:PRO:HG3	5:A:389:HOH:O	1.60	1.02
1:B:39:LEU:HD22	1:B:44:ILE:HB	1.41	1.02
1:A:101:LYS:HB3	1:A:102:PRO:HD2	1.40	1.01
1:E:15:MET:HA	1:F:265:ASN:HB2	1.38	1.01
1:E:218:LYS:HG3	1:E:222:ALA:HB2	1.42	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:MET:N	5:H:360:HOH:O	1.92	1.01
1:A:16:LYS:HD2	1:A:46:ASP:O	1.57	1.01
1:D:215:VAL:CB	1:D:222:ALA:HB1	1.90	1.01
1:A:265:ASN:HB2	1:B:15:MET:HA	1.43	1.01
1:D:215:VAL:HB	1:D:222:ALA:HB1	1.05	1.00
1:E:265:ASN:CB	1:F:15:MET:HA	1.91	1.00
1:E:209:MET:HE3	1:G:305:GLU:H	1.23	1.00
1:H:221:GLU:OE1	1:H:221:GLU:HA	1.58	1.00
1:F:55:GLU:O	1:F:59:ILE:HG13	1.61	1.00
1:B:118:ARG:HB3	1:B:118:ARG:NH1	1.76	1.00
1:A:295:ARG:HD2	1:B:15:MET:HG3	1.43	1.00
1:C:221:GLU:HB3	1:C:224:LYS:HB2	1.39	0.99
1:D:110:VAL:HG13	1:D:142:ILE:HG21	1.43	0.99
1:B:234:ARG:NH1	1:B:235:ASP:OD1	1.94	0.99
1:F:265:ASN:ND2	1:F:295:ARG:HB2	1.77	0.98
1:G:215:VAL:HB	1:G:222:ALA:CB	1.93	0.98
1:F:304:ILE:HA	1:H:209:MET:HE1	1.44	0.98
1:H:215:VAL:CB	1:H:222:ALA:HB1	1.94	0.98
1:E:215:VAL:HB	1:E:222:ALA:CB	1.95	0.97
1:F:145:TYR:CE1	1:F:149:LYS:HD3	2.00	0.97
1:E:264:HIS:HB3	1:F:16:LYS:HZ3	1.27	0.97
1:H:209:MET:CG	1:H:214:LEU:HD21	1.94	0.97
1:H:74:LYS:HD2	1:H:75:PRO:HD2	1.44	0.97
1:G:138:ASN:HB2	4:G:352:NAD:O2D	1.64	0.96
1:E:265:ASN:HB3	1:F:15:MET:HA	1.46	0.95
1:A:206:ILE:CD1	1:A:211:ILE:HD11	1.94	0.95
1:F:304:ILE:HA	1:H:209:MET:CE	1.97	0.95
1:B:70:VAL:HG23	5:B:363:HOH:O	1.65	0.95
1:H:83:TYR:O	1:H:127:SER:HB2	1.66	0.95
1:E:15:MET:HB2	1:E:19:GLY:CA	1.96	0.95
1:G:124:VAL:HG11	1:G:133:PHE:HZ	1.32	0.95
1:F:118:ARG:HH11	1:F:118:ARG:HB3	1.29	0.95
1:E:209:MET:HB3	1:E:214:LEU:HD21	1.49	0.95
1:F:87:ARG:HD3	1:F:127:SER:O	1.67	0.95
1:C:83:TYR:O	1:C:127:SER:HB2	1.67	0.94
1:G:86:CYS:SG	1:G:124:VAL:HG23	2.07	0.94
1:E:251:ILE:HD13	4:E:352:NAD:O7N	1.66	0.94
1:C:16:LYS:HZ1	1:D:264:HIS:HB3	1.30	0.94
1:E:240:ILE:HG12	1:H:63:MET:HE3	1.49	0.94
1:B:112:LYS:HD2	5:B:378:HOH:O	1.65	0.93
1:G:190:ILE:HD13	1:G:200:VAL:HG21	1.50	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:NZ	1:D:264:HIS:O	1.99	0.93
1:G:213:LYS:HA	1:G:216:GLU:HB3	1.49	0.93
1:F:145:TYR:CD1	1:F:329:PHE:HE2	1.85	0.93
1:B:87:ARG:HG3	1:B:127:SER:O	1.69	0.93
1:A:70:VAL:HG13	1:D:182:PRO:HB2	1.50	0.93
1:A:213:LYS:HA	1:A:216:GLU:HB2	1.49	0.93
1:E:16:LYS:HB2	5:F:355:HOH:O	1.67	0.93
1:H:118:ARG:HH11	1:H:118:ARG:HB3	1.31	0.93
1:G:215:VAL:CB	1:G:222:ALA:HB1	1.98	0.92
1:G:16:LYS:H	1:G:16:LYS:HD2	1.28	0.92
1:H:101:LYS:O	1:H:104:GLU:HB2	1.69	0.92
1:E:220:GLU:HA	1:E:223:GLN:HB2	1.51	0.92
1:F:215:VAL:HB	1:F:222:ALA:HB1	1.51	0.92
1:E:118:ARG:HB3	1:E:118:ARG:NH1	1.84	0.92
1:H:240:ILE:CG2	1:H:244:LYS:HD2	2.00	0.92
1:C:15:MET:HB2	1:C:19:GLY:N	1.85	0.92
1:D:74:LYS:HG2	1:D:75:PRO:HD2	1.52	0.92
1:D:22:ARG:CG	1:D:89:ALA:HA	2.00	0.91
1:B:265:ASN:HD22	1:B:295:ARG:H	1.19	0.91
1:G:74:LYS:HD2	1:G:75:PRO:HD2	1.49	0.91
1:F:234:ARG:HD2	1:F:235:ASP:OD1	1.70	0.91
1:B:118:ARG:HH11	1:B:118:ARG:CB	1.81	0.91
1:G:213:LYS:NZ	1:G:213:LYS:HB2	1.86	0.91
1:D:220:GLU:HA	1:D:223:GLN:HB2	1.51	0.91
1:F:166:ASP:OD1	5:F:387:HOH:O	1.89	0.90
1:B:149:LYS:CA	1:B:149:LYS:HE2	1.97	0.90
1:D:138:ASN:HB2	4:D:352:NAD:O2D	1.71	0.90
1:E:15:MET:HA	1:F:265:ASN:CB	2.01	0.90
1:H:309:ASP:O	1:H:313:ARG:HG3	1.71	0.90
1:F:204:ALA:CB	1:F:211:ILE:HD12	2.02	0.90
1:D:16:LYS:HG3	1:D:46:ASP:O	1.72	0.90
1:E:294:ASN:C	1:E:294:ASN:HD22	1.75	0.90
1:E:204:ALA:HB1	1:E:211:ILE:HD12	1.49	0.90
1:B:36:VAL:HG21	1:B:50:LEU:HD21	1.54	0.89
1:B:215:VAL:HB	1:B:222:ALA:CB	2.01	0.89
1:G:209:MET:CG	1:G:214:LEU:HD21	2.02	0.89
1:C:118:ARG:HH11	1:C:118:ARG:HB3	1.38	0.89
1:A:15:MET:CB	1:A:19:GLY:HA3	2.01	0.89
1:F:146:ALA:HA	1:F:329:PHE:CZ	2.07	0.89
1:A:152:GLY:HA2	5:A:381:HOH:O	1.73	0.89
1:E:59:ILE:CG2	1:H:243:LYS:HD3	2.03	0.89

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ALA:O	1:D:322:LYS:HG2	1.71	0.89
1:G:224:LYS:HB2	5:G:501:HOH:O	1.71	0.88
1:G:101:LYS:HB3	1:G:102:PRO:HD2	1.53	0.88
1:F:87:ARG:NH1	1:F:87:ARG:HB2	1.86	0.88
1:H:114:ILE:CG2	1:H:330:THR:HA	2.04	0.88
1:D:223:GLN:HA	1:D:223:GLN:OE1	1.73	0.88
1:C:221:GLU:HG2	1:C:223:GLN:CB	2.04	0.88
1:F:198:LEU:CB	1:F:313:ARG:HD3	2.03	0.88
1:B:138:ASN:HB2	4:B:352:NAD:O2D	1.73	0.87
1:F:146:ALA:CA	1:F:329:PHE:HZ	1.86	0.87
1:A:54:ASN:HD22	1:A:54:ASN:C	1.75	0.87
1:G:209:MET:HG2	1:G:214:LEU:CD2	2.04	0.87
1:A:181:ALA:HB1	1:A:183:GLN:OE1	1.73	0.87
1:F:212:ARG:NH1	1:F:226:LEU:CD1	2.37	0.87
1:F:212:ARG:NH1	1:F:226:LEU:HD12	1.90	0.86
1:F:87:ARG:HG3	1:F:128:GLY:C	1.95	0.86
1:F:70:VAL:CG1	1:G:182:PRO:HB2	2.04	0.86
1:G:283:ARG:O	1:G:322:LYS:HE2	1.75	0.86
1:B:215:VAL:HG11	1:B:226:LEU:HD11	1.58	0.86
1:A:265:ASN:HB3	1:B:16:LYS:H	1.41	0.86
1:H:169:ARG:NH1	5:H:395:HOH:O	2.07	0.86
1:B:289:VAL:CG1	1:B:301:VAL:HG13	2.05	0.86
1:D:83:TYR:O	1:D:86:CYS:HB2	1.76	0.86
1:H:110:VAL:HG21	1:H:324:VAL:HG11	1.58	0.86
1:E:155:HIS:HD2	5:E:378:HOH:O	1.59	0.86
1:C:264:HIS:HB3	1:D:16:LYS:HZ3	1.39	0.85
1:B:161:SER:O	1:B:164:ILE:HG22	1.76	0.85
1:A:294:ASN:C	1:A:294:ASN:HD22	1.79	0.85
1:C:117:PHE:O	1:C:121:VAL:HG23	1.77	0.85
1:D:94:ILE:HG21	1:D:117:PHE:CZ	2.12	0.84
1:C:215:VAL:HA	1:C:218:LYS:HG2	1.58	0.84
1:B:224:LYS:HB2	5:B:418:HOH:O	1.77	0.84
1:D:215:VAL:HG21	1:D:226:LEU:CD1	2.07	0.84
1:A:107:LEU:O	1:A:110:VAL:HG22	1.77	0.84
1:G:107:LEU:O	1:G:110:VAL:HG23	1.77	0.84
1:C:189:ILE:HD12	1:C:230:PHE:HE1	1.41	0.84
1:B:101:LYS:HB3	1:B:102:PRO:HD2	1.58	0.84
1:B:220:GLU:HA	1:B:223:GLN:HB2	1.59	0.84
1:A:154:PRO:HA	5:A:380:HOH:O	1.78	0.84
1:G:16:LYS:HB3	1:G:77:ASP:OD1	1.78	0.83
1:G:215:VAL:HG23	5:G:479:HOH:O	1.76	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:HA	1:D:70:VAL:HG21	1.57	0.83
1:E:36:VAL:HG21	1:E:50:LEU:HD21	1.58	0.83
1:H:118:ARG:HD2	1:H:330:THR:OG1	1.79	0.83
1:A:206:ILE:HD11	1:A:211:ILE:CD1	2.06	0.83
1:F:212:ARG:HH11	1:F:226:LEU:CD1	1.91	0.83
1:A:295:ARG:CD	1:B:15:MET:HE3	2.08	0.83
1:E:221:GLU:HA	5:E:416:HOH:O	1.77	0.83
1:A:264:HIS:HB3	1:B:16:LYS:NZ	1.93	0.83
1:E:70:VAL:HG23	5:E:360:HOH:O	1.77	0.83
1:A:15:MET:HB2	1:A:19:GLY:N	1.94	0.82
1:B:109:LEU:HD22	5:B:378:HOH:O	1.77	0.82
1:F:294:ASN:HD22	1:F:296:ASN:H	1.25	0.82
1:F:87:ARG:HG3	1:F:128:GLY:CA	2.09	0.82
4:E:352:NAD:O7N	5:E:381:HOH:O	1.97	0.82
1:D:221:GLU:OE1	1:D:221:GLU:HA	1.79	0.82
1:E:265:ASN:HB2	1:E:295:ARG:HB2	1.61	0.82
1:D:218:LYS:HG3	1:D:222:ALA:HB2	1.60	0.82
1:B:54:ASN:C	1:B:54:ASN:HD22	1.83	0.82
1:E:118:ARG:HH11	1:E:118:ARG:CB	1.89	0.82
1:C:15:MET:SD	1:C:19:GLY:HA3	2.20	0.82
1:F:70:VAL:HG13	1:G:182:PRO:HB2	1.58	0.81
1:D:228:ARG:HH11	1:D:228:ARG:HB3	1.45	0.81
1:H:244:LYS:HD3	1:H:246:ALA:O	1.80	0.81
1:H:144:THR:HG22	1:H:286:TYR:CD2	2.15	0.81
1:A:43:GLY:O	1:A:74:LYS:HD2	1.81	0.81
1:F:216:GLU:HA	5:F:398:HOH:O	1.78	0.81
1:G:218:LYS:HG3	1:G:222:ALA:HB2	1.60	0.81
1:F:15:MET:N	5:F:354:HOH:O	2.13	0.81
1:G:209:MET:HE2	1:G:209:MET:HA	1.61	0.81
1:F:304:ILE:CA	1:H:209:MET:HE1	2.09	0.81
1:B:15:MET:N	5:B:354:HOH:O	2.12	0.81
1:G:190:ILE:HD13	1:G:200:VAL:CG2	2.09	0.81
1:F:315:HIS:HB2	5:F:400:HOH:O	1.81	0.81
1:C:82:ASP:O	1:C:85:ASP:HB2	1.80	0.81
1:A:264:HIS:O	1:B:16:LYS:HD3	1.81	0.81
1:H:55:GLU:C	1:H:59:ILE:HD12	2.02	0.80
1:F:212:ARG:NH1	1:F:226:LEU:HB2	1.91	0.80
1:H:220:GLU:HA	1:H:223:GLN:HB2	1.61	0.80
1:A:294:ASN:ND2	1:A:296:ASN:H	1.78	0.80
1:B:15:MET:HB2	1:B:19:GLY:N	1.96	0.80
1:D:23:VAL:HG22	1:D:91:LEU:HD23	1.62	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:O	1:A:214:LEU:HG	1.81	0.80
1:D:265:ASN:HB2	1:D:295:ARG:HB2	1.63	0.80
1:F:212:ARG:NH1	1:F:226:LEU:CB	2.42	0.80
1:B:114:ILE:HG21	1:B:330:THR:HA	1.63	0.80
1:B:106:ARG:HB2	5:B:376:HOH:O	1.82	0.80
1:D:107:LEU:O	1:D:110:VAL:HG23	1.82	0.80
1:C:215:VAL:HB	1:C:222:ALA:CB	2.12	0.80
1:G:145:TYR:CE1	1:G:329:PHE:HE2	2.00	0.80
1:G:315:HIS:HB2	5:G:482:HOH:O	1.81	0.80
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.15	0.79
1:A:104:GLU:O	1:A:105:THR:HG22	1.82	0.79
1:E:294:ASN:ND2	1:E:296:ASN:H	1.80	0.79
1:D:319:ALA:O	1:D:322:LYS:HB2	1.82	0.79
1:B:289:VAL:HG13	1:B:301:VAL:HG13	1.64	0.79
1:C:16:LYS:NZ	1:D:264:HIS:HB3	1.96	0.79
1:C:228:ARG:NH1	1:C:232:ASN:ND2	2.31	0.79
1:B:15:MET:HB2	1:B:19:GLY:CA	2.12	0.79
1:H:243:LYS:HB2	1:H:243:LYS:NZ	1.95	0.79
1:G:124:VAL:HG11	1:G:133:PHE:CZ	2.17	0.79
1:G:222:ALA:HB3	5:G:479:HOH:O	1.82	0.79
1:A:54:ASN:ND2	1:A:57:LYS:H	1.80	0.79
1:C:107:LEU:O	1:C:110:VAL:HG23	1.83	0.79
1:E:240:ILE:HG12	1:H:63:MET:CE	2.11	0.79
1:B:177:TYR:CE1	1:B:225:ASP:HB3	2.17	0.78
1:F:16:LYS:HB3	1:F:77:ASP:OD1	1.84	0.78
1:E:264:HIS:CB	1:F:16:LYS:HZ3	1.96	0.78
1:G:227:GLU:O	1:G:231:VAL:HG23	1.83	0.78
1:A:100:GLN:CB	1:A:105:THR:O	2.30	0.78
1:A:213:LYS:HE2	1:C:305:GLU:HG3	1.65	0.78
1:D:265:ASN:ND2	1:D:295:ARG:HB2	1.98	0.78
1:C:180:VAL:HG21	1:C:206:ILE:HG23	1.66	0.78
1:D:294:ASN:HD22	1:D:296:ASN:H	1.29	0.78
1:H:220:GLU:CA	1:H:223:GLN:HB2	2.12	0.78
1:F:194:GLY:O	1:F:197:GLU:HG2	1.83	0.78
1:A:265:ASN:CB	1:B:16:LYS:H	1.96	0.78
1:B:221:GLU:CA	5:B:418:HOH:O	2.31	0.78
1:H:215:VAL:HA	1:H:218:LYS:HE3	1.65	0.78
1:B:213:LYS:O	1:B:213:LYS:HG3	1.84	0.77
1:F:145:TYR:CE1	1:F:329:PHE:HE2	2.02	0.77
1:C:221:GLU:HB3	1:C:224:LYS:H	1.49	0.77
1:A:120:ILE:O	1:A:124:VAL:HG13	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:HB3	1:C:77:ASP:OD1	1.83	0.77
1:G:66:ASN:O	1:G:69:LYS:HG2	1.83	0.77
5:E:423:HOH:O	1:H:71:PHE:HE2	1.67	0.77
1:C:264:HIS:HB3	1:D:16:LYS:NZ	1.99	0.77
1:A:70:VAL:HG22	5:A:360:HOH:O	1.82	0.77
1:B:221:GLU:HA	5:B:418:HOH:O	1.84	0.77
1:D:221:GLU:O	1:D:222:ALA:C	2.24	0.77
1:D:212:ARG:HH11	1:D:226:LEU:HD13	1.50	0.77
1:C:265:ASN:HD22	1:C:295:ARG:HB2	1.49	0.77
1:B:61:ASP:HB3	1:B:65:PHE:CE2	2.20	0.77
1:A:251:ILE:O	1:A:255:LEU:HD22	1.85	0.77
1:D:248:TYR:HA	1:D:251:ILE:HG22	1.67	0.77
4:G:352:NAD:H6N	5:G:450:HOH:O	1.84	0.76
1:A:35:TYR:CZ	1:A:39:LEU:HD11	2.19	0.76
1:A:221:GLU:HA	5:A:417:HOH:O	1.85	0.76
1:H:267:ASN:ND2	1:H:294:ASN:HB3	1.99	0.76
1:F:304:ILE:CB	1:H:209:MET:HE1	2.14	0.76
1:E:244:LYS:HE2	1:H:61:ASP:OD1	1.85	0.76
1:H:254:GLY:O	1:H:258:VAL:HG23	1.85	0.76
1:C:114:ILE:HD13	1:C:143:LEU:HD23	1.68	0.76
1:B:209:MET:HG2	1:B:214:LEU:CD2	2.11	0.76
1:D:265:ASN:HD22	1:D:295:ARG:HB2	1.48	0.76
1:F:304:ILE:HB	1:H:209:MET:HE1	1.68	0.76
1:E:295:ARG:HD2	1:F:15:MET:HG3	1.66	0.76
1:E:59:ILE:HG21	1:H:243:LYS:HD3	1.67	0.76
1:C:189:ILE:HD12	1:C:230:PHE:CE1	2.21	0.76
1:A:91:LEU:HD21	1:A:134:LEU:HD23	1.67	0.76
1:B:15:MET:SD	1:B:19:GLY:HA3	2.26	0.76
1:H:322:LYS:O	1:H:325:LEU:HB2	1.86	0.76
1:E:265:ASN:HB2	1:F:15:MET:HA	1.68	0.75
1:G:22:ARG:HG2	1:G:89:ALA:HA	1.68	0.75
1:H:75:PRO:HA	5:H:370:HOH:O	1.85	0.75
1:E:59:ILE:HG22	1:H:243:LYS:HD3	1.68	0.75
1:E:15:MET:HG3	1:F:295:ARG:HD2	1.68	0.75
1:G:215:VAL:HG11	1:G:226:LEU:HD11	1.69	0.75
1:D:253:MET:HE3	5:D:354:HOH:O	1.86	0.75
1:A:315:HIS:HB2	5:A:400:HOH:O	1.86	0.75
1:B:227:GLU:O	1:B:231:VAL:HG23	1.86	0.75
1:F:125:MET:CE	1:F:125:MET:HA	2.16	0.75
1:H:309:ASP:O	1:H:313:ARG:CG	2.34	0.75
1:C:174:LEU:HD23	1:C:229:ILE:HD13	1.67	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:GLY:O	1:E:197:GLU:HG2	1.86	0.75
1:A:266:GLU:HG3	1:B:75:PRO:HG3	1.69	0.75
1:A:16:LYS:HE3	1:A:46:ASP:HA	1.66	0.75
1:A:192:GLU:O	1:A:197:GLU:HB3	1.87	0.75
1:B:243:LYS:HG2	1:C:56:SER:O	1.86	0.75
1:H:144:THR:CG2	1:H:286:TYR:CD2	2.70	0.75
1:H:55:GLU:O	1:H:59:ILE:HD12	1.87	0.75
1:A:275:TYR:CE1	1:A:284:ASP:HA	2.22	0.75
1:E:15:MET:CG	1:E:19:GLY:HA3	2.17	0.74
1:G:210:PRO:O	1:G:213:LYS:HG2	1.88	0.74
1:C:35:TYR:CZ	1:C:39:LEU:HD11	2.22	0.74
1:E:15:MET:HB2	1:E:19:GLY:HA3	1.67	0.74
4:C:352:NAD:O2D	5:C:373:HOH:O	2.05	0.74
1:B:315:HIS:HB2	5:B:402:HOH:O	1.86	0.74
1:H:221:GLU:O	1:H:222:ALA:C	2.26	0.74
1:B:39:LEU:HD23	1:B:44:ILE:HD12	1.69	0.74
1:D:209:MET:HA	1:D:209:MET:CE	2.15	0.74
1:E:212:ARG:HH12	1:E:226:LEU:HD12	1.52	0.74
1:C:265:ASN:ND2	1:C:295:ARG:HB2	2.03	0.74
1:C:228:ARG:HH12	1:C:232:ASN:ND2	1.85	0.74
1:H:39:LEU:HD12	1:H:48:ILE:HD13	1.69	0.74
1:D:174:LEU:O	1:D:178:PHE:HD1	1.70	0.74
1:F:132:LEU:HD12	1:F:157:ARG:HB3	1.69	0.74
1:B:64:ASP:OD2	1:C:244:LYS:CE	2.36	0.74
1:C:264:HIS:CB	1:D:16:LYS:HZ3	2.01	0.74
1:F:313:ARG:HH11	1:F:313:ARG:HG2	1.50	0.74
1:B:98:ALA:O	1:B:109:LEU:HD13	1.88	0.74
1:A:107:LEU:O	1:A:110:VAL:CG2	2.36	0.74
1:G:15:MET:HA	1:H:265:ASN:HB3	1.70	0.74
1:E:110:VAL:HG12	1:E:111:ASP:N	2.03	0.74
1:A:234:ARG:O	5:A:385:HOH:O	2.06	0.73
1:E:16:LYS:H	1:F:265:ASN:HB3	1.53	0.73
1:A:106:ARG:O	1:A:109:LEU:HG	1.88	0.73
1:A:54:ASN:HD21	1:A:57:LYS:H	1.33	0.73
1:G:283:ARG:O	1:G:322:LYS:CE	2.36	0.73
1:C:309:ASP:O	1:C:312:ASN:HB3	1.88	0.73
1:A:295:ARG:HD3	1:B:15:MET:HE3	1.70	0.73
1:H:15:MET:HB2	1:H:19:GLY:N	2.03	0.73
1:F:213:LYS:HA	1:F:216:GLU:HB3	1.71	0.73
1:B:141:ASP:OD1	1:B:273:SER:OG	2.05	0.73
1:A:180:VAL:HG11	1:C:269:ILE:HD11	1.70	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASN:HB2	1:D:15:MET:HA	1.69	0.73
1:C:215:VAL:HB	1:C:222:ALA:HB3	1.70	0.73
1:E:212:ARG:NH1	1:E:226:LEU:HD12	2.04	0.73
1:C:247:THR:HG21	3:C:351:OXM:O3	1.89	0.73
1:E:218:LYS:CG	1:E:222:ALA:HB2	2.19	0.73
1:D:74:LYS:CG	1:D:75:PRO:HD2	2.18	0.73
1:A:211:ILE:HA	1:A:214:LEU:HD12	1.68	0.73
1:H:210:PRO:CG	1:H:213:LYS:HD3	2.08	0.73
1:C:167:THR:O	1:C:171:ARG:HG2	1.89	0.73
1:H:22:ARG:HA	1:H:47:GLU:O	1.89	0.73
1:B:265:ASN:ND2	1:B:294:ASN:HB2	2.03	0.73
1:D:113:ASN:ND2	1:D:138:ASN:O	2.21	0.73
1:E:15:MET:HG3	1:E:19:GLY:HA3	1.71	0.72
1:E:213:LYS:HA	1:E:216:GLU:HB3	1.69	0.72
1:H:94:ILE:HG21	1:H:117:PHE:CZ	2.24	0.72
1:H:254:GLY:N	5:H:358:HOH:O	2.22	0.72
1:C:16:LYS:HB3	1:C:77:ASP:HB2	1.69	0.72
1:F:57:LYS:NZ	1:F:61:ASP:OD2	2.21	0.72
1:D:165:LEU:O	1:D:165:LEU:HD12	1.90	0.72
1:E:240:ILE:HD11	1:H:67:HIS:CE1	2.25	0.72
1:E:15:MET:N	5:E:417:HOH:O	2.22	0.72
1:G:145:TYR:HA	1:G:286:TYR:CD1	2.24	0.72
1:F:43:GLY:HA2	5:F:361:HOH:O	1.90	0.72
1:C:286:TYR:HB2	5:C:380:HOH:O	1.87	0.72
1:C:15:MET:CG	1:C:19:GLY:HA3	2.19	0.72
1:F:29:GLY:HA3	4:F:352:NAD:O5B	1.89	0.72
1:D:22:ARG:HG2	1:D:89:ALA:CA	2.17	0.72
1:B:87:ARG:HG3	1:B:127:SER:C	2.10	0.72
1:B:54:ASN:C	1:B:54:ASN:ND2	2.42	0.72
1:C:315:HIS:HB2	5:C:401:HOH:O	1.89	0.72
1:D:110:VAL:CG1	1:D:142:ILE:HG21	2.18	0.72
1:F:125:MET:HA	1:F:125:MET:HE3	1.70	0.72
5:B:421:HOH:O	1:C:70:VAL:HG22	1.89	0.72
1:D:164:ILE:HD11	1:D:270:LEU:HD22	1.72	0.72
1:H:80:HIS:NE2	5:H:368:HOH:O	2.23	0.72
1:F:112:LYS:N	5:F:375:HOH:O	2.01	0.71
1:E:41:ASN:O	1:E:73:PRO:CG	2.38	0.71
1:A:15:MET:CG	1:A:19:GLY:HA3	2.20	0.71
1:H:240:ILE:HG22	1:H:244:LYS:HD2	1.72	0.71
1:E:74:LYS:HD2	1:E:75:PRO:HD2	1.72	0.71
1:E:59:ILE:HG22	1:H:243:LYS:CD	2.20	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:MET:SD	1:G:19:GLY:HA3	2.30	0.71
1:C:298:ILE:HD12	5:C:382:HOH:O	1.89	0.71
1:B:215:VAL:CB	1:B:222:ALA:HB1	2.12	0.71
1:F:145:TYR:CD1	1:F:329:PHE:CE2	2.76	0.71
1:F:112:LYS:HE2	1:F:112:LYS:HA	1.72	0.71
1:C:16:LYS:HZ3	1:D:264:HIS:C	1.93	0.71
1:H:294:ASN:ND2	1:H:296:ASN:H	1.89	0.71
1:G:15:MET:HB2	1:G:19:GLY:C	2.11	0.71
1:E:92:VAL:HG23	1:E:129:PHE:CZ	2.25	0.71
1:A:206:ILE:HG13	1:A:214:LEU:CD1	2.21	0.71
1:A:294:ASN:HD22	1:A:296:ASN:H	1.37	0.71
1:A:212:ARG:HH11	1:A:226:LEU:HD12	1.56	0.71
1:E:289:VAL:HG22	1:E:290:PRO:HD2	1.73	0.71
1:F:294:ASN:ND2	1:F:296:ASN:H	1.88	0.71
1:H:228:ARG:O	1:H:228:ARG:NH1	2.24	0.71
1:D:107:LEU:HD13	1:D:324:VAL:HG21	1.72	0.70
1:E:75:PRO:HA	5:H:356:HOH:O	1.91	0.70
1:F:59:ILE:O	1:F:63:MET:HG3	1.91	0.70
1:D:110:VAL:HG22	1:D:139:PRO:HG2	1.74	0.70
1:F:87:ARG:CD	1:F:128:GLY:HA3	2.21	0.70
1:B:258:VAL:O	1:B:261:ALA:N	2.25	0.70
1:D:225:ASP:O	1:D:228:ARG:HB2	1.91	0.70
1:E:15:MET:CB	1:E:19:GLY:HA3	2.20	0.70
1:B:15:MET:CG	1:B:19:GLY:HA3	2.22	0.70
1:D:213:LYS:HG3	1:D:213:LYS:O	1.91	0.70
1:G:138:ASN:CB	4:G:352:NAD:O2D	2.39	0.70
1:A:218:LYS:HG3	1:A:222:ALA:CB	2.21	0.70
1:C:116:ILE:CG2	1:C:120:ILE:HD12	2.21	0.70
1:G:54:ASN:C	1:G:54:ASN:HD22	1.94	0.70
1:B:55:GLU:HB3	1:B:59:ILE:HD11	1.73	0.70
1:E:15:MET:HB3	1:E:17:ASN:C	2.12	0.70
1:D:287:ILE:HG13	1:D:321:LEU:HD12	1.73	0.70
1:E:15:MET:HG3	1:F:295:ARG:CD	2.22	0.70
1:F:39:LEU:HD23	1:F:44:ILE:HD12	1.72	0.70
1:G:138:ASN:HB2	4:G:352:NAD:HO2N	1.55	0.70
1:G:101:LYS:HD2	5:G:499:HOH:O	1.92	0.70
1:E:49:VAL:HA	1:E:79:TRP:O	1.91	0.70
1:C:145:TYR:HD1	1:C:329:PHE:HZ	1.38	0.70
1:F:66:ASN:O	1:F:69:LYS:HG2	1.91	0.70
1:H:45:ALA:O	1:H:76:VAL:HG23	1.92	0.70
1:B:114:ILE:HD11	1:B:328:ALA:HB1	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:VAL:HB	1:F:222:ALA:CB	2.21	0.70
1:H:240:ILE:CG2	1:H:244:LYS:CD	2.70	0.70
1:C:240:ILE:CG2	1:C:244:LYS:HD3	2.22	0.70
1:H:167:THR:O	1:H:171:ARG:HG3	1.92	0.70
1:A:264:HIS:HB3	1:B:16:LYS:HZ1	1.54	0.69
1:H:161:SER:OG	5:H:391:HOH:O	2.10	0.69
1:E:170:PHE:CE2	1:E:187:ALA:HB1	2.27	0.69
1:G:92:VAL:HG12	1:G:133:PHE:CE1	2.27	0.69
1:E:274:ALA:O	1:E:286:TYR:HA	1.92	0.69
1:C:229:ILE:HG22	1:C:230:PHE:N	2.08	0.69
1:F:15:MET:HB2	1:F:19:GLY:CA	2.21	0.69
1:A:224:LYS:HB2	5:A:417:HOH:O	1.91	0.69
1:G:211:ILE:O	1:G:215:VAL:HG13	1.92	0.69
1:H:83:TYR:O	1:H:127:SER:CB	2.41	0.69
1:F:323:SER:O	1:F:327:ARG:HG3	1.92	0.69
1:G:294:ASN:ND2	1:G:296:ASN:H	1.91	0.69
1:B:80:HIS:NE2	5:B:361:HOH:O	2.25	0.69
1:H:210:PRO:HB2	1:H:213:LYS:HB2	1.74	0.69
1:E:294:ASN:HD22	1:E:296:ASN:H	1.40	0.69
1:G:327:ARG:NH2	1:G:328:ALA:HB2	2.07	0.69
1:B:265:ASN:HB2	1:B:295:ARG:CG	2.22	0.69
1:B:287:ILE:HG13	1:B:321:LEU:HD11	1.72	0.69
1:G:299:ARG:NH2	1:G:300:GLU:OE2	2.25	0.69
1:G:124:VAL:CG1	1:G:133:PHE:HZ	2.04	0.69
1:F:87:ARG:HH11	1:F:87:ARG:HB2	1.53	0.69
1:A:145:TYR:CD1	1:A:329:PHE:HE2	2.11	0.69
1:G:309:ASP:O	1:G:313:ARG:HG3	1.92	0.69
1:E:145:TYR:CE1	1:E:329:PHE:HE2	2.11	0.69
1:G:213:LYS:CB	1:G:213:LYS:NZ	2.56	0.68
1:E:204:ALA:CB	1:E:211:ILE:HD12	2.24	0.68
1:B:221:GLU:O	5:B:418:HOH:O	2.11	0.68
1:C:145:TYR:HD1	1:C:329:PHE:CZ	2.12	0.68
1:G:237:ALA:O	1:G:241:ILE:HD12	1.93	0.68
1:H:94:ILE:CG2	1:H:117:PHE:CZ	2.76	0.68
1:C:15:MET:HA	1:D:265:ASN:HB3	1.75	0.68
1:B:138:ASN:CB	4:B:352:NAD:O2D	2.41	0.68
1:D:294:ASN:ND2	1:D:296:ASN:H	1.92	0.68
1:F:289:VAL:HG13	1:F:301:VAL:HG13	1.74	0.68
1:C:265:ASN:CB	1:D:15:MET:HA	2.23	0.68
1:E:43:GLY:HA2	5:E:357:HOH:O	1.94	0.68
1:H:292:VAL:C	1:H:293:ILE:HD13	2.14	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HA	1:A:218:LYS:HD2	1.76	0.68
1:B:55:GLU:O	1:B:58:ALA:N	2.26	0.68
1:A:41:ASN:O	1:A:73:PRO:HG3	1.92	0.68
1:D:16:LYS:HB3	1:D:77:ASP:HB2	1.76	0.68
1:C:264:HIS:CE1	1:D:74:LYS:HD3	2.29	0.68
1:D:91:LEU:CD2	1:D:259:THR:HG23	2.23	0.68
1:F:256:ALA:HB3	5:F:420:HOH:O	1.92	0.68
1:H:222:ALA:HB3	5:H:405:HOH:O	1.94	0.68
1:G:16:LYS:N	1:G:16:LYS:CD	2.49	0.68
1:E:265:ASN:CB	1:E:295:ARG:HB2	2.24	0.68
1:F:87:ARG:CD	1:F:127:SER:O	2.39	0.68
1:E:193:HIS:NE2	3:E:351:OXM:O1	2.24	0.68
1:D:54:ASN:HD21	1:D:56:SER:HB2	1.58	0.68
1:H:238:TYR:CD1	5:H:380:HOH:O	2.47	0.68
1:D:210:PRO:HB3	5:D:403:HOH:O	1.92	0.68
1:D:295:ARG:HD3	1:D:295:ARG:O	1.93	0.68
1:B:299:ARG:NH2	1:B:300:GLU:OE2	2.26	0.68
1:H:220:GLU:N	1:H:223:GLN:HB2	2.09	0.67
1:G:264:HIS:O	1:H:16:LYS:NZ	2.28	0.67
1:H:209:MET:HG3	1:H:214:LEU:CD2	2.22	0.67
1:B:55:GLU:C	1:B:59:ILE:HD13	2.15	0.67
1:G:132:LEU:HD22	1:G:132:LEU:N	2.08	0.67
1:G:22:ARG:CG	1:G:89:ALA:HA	2.24	0.67
1:A:189:ILE:HD13	1:A:199:PRO:HA	1.76	0.67
1:G:221:GLU:O	1:G:222:ALA:C	2.33	0.67
1:G:77:ASP:HB3	1:G:79:TRP:HZ3	1.58	0.67
1:C:16:LYS:CB	1:C:77:ASP:HB2	2.24	0.67
1:E:63:MET:CE	1:H:243:LYS:HD2	2.24	0.67
1:C:260:ARG:HH22	1:D:75:PRO:CD	2.07	0.67
1:A:54:ASN:ND2	1:A:54:ASN:C	2.48	0.67
1:F:138:ASN:HD22	1:F:139:PRO:HA	1.60	0.67
1:D:22:ARG:NH1	1:D:85:ASP:O	2.27	0.67
1:A:247:THR:OG1	3:A:351:OXM:O3	2.09	0.67
1:H:293:ILE:HD13	1:H:293:ILE:N	2.08	0.67
1:F:148:TRP:HB2	1:F:158:VAL:HG21	1.75	0.67
1:B:180:VAL:HG21	1:B:206:ILE:HG23	1.75	0.67
1:E:16:LYS:HD3	1:F:264:HIS:O	1.94	0.67
1:G:16:LYS:HB3	1:G:77:ASP:CG	2.15	0.67
1:B:39:LEU:CD2	1:B:44:ILE:HB	2.23	0.67
1:C:279:LEU:HD23	1:C:301:VAL:HB	1.77	0.67
1:A:15:MET:HG2	1:B:295:ARG:HG3	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:PRO:HG2	1:F:304:ILE:HG23	1.77	0.67
1:H:323:SER:O	1:H:324:VAL:C	2.32	0.67
1:C:116:ILE:HG22	1:C:120:ILE:HD12	1.76	0.67
1:C:294:ASN:C	1:C:294:ASN:HD22	1.97	0.67
1:C:218:LYS:HG3	1:C:222:ALA:HB2	1.77	0.67
1:F:141:ASP:OD1	1:F:273:SER:OG	2.13	0.67
1:A:55:GLU:O	1:A:59:ILE:HD12	1.94	0.67
1:A:63:MET:HE1	1:D:243:LYS:HD3	1.75	0.67
1:E:237:ALA:O	1:E:241:ILE:HG13	1.95	0.67
1:D:114:ILE:HG22	5:D:415:HOH:O	1.94	0.67
1:H:276:LEU:CD2	1:H:279:LEU:HB3	2.25	0.67
1:A:35:TYR:OH	1:A:39:LEU:HD11	1.95	0.67
1:B:316:HIS:O	1:B:319:ALA:HB3	1.95	0.67
1:F:244:LYS:O	1:F:244:LYS:HG2	1.93	0.67
1:B:109:LEU:O	1:B:112:LYS:HB2	1.94	0.66
1:A:212:ARG:HH12	1:A:226:LEU:HB3	1.59	0.66
1:F:87:ARG:O	5:F:367:HOH:O	2.13	0.66
1:H:162:GLY:O	5:H:391:HOH:O	2.13	0.66
1:F:55:GLU:O	1:F:59:ILE:CG1	2.40	0.66
1:E:117:PHE:O	1:E:121:VAL:HG23	1.95	0.66
1:E:244:LYS:HD2	1:H:60:GLY:HA3	1.77	0.66
1:F:188:TYR:O	1:F:189:ILE:HD13	1.95	0.66
1:E:265:ASN:HB3	1:F:16:LYS:H	1.58	0.66
1:F:145:TYR:CE1	1:F:149:LYS:CD	2.77	0.66
1:B:279:LEU:HD23	1:B:301:VAL:HB	1.77	0.66
1:H:167:THR:O	1:H:171:ARG:CG	2.43	0.66
1:A:212:ARG:HH12	1:A:226:LEU:CB	2.08	0.66
1:A:55:GLU:C	1:A:59:ILE:HD12	2.16	0.66
1:E:141:ASP:OD1	1:E:273:SER:OG	2.13	0.66
1:G:164:ILE:HD12	1:G:258:VAL:HG23	1.78	0.66
1:B:26:ILE:HG21	1:B:120:ILE:CG2	2.26	0.66
1:A:264:HIS:CA	1:B:16:LYS:HZ3	2.09	0.66
1:A:294:ASN:HD22	1:A:295:ARG:N	1.94	0.66
1:A:251:ILE:HG13	1:A:255:LEU:CD2	2.25	0.66
1:C:40:MET:CE	1:C:69:LYS:HB3	2.25	0.66
1:G:170:PHE:CE2	1:G:187:ALA:HB1	2.31	0.66
1:A:16:LYS:HE2	1:A:75:PRO:O	1.95	0.66
1:C:221:GLU:CB	1:C:224:LYS:HB2	2.21	0.66
1:C:15:MET:O	1:C:47:GLU:OE2	2.13	0.66
1:H:227:GLU:O	1:H:231:VAL:HG23	1.95	0.66
1:A:209:MET:HE1	1:C:305:GLU:H	1.59	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:ILE:CG2	1:F:330:THR:HA	2.25	0.66
1:F:329:PHE:HD1	1:F:330:THR:N	1.93	0.66
1:H:299:ARG:NH2	1:H:300:GLU:OE2	2.28	0.66
1:A:304:ILE:HB	1:C:209:MET:HE1	1.77	0.66
1:D:199:PRO:HG3	1:D:230:PHE:CD1	2.31	0.66
1:F:251:ILE:O	1:F:255:LEU:HD22	1.96	0.66
1:F:257:ARG:HG2	1:G:71:PHE:CD1	2.31	0.66
1:H:229:ILE:O	1:H:233:VAL:HG23	1.95	0.66
1:B:202:SER:HB3	1:B:310:GLU:OE2	1.96	0.66
1:E:16:LYS:NZ	1:E:46:ASP:OD1	2.28	0.66
1:D:170:PHE:CD2	1:D:189:ILE:CD1	2.79	0.66
1:B:289:VAL:HG11	1:B:301:VAL:HG13	1.79	0.65
1:E:66:ASN:O	1:E:69:LYS:HG2	1.94	0.65
1:G:209:MET:CE	1:G:209:MET:HA	2.25	0.65
1:C:16:LYS:N	1:C:16:LYS:HD3	2.11	0.65
1:H:294:ASN:HD22	1:H:296:ASN:H	1.43	0.65
1:A:213:LYS:O	1:A:213:LYS:HG3	1.95	0.65
1:E:94:ILE:HG21	1:E:117:PHE:CE2	2.32	0.65
1:B:138:ASN:CG	4:B:352:NAD:HO2N	1.99	0.65
1:A:295:ARG:O	1:A:295:ARG:HG2	1.96	0.65
1:G:74:LYS:CD	1:G:75:PRO:HD2	2.26	0.65
1:B:243:LYS:HG3	1:C:56:SER:HB3	1.79	0.65
1:H:218:LYS:O	1:H:218:LYS:CG	2.43	0.65
1:C:260:ARG:HH22	1:D:75:PRO:HD3	1.61	0.65
1:A:109:LEU:HB3	1:A:113:ASN:ND2	2.12	0.65
1:B:70:VAL:HG22	1:C:182:PRO:HB3	1.78	0.65
1:E:116:ILE:HG22	1:E:120:ILE:HD11	1.76	0.65
1:A:91:LEU:HD11	1:A:134:LEU:HB2	1.79	0.65
1:E:54:ASN:ND2	1:E:57:LYS:H	1.94	0.65
1:G:228:ARG:HD3	1:G:228:ARG:O	1.96	0.65
1:A:16:LYS:HE3	1:A:46:ASP:CA	2.27	0.65
1:F:145:TYR:HD1	1:F:329:PHE:HE2	1.40	0.65
1:E:304:ILE:HG13	1:E:306:LEU:CD2	2.27	0.65
1:E:170:PHE:HE2	1:E:187:ALA:HB1	1.60	0.65
1:E:132:LEU:HD22	1:E:132:LEU:N	2.12	0.65
1:F:87:ARG:CZ	1:F:87:ARG:CB	2.73	0.65
1:F:313:ARG:HG2	1:F:313:ARG:NH1	2.11	0.65
1:A:266:GLU:CG	1:B:75:PRO:HG3	2.26	0.65
1:C:35:TYR:CD1	1:C:255:LEU:HB3	2.31	0.65
1:E:253:MET:SD	1:H:41:ASN:OD1	2.54	0.65
1:C:16:LYS:HB3	1:C:77:ASP:CG	2.17	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MET:O	5:E:358:HOH:O	2.14	0.65
1:A:313:ARG:O	1:A:316:HIS:HB3	1.97	0.65
1:G:213:LYS:CA	1:G:216:GLU:HB3	2.26	0.65
1:F:15:MET:HB2	1:F:19:GLY:C	2.16	0.65
1:F:87:ARG:NH1	1:F:87:ARG:CB	2.60	0.65
1:E:41:ASN:O	1:E:73:PRO:HG3	1.96	0.65
1:G:159:ILE:HD13	1:G:298:ILE:HG12	1.79	0.65
1:E:220:GLU:CA	1:E:223:GLN:HB2	2.26	0.64
1:G:291:ALA:HB1	1:G:298:ILE:HG23	1.79	0.64
1:C:101:LYS:NZ	1:C:101:LYS:HB3	2.12	0.64
1:B:294:ASN:C	1:B:294:ASN:HD22	2.00	0.64
1:G:264:HIS:O	1:G:265:ASN:C	2.35	0.64
1:C:117:PHE:HD2	1:C:147:THR:OG1	1.81	0.64
1:C:148:TRP:HA	1:C:158:VAL:HG21	1.77	0.64
1:A:151:SER:HB2	1:A:153:LEU:HD12	1.79	0.64
1:D:228:ARG:CB	1:D:228:ARG:HH11	2.10	0.64
1:E:215:VAL:HA	1:E:218:LYS:CD	2.17	0.64
1:C:221:GLU:OE1	1:C:224:LYS:CG	2.41	0.64
1:F:147:THR:O	1:F:151:SER:HB3	1.96	0.64
1:F:162:GLY:O	1:F:193:HIS:HB2	1.98	0.64
1:D:224:LYS:HB2	5:D:425:HOH:O	1.96	0.64
1:H:243:LYS:HB2	1:H:243:LYS:HZ3	1.61	0.64
1:G:36:VAL:HG21	1:G:50:LEU:HD21	1.78	0.64
1:B:209:MET:HE1	1:D:305:GLU:H	1.63	0.64
1:A:264:HIS:CB	1:B:16:LYS:NZ	2.59	0.64
1:A:257:ARG:O	1:A:260:ARG:HG3	1.98	0.64
1:F:100:GLN:HG3	5:F:371:HOH:O	1.97	0.64
5:A:419:HOH:O	1:B:295:ARG:CG	2.45	0.64
1:A:221:GLU:CA	5:A:417:HOH:O	2.43	0.64
1:G:299:ARG:O	1:G:300:GLU:HG3	1.97	0.64
1:C:101:LYS:HB3	1:C:102:PRO:HD2	1.80	0.64
1:A:213:LYS:CA	1:A:216:GLU:HB2	2.24	0.64
1:G:101:LYS:HB3	1:G:102:PRO:CD	2.27	0.64
1:E:98:ALA:HB1	5:E:374:HOH:O	1.97	0.64
1:A:148:TRP:CZ3	1:A:149:LYS:NZ	2.60	0.64
1:D:32:GLY:O	1:D:35:TYR:HB3	1.97	0.64
1:B:265:ASN:HB2	1:B:295:ARG:HG3	1.79	0.63
1:F:87:ARG:HG3	1:F:128:GLY:HA3	1.79	0.63
1:C:16:LYS:HB3	1:C:77:ASP:CB	2.26	0.63
1:C:147:THR:O	1:C:151:SER:HB3	1.99	0.63
1:B:215:VAL:HG23	5:B:399:HOH:O	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ARG:HD2	1:B:15:MET:HG2	1.77	0.63
1:B:100:GLN:HG3	5:B:373:HOH:O	1.98	0.63
1:F:15:MET:SD	1:F:19:GLY:HA3	2.38	0.63
1:G:15:MET:HA	1:H:265:ASN:CB	2.27	0.63
1:F:167:THR:O	1:F:171:ARG:HG3	1.98	0.63
1:A:119:SER:O	1:A:122:GLU:HB2	1.99	0.63
1:H:220:GLU:HA	1:H:223:GLN:CB	2.28	0.63
1:G:98:ALA:O	4:G:352:NAD:H3D	1.98	0.63
5:C:420:HOH:O	1:D:295:ARG:HG2	1.99	0.63
1:A:219:GLY:O	1:A:221:GLU:HG2	1.98	0.63
1:D:274:ALA:HB3	1:D:289:VAL:CG1	2.28	0.63
1:C:324:VAL:HG13	1:C:327:ARG:NH1	2.14	0.63
1:E:161:SER:O	1:E:164:ILE:HG22	1.98	0.63
1:F:120:ILE:O	1:F:124:VAL:HG12	1.99	0.63
1:F:188:TYR:CE2	1:F:290:PRO:HG3	2.34	0.63
1:E:295:ARG:HG3	1:F:15:MET:CG	2.28	0.63
1:H:74:LYS:CD	1:H:75:PRO:HD2	2.22	0.63
1:C:215:VAL:HA	1:C:218:LYS:CG	2.28	0.63
1:C:16:LYS:CE	1:D:264:HIS:O	2.46	0.63
1:A:159:ILE:HD11	1:A:297:GLY:HA2	1.81	0.63
1:G:31:VAL:HG23	4:G:352:NAD:PN	2.39	0.63
1:H:265:ASN:HD22	1:H:295:ARG:H	1.46	0.63
1:F:136:ALA:O	4:F:352:NAD:H2N	1.97	0.63
1:A:148:TRP:HA	1:A:158:VAL:HG21	1.81	0.63
1:F:114:ILE:HG21	1:F:330:THR:HA	1.81	0.63
1:H:110:VAL:HG21	1:H:324:VAL:CG1	2.28	0.63
1:C:145:TYR:CD1	1:C:329:PHE:CZ	2.87	0.63
1:D:199:PRO:HG3	1:D:230:PHE:CG	2.34	0.63
1:C:311:LYS:CB	5:C:402:HOH:O	2.47	0.63
1:E:203:GLN:NE2	1:G:209:MET:HE1	2.14	0.63
1:F:215:VAL:CB	1:F:222:ALA:HB1	2.27	0.63
1:B:29:GLY:HA3	4:B:352:NAD:O5B	1.98	0.63
1:A:234:ARG:HG2	1:A:234:ARG:O	1.99	0.62
1:H:166:ASP:OD1	1:H:193:HIS:ND1	2.30	0.62
5:A:419:HOH:O	1:B:295:ARG:HD2	1.98	0.62
1:B:101:LYS:O	1:B:104:GLU:HB2	1.99	0.62
1:A:31:VAL:HG12	1:A:95:CYS:HB3	1.80	0.62
1:C:309:ASP:O	1:C:313:ARG:CG	2.47	0.62
1:G:152:GLY:HA2	5:G:463:HOH:O	1.99	0.62
1:B:241:ILE:O	1:B:245:GLY:HA2	1.99	0.62
1:D:223:GLN:CA	1:D:223:GLN:OE1	2.42	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:ND2	1:B:295:ARG:HB2	2.13	0.62
1:A:70:VAL:CG2	5:A:360:HOH:O	2.45	0.62
1:A:291:ALA:HB1	1:A:298:ILE:HG23	1.81	0.62
1:F:228:ARG:NH2	1:F:231:VAL:HG11	2.14	0.62
1:E:15:MET:SD	1:E:18:ASN:O	2.58	0.62
1:G:218:LYS:CG	1:G:222:ALA:HB2	2.27	0.62
1:E:222:ALA:HB3	5:E:396:HOH:O	1.98	0.62
1:H:118:ARG:HB3	1:H:118:ARG:NH1	2.10	0.62
1:B:39:LEU:HD22	1:B:44:ILE:CB	2.23	0.62
1:A:101:LYS:CB	1:A:102:PRO:HD2	2.23	0.62
1:G:236:ALA:O	1:G:240:ILE:HG13	2.00	0.62
1:C:87:ARG:NH1	1:C:87:ARG:HB2	2.15	0.62
1:A:215:VAL:HG23	5:A:398:HOH:O	1.99	0.62
1:A:93:VAL:HA	1:A:134:LEU:O	1.99	0.62
1:A:59:ILE:O	1:A:63:MET:HG2	2.00	0.62
1:G:93:VAL:HA	1:G:134:LEU:O	2.00	0.62
1:A:208:VAL:O	1:C:203:GLN:HG3	2.00	0.62
1:C:36:VAL:HG21	1:C:50:LEU:HD21	1.81	0.62
1:E:200:VAL:HG12	1:E:203:GLN:HB2	1.80	0.62
1:G:112:LYS:CA	1:G:112:LYS:HE2	2.21	0.62
1:A:220:GLU:HA	1:A:223:GLN:HB2	1.82	0.62
1:H:121:VAL:O	1:H:125:MET:HG2	1.98	0.62
1:F:209:MET:HE1	1:H:305:GLU:H	1.65	0.62
1:H:294:ASN:HD22	1:H:294:ASN:C	2.03	0.62
1:D:218:LYS:CG	1:D:222:ALA:HB2	2.30	0.62
1:E:15:MET:HB2	1:E:18:ASN:C	2.19	0.62
1:G:264:HIS:C	1:H:16:LYS:HZ3	2.03	0.62
1:B:64:ASP:OD2	1:C:244:LYS:HE3	2.00	0.62
1:H:238:TYR:HD1	5:H:380:HOH:O	1.83	0.62
1:G:170:PHE:HE2	1:G:187:ALA:HB1	1.64	0.62
1:C:15:MET:HE3	1:D:295:ARG:HB3	1.81	0.61
1:C:311:LYS:HB3	5:C:402:HOH:O	2.00	0.61
1:E:200:VAL:CG1	1:E:203:GLN:HB2	2.30	0.61
1:E:150:PHE:HZ	1:E:330:THR:HB	1.65	0.61
1:B:26:ILE:HG21	1:B:120:ILE:HG21	1.82	0.61
1:G:186:HIS:O	1:G:204:ALA:HA	2.00	0.61
1:E:15:MET:C	1:E:17:ASN:N	2.47	0.61
1:H:114:ILE:HD12	1:H:328:ALA:O	1.99	0.61
1:B:194:GLY:O	1:B:197:GLU:HG2	2.00	0.61
1:D:209:MET:HA	1:D:209:MET:HE2	1.81	0.61
1:C:66:ASN:O	1:C:69:LYS:HG2	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ILE:HA	1:G:214:LEU:HD12	1.82	0.61
1:F:145:TYR:CE1	1:F:329:PHE:CE2	2.87	0.61
1:A:101:LYS:HB3	1:A:102:PRO:CD	2.23	0.61
1:G:183:GLN:NE2	5:G:369:HOH:O	2.03	0.61
1:H:31:VAL:HG22	1:H:251:ILE:HG21	1.81	0.61
1:E:298:ILE:HG22	1:E:298:ILE:O	1.99	0.61
1:H:219:GLY:HA2	5:H:405:HOH:O	1.98	0.61
1:G:77:ASP:HB3	1:G:79:TRP:CZ3	2.36	0.61
1:C:145:TYR:CE1	1:C:329:PHE:CE2	2.89	0.61
1:C:209:MET:CG	1:C:214:LEU:HD21	2.30	0.61
5:A:423:HOH:O	1:D:75:PRO:HA	2.00	0.61
1:E:294:ASN:HD22	1:E:295:ARG:N	1.99	0.61
1:G:145:TYR:CE1	1:G:329:PHE:CE2	2.87	0.61
1:H:215:VAL:HB	1:H:222:ALA:HB2	1.78	0.61
1:H:116:ILE:HD12	1:H:116:ILE:H	1.66	0.61
1:E:138:ASN:HB2	4:E:352:NAD:O2D	2.01	0.61
1:E:69:LYS:C	1:E:71:PHE:N	2.54	0.61
1:H:29:GLY:HA3	4:H:352:NAD:O5B	2.01	0.61
1:H:82:ASP:O	1:H:85:ASP:HB2	2.01	0.61
1:B:94:ILE:HG21	1:B:117:PHE:CZ	2.36	0.61
1:H:54:ASN:HD22	1:H:54:ASN:C	2.03	0.61
1:A:94:ILE:HG21	1:A:117:PHE:CE2	2.35	0.61
1:A:230:PHE:O	1:A:233:VAL:HB	2.00	0.61
1:D:171:ARG:HD2	1:D:185:VAL:O	2.00	0.61
1:B:264:HIS:O	1:B:265:ASN:C	2.36	0.61
1:C:264:HIS:CB	1:D:16:LYS:NZ	2.63	0.61
1:H:257:ARG:NH2	1:H:266:GLU:OE2	2.31	0.61
1:A:234:ARG:HD2	1:A:235:ASP:OD1	2.01	0.61
1:F:16:LYS:NZ	1:F:46:ASP:OD1	2.26	0.60
1:D:202:SER:HB3	1:D:310:GLU:OE2	2.01	0.60
1:A:228:ARG:HH11	1:A:228:ARG:HB3	1.66	0.60
1:E:150:PHE:CZ	1:E:330:THR:HB	2.37	0.60
1:F:74:LYS:HD3	5:F:418:HOH:O	2.01	0.60
1:C:279:LEU:O	1:C:303:GLU:OE2	2.20	0.60
1:G:186:HIS:O	1:G:205:TYR:N	2.30	0.60
1:B:86:CYS:O	1:B:129:PHE:HD1	1.83	0.60
1:F:211:ILE:HG22	1:F:212:ARG:HG2	1.81	0.60
1:C:295:ARG:HG3	1:D:15:MET:HG2	1.82	0.60
1:C:215:VAL:HB	1:C:222:ALA:HB1	1.82	0.60
1:F:204:ALA:HB1	1:F:211:ILE:CD1	2.18	0.60
1:A:287:ILE:HG13	1:A:321:LEU:HD13	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:CD1	1:B:328:ALA:HB1	2.30	0.60
1:E:295:ARG:CG	1:F:15:MET:HG2	2.31	0.60
1:F:213:LYS:HE2	1:H:305:GLU:OE2	2.01	0.60
1:D:116:ILE:HG22	1:D:120:ILE:CD1	2.31	0.60
1:E:169:ARG:O	1:E:173:LEU:HG	2.01	0.60
1:A:36:VAL:HG21	1:A:50:LEU:HD21	1.83	0.60
1:H:313:ARG:O	5:H:402:HOH:O	2.16	0.60
1:B:101:LYS:CB	1:B:102:PRO:HD2	2.30	0.60
1:A:49:VAL:HG22	1:A:79:TRP:CE2	2.36	0.60
1:F:87:ARG:CG	1:F:128:GLY:HA3	2.31	0.60
1:H:280:TYR:CE1	1:H:289:VAL:HG21	2.37	0.60
1:F:243:LYS:HG2	1:G:56:SER:O	2.02	0.60
1:H:54:ASN:C	1:H:54:ASN:ND2	2.55	0.60
1:E:116:ILE:HG23	4:E:352:NAD:N6A	2.16	0.60
1:A:218:LYS:HG3	1:A:222:ALA:HB2	1.83	0.60
1:F:169:ARG:HG2	1:G:67:HIS:CG	2.37	0.60
1:A:15:MET:HA	1:B:265:ASN:CB	2.30	0.60
1:A:212:ARG:NH1	1:A:226:LEU:CB	2.65	0.60
1:H:112:LYS:CA	1:H:112:LYS:HE2	2.29	0.60
1:B:244:LYS:HD3	1:B:246:ALA:O	2.02	0.60
1:B:121:VAL:HG11	1:B:150:PHE:HB2	1.84	0.60
1:E:210:PRO:O	1:E:214:LEU:HG	2.02	0.59
1:F:43:GLY:O	1:F:74:LYS:HD2	2.01	0.59
1:G:132:LEU:N	1:G:132:LEU:CD2	2.65	0.59
1:G:234:ARG:NH1	1:G:235:ASP:OD1	2.34	0.59
1:E:63:MET:HE1	1:H:243:LYS:HD2	1.82	0.59
1:F:272:VAL:O	1:F:288:GLY:HA2	2.01	0.59
1:G:308:ASP:O	1:G:312:ASN:HB2	2.01	0.59
1:D:38:ALA:O	1:D:42:GLN:HB2	2.02	0.59
1:A:209:MET:CG	1:A:214:LEU:HD21	2.33	0.59
1:F:112:LYS:HE2	1:F:112:LYS:CA	2.31	0.59
1:D:39:LEU:HD22	1:D:44:ILE:HB	1.84	0.59
1:A:294:ASN:C	1:A:294:ASN:ND2	2.52	0.59
1:E:41:ASN:O	1:E:73:PRO:HG2	2.02	0.59
1:G:26:ILE:HG21	1:G:120:ILE:CG2	2.32	0.59
1:D:228:ARG:CA	1:D:228:ARG:NH1	2.66	0.59
1:E:203:GLN:HE21	1:G:209:MET:HE1	1.67	0.59
1:F:218:LYS:HG3	1:F:222:ALA:HB2	1.85	0.59
1:G:237:ALA:C	1:G:241:ILE:HD12	2.23	0.59
1:B:280:TYR:OH	1:B:302:ILE:O	2.15	0.59
1:G:279:LEU:HD23	1:G:301:VAL:HB	1.84	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:ARG:O	1:G:22:ARG:HG3	2.03	0.59
1:A:159:ILE:HD12	1:A:262:ILE:HD11	1.85	0.59
1:D:269:ILE:CG2	1:D:302:ILE:HD12	2.33	0.59
5:A:419:HOH:O	1:B:295:ARG:HG2	2.01	0.59
1:C:309:ASP:O	1:C:313:ARG:HG3	2.02	0.59
1:D:290:PRO:HB2	1:D:302:ILE:HB	1.83	0.59
1:C:202:SER:OG	1:C:310:GLU:OE1	2.21	0.59
1:A:22:ARG:NH2	1:A:47:GLU:OE1	2.33	0.59
1:F:251:ILE:HG13	1:F:255:LEU:CD2	2.32	0.59
1:H:149:LYS:N	1:H:149:LYS:HD2	2.17	0.59
1:H:215:VAL:CG2	1:H:222:ALA:HB1	2.33	0.59
1:B:224:LYS:CB	5:B:418:HOH:O	2.45	0.59
1:A:165:LEU:O	1:A:169:ARG:HG3	2.03	0.59
1:E:294:ASN:C	1:E:294:ASN:ND2	2.50	0.59
1:E:138:ASN:HD21	1:E:193:HIS:HD2	1.50	0.59
1:E:29:GLY:HA3	4:E:352:NAD:O5B	2.03	0.59
1:B:193:HIS:NE2	3:B:351:OXM:O1	2.36	0.59
1:F:132:LEU:CD1	1:F:157:ARG:HB3	2.33	0.59
1:D:280:TYR:CE1	1:D:289:VAL:CG2	2.86	0.59
1:B:105:THR:HG23	1:B:108:ASP:OD2	2.03	0.58
1:A:209:MET:HE3	1:C:304:ILE:HA	1.83	0.58
1:F:146:ALA:CA	1:F:329:PHE:CZ	2.78	0.58
1:G:192:GLU:O	1:G:197:GLU:HB3	2.04	0.58
1:E:164:ILE:HD12	1:E:258:VAL:HG23	1.85	0.58
1:E:21:ALA:CB	1:E:263:LEU:HD13	2.33	0.58
1:F:205:TYR:HE1	1:H:208:VAL:HB	1.67	0.58
1:G:262:ILE:O	1:G:264:HIS:N	2.35	0.58
1:C:240:ILE:HG23	1:C:244:LYS:HD3	1.85	0.58
1:C:209:MET:HG2	1:C:214:LEU:HD21	1.85	0.58
1:D:261:ALA:HA	1:D:266:GLU:HB2	1.85	0.58
1:B:169:ARG:NH1	5:B:389:HOH:O	2.35	0.58
1:G:275:TYR:CE1	1:G:284:ASP:HA	2.38	0.58
1:E:80:HIS:NE2	5:E:359:HOH:O	2.26	0.58
1:B:35:TYR:CE2	1:B:93:VAL:HG21	2.37	0.58
1:G:295:ARG:HG3	1:H:15:MET:HG3	1.85	0.58
1:B:16:LYS:HB3	1:B:77:ASP:OD1	2.03	0.58
1:C:181:ALA:O	1:C:182:PRO:C	2.41	0.58
1:A:218:LYS:HG3	1:A:222:ALA:HB3	1.83	0.58
1:B:59:ILE:HG22	1:B:63:MET:HE3	1.83	0.58
1:A:15:MET:HA	1:B:295:ARG:HG3	1.84	0.58
1:G:220:GLU:HA	1:G:223:GLN:HB2	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASP:O	1:G:85:ASP:HB2	2.04	0.58
1:E:244:LYS:CE	1:H:61:ASP:OD1	2.50	0.58
1:F:289:VAL:CG1	1:F:301:VAL:HG13	2.34	0.58
1:A:60:GLY:HA2	1:A:63:MET:HG3	1.85	0.58
1:C:101:LYS:H	1:C:104:GLU:HB2	1.68	0.58
1:A:267:ASN:HD22	1:A:292:VAL:CG1	2.17	0.58
1:D:221:GLU:O	1:D:222:ALA:O	2.22	0.58
1:E:15:MET:C	1:E:17:ASN:H	2.01	0.58
1:A:104:GLU:C	1:A:105:THR:CG2	2.71	0.58
1:G:40:MET:CE	1:G:69:LYS:HA	2.33	0.58
1:E:205:TYR:O	1:E:206:ILE:HD13	2.02	0.58
1:E:138:ASN:HD22	1:E:140:VAL:H	1.50	0.58
1:D:177:TYR:HD2	1:D:178:PHE:CE1	2.21	0.58
1:A:151:SER:CB	1:A:153:LEU:HD12	2.34	0.58
1:E:15:MET:HB3	1:E:17:ASN:O	2.04	0.58
1:C:228:ARG:O	1:C:228:ARG:NH1	2.37	0.58
1:A:212:ARG:NH1	1:A:226:LEU:HB3	2.19	0.58
1:D:258:VAL:HG22	1:D:270:LEU:HD13	1.86	0.58
1:A:125:MET:SD	1:A:151:SER:HB2	2.44	0.58
1:H:189:ILE:HD13	1:H:230:PHE:HE1	1.69	0.58
1:H:315:HIS:HB2	5:H:408:HOH:O	2.02	0.58
1:F:208:VAL:HG23	1:H:203:GLN:HG3	1.84	0.58
1:B:265:ASN:HD22	1:B:295:ARG:N	1.94	0.58
1:H:209:MET:HG2	1:H:214:LEU:HD21	1.84	0.58
1:G:265:ASN:HB2	1:G:295:ARG:HB2	1.86	0.58
1:E:215:VAL:HG23	5:E:396:HOH:O	2.02	0.58
1:C:153:LEU:HB3	1:C:154:PRO:HD2	1.86	0.58
1:G:306:LEU:HB2	1:G:311:LYS:HG2	1.86	0.58
1:F:275:TYR:CE1	1:F:284:ASP:HA	2.38	0.58
1:G:149:LYS:HE2	1:G:149:LYS:HA	1.86	0.58
1:H:311:LYS:HG2	5:H:409:HOH:O	2.02	0.58
1:A:16:LYS:NZ	1:B:264:HIS:O	2.36	0.57
1:C:181:ALA:HB3	5:C:417:HOH:O	2.02	0.57
1:C:185:VAL:HG22	1:C:206:ILE:HD13	1.86	0.57
1:E:132:LEU:CD2	1:E:132:LEU:N	2.67	0.57
1:D:24:VAL:HG22	1:D:49:VAL:HB	1.86	0.57
1:D:129:PHE:CZ	1:D:131:GLY:N	2.72	0.57
1:B:118:ARG:NE	1:B:330:THR:OG1	2.37	0.57
1:D:265:ASN:CB	1:D:295:ARG:HB2	2.33	0.57
1:E:64:ASP:OD2	1:H:244:LYS:HE3	2.03	0.57
1:C:324:VAL:HA	1:C:327:ARG:HG3	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:TRP:CH2	1:H:226:LEU:HB3	2.40	0.57
1:G:16:LYS:HG3	1:G:46:ASP:O	2.05	0.57
1:A:138:ASN:HD22	1:A:140:VAL:H	1.51	0.57
1:C:138:ASN:OD1	4:C:352:NAD:O2D	2.11	0.57
1:A:83:TYR:O	1:A:127:SER:HB2	2.04	0.57
1:B:59:ILE:N	1:B:59:ILE:HD12	2.18	0.57
1:C:299:ARG:C	1:C:300:GLU:HG3	2.24	0.57
1:G:174:LEU:O	1:G:178:PHE:HD2	1.87	0.57
1:G:315:HIS:O	1:G:319:ALA:HB2	2.05	0.57
1:H:159:ILE:HG23	1:H:298:ILE:HD11	1.85	0.57
1:H:210:PRO:HG2	1:H:213:LYS:CD	2.09	0.57
1:G:216:GLU:CG	1:G:217:SER:N	2.67	0.57
1:G:138:ASN:HD22	1:G:140:VAL:H	1.50	0.57
1:C:215:VAL:HG11	1:C:226:LEU:HD11	1.85	0.57
1:G:15:MET:HB2	1:G:19:GLY:CA	2.34	0.57
1:C:75:PRO:HG3	1:D:266:GLU:HG2	1.86	0.57
1:H:200:VAL:HG12	1:H:203:GLN:HB2	1.87	0.57
1:D:118:ARG:NE	1:D:330:THR:OG1	2.37	0.57
1:G:215:VAL:HG23	1:G:222:ALA:HB3	1.86	0.57
1:C:200:VAL:HG21	1:C:304:ILE:HD11	1.86	0.57
1:C:16:LYS:HB2	5:D:360:HOH:O	2.05	0.57
4:A:352:NAD:H6N	5:A:368:HOH:O	2.04	0.57
1:E:93:VAL:HA	1:E:134:LEU:O	2.04	0.57
1:E:169:ARG:NH1	5:E:385:HOH:O	2.27	0.57
1:B:165:LEU:HD11	1:B:250:GLY:HA3	1.85	0.57
1:G:130:GLN:O	1:G:157:ARG:NH1	2.37	0.57
1:E:203:GLN:HG3	1:G:208:VAL:CG2	2.34	0.57
1:D:15:MET:HG3	1:D:19:GLY:HA3	1.87	0.57
1:E:266:GLU:CG	1:F:75:PRO:HG3	2.35	0.57
1:D:29:GLY:HA3	4:D:352:NAD:O1A	2.04	0.57
1:B:36:VAL:HG21	1:B:50:LEU:CD2	2.31	0.57
1:C:118:ARG:O	1:C:122:GLU:HG3	2.05	0.57
1:B:96:ALA:HB1	4:B:352:NAD:C4A	2.34	0.57
1:G:67:HIS:ND1	5:G:444:HOH:O	2.12	0.57
1:E:18:ASN:HA	5:E:355:HOH:O	2.04	0.57
1:H:15:MET:HB2	1:H:19:GLY:H	1.68	0.57
1:F:107:LEU:O	1:F:110:VAL:HG23	2.05	0.57
1:E:295:ARG:HG3	1:F:15:MET:HG2	1.85	0.57
1:D:265:ASN:HD22	1:D:295:ARG:H	1.53	0.57
1:A:168:ALA:HB1	1:D:70:VAL:HG23	1.87	0.57
1:A:251:ILE:HG13	1:A:255:LEU:HD22	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:PHE:O	1:D:233:VAL:HB	2.05	0.57
1:E:173:LEU:HB3	1:E:229:ILE:HG23	1.87	0.57
1:G:59:ILE:O	1:G:60:GLY:C	2.41	0.57
1:E:251:ILE:CD1	4:E:352:NAD:O7N	2.49	0.57
1:C:15:MET:HB2	1:C:19:GLY:CA	2.35	0.57
1:H:276:LEU:HD12	1:H:287:ILE:HG22	1.87	0.57
1:G:309:ASP:O	1:G:313:ARG:CG	2.52	0.57
1:F:240:ILE:CG2	1:F:244:LYS:HD3	2.35	0.57
1:H:149:LYS:HA	1:H:149:LYS:HE2	1.87	0.57
1:B:101:LYS:HB3	1:B:102:PRO:CD	2.28	0.57
1:F:172:PHE:CE1	1:G:66:ASN:HB3	2.40	0.57
1:A:275:TYR:HE1	1:A:284:ASP:HA	1.69	0.57
1:E:279:LEU:O	1:E:303:GLU:HG3	2.05	0.56
1:G:209:MET:CA	1:G:209:MET:CE	2.82	0.56
1:G:22:ARG:HB2	1:G:47:GLU:HB2	1.87	0.56
1:C:221:GLU:HB3	1:C:224:LYS:CB	2.26	0.56
1:E:26:ILE:HG21	1:E:120:ILE:HG23	1.87	0.56
1:A:107:LEU:HA	1:A:139:PRO:HG3	1.86	0.56
1:C:95:CYS:O	5:C:361:HOH:O	2.17	0.56
1:E:279:LEU:CB	5:E:398:HOH:O	2.16	0.56
1:D:206:ILE:HG12	1:D:211:ILE:HG12	1.87	0.56
1:F:119:SER:O	1:F:122:GLU:HB2	2.04	0.56
1:H:98:ALA:O	1:H:109:LEU:HD13	2.05	0.56
1:F:242:GLU:HG2	1:F:242:GLU:O	2.03	0.56
1:E:265:ASN:HB3	1:F:15:MET:CA	2.28	0.56
1:C:218:LYS:HG3	1:C:222:ALA:CB	2.35	0.56
4:C:352:NAD:H6N	5:C:371:HOH:O	2.05	0.56
1:B:59:ILE:HG22	1:B:63:MET:CE	2.35	0.56
1:G:294:ASN:HD22	1:G:296:ASN:H	1.53	0.56
1:F:272:VAL:HG21	1:F:293:ILE:HD11	1.86	0.56
1:E:202:SER:OG	1:E:310:GLU:OE1	2.23	0.56
1:E:165:LEU:O	1:E:168:ALA:HB3	2.05	0.56
1:D:132:LEU:CD2	1:D:132:LEU:N	2.68	0.56
1:B:211:ILE:HA	1:B:214:LEU:HD12	1.86	0.56
1:G:215:VAL:CB	1:G:222:ALA:CB	2.71	0.56
1:H:274:ALA:HB3	1:H:289:VAL:HG12	1.87	0.56
1:A:138:ASN:HB2	4:A:352:NAD:O2D	2.06	0.56
1:A:184:ASN:HB3	1:C:269:ILE:HD12	1.87	0.56
1:A:242:GLU:O	1:A:242:GLU:CG	2.49	0.56
1:D:212:ARG:HH11	1:D:226:LEU:CD1	2.18	0.56
1:E:295:ARG:HD2	1:F:15:MET:CG	2.36	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:PHE:O	1:H:121:VAL:HG23	2.06	0.56
1:C:138:ASN:HD22	1:C:140:VAL:H	1.54	0.56
1:D:39:LEU:O	1:D:43:GLY:N	2.39	0.56
1:E:167:THR:O	1:E:171:ARG:CG	2.53	0.56
1:D:215:VAL:CG2	1:D:222:ALA:HB1	2.35	0.56
1:E:18:ASN:N	1:E:47:GLU:OE2	2.38	0.56
1:H:222:ALA:O	1:H:225:ASP:HB2	2.05	0.56
1:F:117:PHE:O	1:F:118:ARG:C	2.44	0.56
1:B:99:ASN:HA	4:B:352:NAD:H3D	1.87	0.56
1:A:177:TYR:OH	1:A:222:ALA:HA	2.05	0.56
1:D:118:ARG:CG	1:D:118:ARG:HH11	2.19	0.56
1:F:27:GLY:O	1:F:32:GLY:HA3	2.06	0.56
1:H:219:GLY:O	1:H:221:GLU:HG2	2.05	0.56
1:F:313:ARG:HH11	1:F:313:ARG:CG	2.13	0.56
1:H:189:ILE:CD1	1:H:230:PHE:HE1	2.18	0.56
1:G:159:ILE:HD13	1:G:298:ILE:CG1	2.36	0.56
1:G:186:HIS:HD2	1:G:207:GLY:O	1.89	0.56
1:A:32:GLY:O	1:A:36:VAL:HG23	2.05	0.56
1:A:49:VAL:HG22	1:A:79:TRP:CZ2	2.41	0.56
1:A:203:GLN:HA	5:A:395:HOH:O	2.06	0.56
1:E:16:LYS:HB3	1:E:77:ASP:OD1	2.05	0.56
1:C:260:ARG:NH2	1:D:75:PRO:CD	2.69	0.56
1:A:100:GLN:HA	1:A:109:LEU:HD21	1.87	0.56
1:C:15:MET:HG3	1:C:19:GLY:HA3	1.88	0.56
1:B:166:ASP:OD1	1:B:193:HIS:ND1	2.31	0.56
1:H:240:ILE:HG22	1:H:244:LYS:CD	2.35	0.56
1:C:166:ASP:HB3	1:C:189:ILE:HG21	1.88	0.56
1:A:264:HIS:CB	1:B:16:LYS:HZ3	2.17	0.56
1:E:209:MET:CB	1:E:214:LEU:HD21	2.30	0.56
1:D:283:ARG:O	1:D:322:LYS:HE2	2.05	0.56
1:H:182:PRO:O	1:H:185:VAL:HB	2.06	0.56
1:C:185:VAL:HG22	1:C:206:ILE:CD1	2.36	0.56
1:H:218:LYS:HG2	1:H:222:ALA:HB2	1.87	0.56
1:G:264:HIS:O	1:H:16:LYS:HE2	2.06	0.56
1:A:83:TYR:CE2	1:A:124:VAL:HG12	2.40	0.56
1:D:307:ASN:O	1:D:311:LYS:HG2	2.06	0.56
1:A:16:LYS:CD	1:A:46:ASP:O	2.42	0.55
1:A:15:MET:CG	1:B:295:ARG:HG3	2.36	0.55
1:A:142:ILE:HD12	1:A:325:LEU:CD2	2.36	0.55
1:A:280:TYR:CE1	1:A:289:VAL:CG2	2.89	0.55
1:B:222:ALA:O	1:B:226:LEU:HG	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ARG:NH1	1:C:295:ARG:O	2.39	0.55
1:G:15:MET:HB2	1:G:20:GLY:N	2.20	0.55
1:F:228:ARG:HH22	1:F:231:VAL:HG11	1.71	0.55
1:B:121:VAL:HG11	1:B:150:PHE:CB	2.36	0.55
1:D:15:MET:N	1:D:20:GLY:CA	2.70	0.55
1:G:92:VAL:CG1	1:G:133:PHE:CE1	2.89	0.55
1:A:176:GLU:O	1:A:177:TYR:C	2.44	0.55
1:B:31:VAL:HG13	1:B:251:ILE:HG23	1.88	0.55
1:G:142:ILE:HG13	1:G:324:VAL:HG11	1.87	0.55
1:E:15:MET:O	1:E:47:GLU:OE2	2.23	0.55
1:G:18:ASN:OD1	1:G:18:ASN:N	2.40	0.55
1:H:113:ASN:HA	1:H:116:ILE:HD13	1.89	0.55
1:B:118:ARG:O	1:B:122:GLU:HB2	2.06	0.55
1:D:94:ILE:CG2	1:D:117:PHE:CZ	2.85	0.55
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.88	0.55
1:F:209:MET:CE	1:H:304:ILE:HA	2.36	0.55
1:E:109:LEU:HD23	5:E:374:HOH:O	2.05	0.55
1:D:55:GLU:O	1:D:59:ILE:HG13	2.07	0.55
1:A:243:LYS:HD3	1:D:59:ILE:CG2	2.36	0.55
1:D:269:ILE:HG23	1:D:302:ILE:HD12	1.89	0.55
1:H:148:TRP:HA	1:H:158:VAL:HG21	1.88	0.55
1:H:107:LEU:HD11	1:H:192:GLU:OE2	2.07	0.55
1:D:309:ASP:O	1:D:313:ARG:HG2	2.07	0.55
1:A:209:MET:CE	1:C:304:ILE:HA	2.37	0.55
1:H:240:ILE:HG23	1:H:244:LYS:HD2	1.84	0.55
1:A:136:ALA:O	4:A:352:NAD:H2N	2.06	0.55
1:B:61:ASP:HB3	1:B:65:PHE:HE2	1.69	0.55
1:C:40:MET:HE2	1:C:69:LYS:HB3	1.89	0.55
1:E:280:TYR:CE1	1:E:302:ILE:O	2.60	0.55
1:H:187:ALA:HB2	1:H:204:ALA:HB1	1.89	0.55
1:E:16:LYS:HD2	1:E:16:LYS:N	2.21	0.55
1:C:264:HIS:CA	1:D:16:LYS:HZ3	2.20	0.55
1:F:114:ILE:HD12	1:F:328:ALA:O	2.07	0.55
1:H:65:PHE:O	1:H:68:GLY:N	2.36	0.55
1:B:299:ARG:NE	1:B:300:GLU:OE2	2.39	0.55
1:F:71:PHE:HE2	5:G:373:HOH:O	1.89	0.55
1:F:305:GLU:OE1	1:H:213:LYS:HD2	2.07	0.55
1:B:322:LYS:HG2	5:B:408:HOH:O	2.06	0.55
1:H:220:GLU:H	1:H:223:GLN:HB2	1.71	0.55
1:E:155:HIS:HB2	1:E:286:TYR:OH	2.06	0.55
1:B:55:GLU:O	1:B:58:ALA:HB3	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:O	1:E:178:PHE:HD1	1.89	0.55
1:D:100:GLN:HG3	5:D:378:HOH:O	2.07	0.55
1:A:100:GLN:HB3	1:A:109:LEU:HD11	1.89	0.55
1:C:184:ASN:OD1	5:C:417:HOH:O	2.17	0.55
1:B:221:GLU:C	5:B:418:HOH:O	2.43	0.55
1:C:93:VAL:HA	1:C:134:LEU:O	2.07	0.55
1:E:203:GLN:HG3	1:G:208:VAL:HG23	1.89	0.55
1:G:86:CYS:HG	1:G:124:VAL:HG23	1.68	0.55
1:H:114:ILE:HD13	1:H:329:PHE:CE1	2.41	0.55
1:B:74:LYS:HD2	1:B:75:PRO:O	2.07	0.55
4:E:352:NAD:H6N	5:E:367:HOH:O	2.07	0.55
1:A:63:MET:CE	1:D:243:LYS:HD3	2.36	0.55
1:C:327:ARG:CZ	1:C:328:ALA:HB2	2.37	0.55
1:A:170:PHE:CE2	1:A:187:ALA:HB1	2.42	0.55
1:G:39:LEU:HD22	1:G:44:ILE:HB	1.89	0.55
1:B:187:ALA:HB2	1:B:204:ALA:HB1	1.89	0.55
1:H:205:TYR:CD1	1:H:205:TYR:N	2.74	0.54
1:F:329:PHE:C	1:F:329:PHE:HD1	2.11	0.54
1:E:265:ASN:HB3	1:F:16:LYS:N	2.22	0.54
1:D:209:MET:CA	1:D:209:MET:CE	2.80	0.54
1:E:290:PRO:HG3	1:E:304:ILE:CG2	2.36	0.54
1:A:280:TYR:CE1	1:A:289:VAL:HG21	2.42	0.54
1:E:276:LEU:O	1:E:283:ARG:HA	2.07	0.54
1:A:264:HIS:HB3	1:B:16:LYS:HZ3	1.71	0.54
1:E:295:ARG:CB	1:F:15:MET:HG2	2.37	0.54
1:C:153:LEU:HB3	1:C:154:PRO:CD	2.36	0.54
1:E:289:VAL:HG13	1:E:301:VAL:HG13	1.88	0.54
1:G:52:ASP:OD1	1:G:54:ASN:N	2.34	0.54
1:E:148:TRP:HA	1:E:158:VAL:HG21	1.89	0.54
1:G:249:TYR:O	1:G:253:MET:HG2	2.06	0.54
1:H:150:PHE:HZ	1:H:330:THR:HB	1.73	0.54
1:C:221:GLU:CB	1:C:224:LYS:H	2.20	0.54
1:B:70:VAL:HG22	1:C:182:PRO:CB	2.37	0.54
1:E:116:ILE:HG22	1:E:120:ILE:CD1	2.38	0.54
1:E:240:ILE:HD11	1:H:67:HIS:HE1	1.72	0.54
1:C:189:ILE:CD1	1:C:230:PHE:CE1	2.90	0.54
1:G:282:GLU:HG3	1:G:318:ALA:HB1	1.89	0.54
1:F:220:GLU:HA	1:F:223:GLN:HB2	1.88	0.54
1:B:211:ILE:O	1:B:213:LYS:N	2.41	0.54
1:G:218:LYS:HD2	1:G:222:ALA:HB2	1.89	0.54
1:G:264:HIS:C	1:H:16:LYS:NZ	2.60	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:363:HOH:O	1:C:172:PHE:HB2	2.07	0.54
1:B:87:ARG:CZ	1:B:87:ARG:HB3	2.37	0.54
1:D:220:GLU:CA	1:D:223:GLN:HB2	2.31	0.54
1:A:74:LYS:HG2	5:A:418:HOH:O	2.07	0.54
1:C:167:THR:O	1:C:171:ARG:CG	2.56	0.54
1:H:248:TYR:O	1:H:251:ILE:HG22	2.07	0.54
1:C:75:PRO:HG3	1:D:266:GLU:CG	2.37	0.54
1:B:265:ASN:HD22	1:B:294:ASN:HB2	1.71	0.54
1:H:216:GLU:HG2	1:H:217:SER:N	2.22	0.54
1:E:265:ASN:OD1	1:F:17:ASN:N	2.37	0.54
1:E:295:ARG:O	1:E:295:ARG:HD3	2.08	0.54
1:B:87:ARG:CG	1:B:127:SER:O	2.51	0.54
1:G:232:ASN:O	1:G:236:ALA:HB2	2.07	0.54
1:G:278:GLY:N	1:G:282:GLU:O	2.35	0.54
1:F:212:ARG:CD	1:F:223:GLN:HE22	2.20	0.54
1:C:15:MET:HB2	1:C:19:GLY:H	1.68	0.54
1:G:190:ILE:CD1	1:G:200:VAL:HG21	2.30	0.54
1:D:94:ILE:HG21	1:D:117:PHE:CE2	2.42	0.54
1:G:145:TYR:CD1	1:G:329:PHE:CE2	2.96	0.54
1:D:109:LEU:O	1:D:112:LYS:HB2	2.08	0.54
1:G:57:LYS:HG2	5:G:492:HOH:O	2.07	0.54
1:F:265:ASN:HA	1:F:295:ARG:H	1.71	0.54
1:B:114:ILE:CG2	1:B:330:THR:HA	2.37	0.54
1:A:295:ARG:HB3	1:B:15:MET:HE3	1.90	0.54
1:H:276:LEU:HD22	1:H:279:LEU:HB3	1.89	0.54
1:B:54:ASN:ND2	1:B:57:LYS:H	2.05	0.54
1:C:240:ILE:HG22	1:C:244:LYS:HD3	1.88	0.54
1:A:173:LEU:HD12	1:A:233:VAL:CG2	2.38	0.54
1:G:100:GLN:HA	1:G:109:LEU:HD21	1.90	0.54
1:A:265:ASN:OD1	1:B:17:ASN:CB	2.56	0.54
1:F:87:ARG:CG	1:F:127:SER:O	2.55	0.54
1:F:139:PRO:HD2	1:F:143:LEU:HD12	1.90	0.54
1:B:59:ILE:HB	1:C:243:LYS:HD3	1.88	0.54
1:D:118:ARG:NH1	1:D:118:ARG:HG2	2.23	0.54
1:D:240:ILE:HG22	1:D:244:LYS:HD3	1.90	0.54
1:B:76:VAL:HB	5:B:359:HOH:O	2.08	0.54
1:E:215:VAL:HG21	1:E:226:LEU:HD11	1.90	0.54
1:B:15:MET:C	1:B:17:ASN:H	2.05	0.54
1:B:138:ASN:CB	4:B:352:NAD:HO2N	2.21	0.54
1:G:315:HIS:O	1:G:319:ALA:CB	2.56	0.54
1:C:228:ARG:HH12	1:C:232:ASN:CG	2.11	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ALA:H	1:D:46:ASP:HB2	1.73	0.54
1:G:16:LYS:O	1:G:77:ASP:OD2	2.26	0.54
1:C:280:TYR:OH	1:C:304:ILE:HG12	2.08	0.54
1:H:112:LYS:HE2	1:H:112:LYS:HA	1.89	0.54
1:F:77:ASP:HB3	1:F:79:TRP:HZ3	1.73	0.54
1:D:110:VAL:HG12	1:D:114:ILE:HD12	1.89	0.54
1:H:280:TYR:O	1:H:282:GLU:HG2	2.08	0.54
1:A:142:ILE:HD12	1:A:325:LEU:HD21	1.88	0.54
1:E:40:MET:CE	1:E:72:ALA:HB2	2.38	0.54
1:B:37:PHE:HD2	1:C:37:PHE:HD2	1.56	0.54
1:F:145:TYR:HD1	1:F:329:PHE:CE2	2.19	0.53
1:A:87:ARG:HB2	1:A:127:SER:O	2.08	0.53
1:D:15:MET:HB2	1:D:19:GLY:N	2.24	0.53
1:E:70:VAL:HG22	1:H:182:PRO:HB2	1.88	0.53
1:B:54:ASN:O	1:B:54:ASN:ND2	2.40	0.53
1:A:306:LEU:O	1:A:311:LYS:HE2	2.08	0.53
1:H:218:LYS:O	1:H:218:LYS:HG2	2.07	0.53
1:H:120:ILE:O	1:H:124:VAL:HG12	2.08	0.53
1:A:15:MET:HG3	1:A:19:GLY:HA3	1.91	0.53
1:D:222:ALA:HB3	5:D:405:HOH:O	2.07	0.53
1:G:221:GLU:HA	1:G:221:GLU:OE1	2.08	0.53
1:D:22:ARG:HB2	1:D:47:GLU:HB2	1.89	0.53
1:B:149:LYS:HA	1:B:149:LYS:CE	2.25	0.53
1:C:117:PHE:CD2	1:C:147:THR:OG1	2.60	0.53
1:C:215:VAL:CA	1:C:218:LYS:HG2	2.36	0.53
1:H:228:ARG:O	1:H:231:VAL:HB	2.07	0.53
1:C:145:TYR:CD1	1:C:329:PHE:CE2	2.97	0.53
1:G:299:ARG:NE	1:G:300:GLU:OE2	2.41	0.53
1:E:205:TYR:C	1:E:206:ILE:HG12	2.29	0.53
1:A:279:LEU:HD23	1:A:301:VAL:CG1	2.38	0.53
1:E:212:ARG:NH1	1:E:226:LEU:CD1	2.72	0.53
1:C:257:ARG:O	1:C:257:ARG:HG3	2.00	0.53
1:A:247:THR:OG1	4:A:352:NAD:H5N	2.08	0.53
1:B:203:GLN:HE22	1:B:305:GLU:HB3	1.74	0.53
1:B:304:ILE:HB	1:D:209:MET:HE1	1.89	0.53
1:B:241:ILE:O	1:B:245:GLY:CA	2.57	0.53
1:D:309:ASP:O	1:D:313:ARG:CG	2.57	0.53
1:F:219:GLY:HA2	5:F:397:HOH:O	2.07	0.53
1:G:16:LYS:NZ	1:H:264:HIS:O	2.33	0.53
1:B:162:GLY:O	1:B:193:HIS:HB2	2.08	0.53
1:A:168:ALA:CA	1:D:70:VAL:HG21	2.32	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:THR:O	1:H:151:SER:HB3	2.08	0.53
1:E:224:LYS:NZ	1:E:224:LYS:HB3	2.24	0.53
1:A:202:SER:OG	1:A:310:GLU:OE1	2.26	0.53
1:A:264:HIS:O	1:B:16:LYS:CD	2.54	0.53
1:E:56:SER:O	1:H:243:LYS:HG2	2.07	0.53
1:E:110:VAL:CG1	1:E:111:ASP:N	2.69	0.53
1:D:216:GLU:HA	5:D:406:HOH:O	2.09	0.53
1:A:61:ASP:OD1	1:D:244:LYS:HE2	2.09	0.53
1:E:207:GLY:HA3	5:E:395:HOH:O	2.08	0.53
1:D:27:GLY:O	1:D:95:CYS:HB2	2.09	0.53
1:C:24:VAL:CG1	1:C:51:ILE:HD11	2.38	0.53
1:F:112:LYS:O	1:F:115:ALA:HB3	2.08	0.53
1:B:15:MET:HB2	1:B:19:GLY:HA3	1.89	0.53
1:F:217:SER:O	1:F:218:LYS:HB3	2.08	0.53
1:C:118:ARG:HH11	1:C:118:ARG:CB	2.16	0.53
1:A:234:ARG:HG2	5:A:385:HOH:O	2.07	0.53
1:C:209:MET:HE2	1:C:209:MET:CA	2.39	0.53
1:D:329:PHE:HD1	1:D:330:THR:N	2.07	0.53
1:D:17:ASN:HA	5:D:419:HOH:O	2.09	0.53
1:A:15:MET:HA	1:B:265:ASN:HB2	1.91	0.53
1:G:137:THR:HG23	4:G:352:NAD:O3D	2.08	0.53
1:C:15:MET:CG	1:D:295:ARG:HG3	2.39	0.53
1:D:280:TYR:CZ	1:D:303:GLU:HA	2.44	0.53
1:C:87:ARG:CZ	1:C:87:ARG:CB	2.86	0.53
1:H:307:ASN:O	1:H:311:LYS:HG3	2.09	0.53
1:F:174:LEU:HD23	1:F:229:ILE:HD13	1.91	0.53
1:G:264:HIS:O	1:H:16:LYS:CE	2.56	0.53
1:F:138:ASN:HA	1:F:140:VAL:H	1.74	0.53
1:A:173:LEU:HD12	1:A:233:VAL:HG23	1.91	0.53
1:E:30:PHE:HB3	1:E:248:TYR:CD2	2.44	0.53
1:H:112:LYS:O	1:H:115:ALA:CB	2.43	0.52
1:A:55:GLU:HB3	1:A:59:ILE:HD11	1.89	0.52
1:A:159:ILE:HG12	1:A:298:ILE:HD11	1.90	0.52
1:A:114:ILE:HD12	1:A:328:ALA:O	2.09	0.52
1:A:160:GLY:HA3	1:A:273:SER:HB3	1.91	0.52
1:G:288:GLY:O	1:G:289:VAL:HB	2.08	0.52
1:G:219:GLY:O	1:G:221:GLU:N	2.42	0.52
1:E:295:ARG:CG	1:F:15:MET:CG	2.86	0.52
1:D:52:ASP:OD1	4:D:352:NAD:O2B	2.27	0.52
1:G:145:TYR:CD1	1:G:329:PHE:HE2	2.26	0.52
1:E:304:ILE:HG13	1:E:306:LEU:HD21	1.89	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ARG:HA	1:E:316:HIS:HB3	1.90	0.52
1:B:209:MET:HE1	1:D:203:GLN:NE2	2.23	0.52
1:E:118:ARG:O	1:E:122:GLU:HB2	2.10	0.52
1:D:324:VAL:O	1:D:328:ALA:CB	2.57	0.52
1:B:243:LYS:CD	1:C:59:ILE:HG22	2.39	0.52
1:E:167:THR:O	1:E:171:ARG:HG2	2.09	0.52
1:D:323:SER:O	1:D:326:ALA:HB3	2.09	0.52
1:E:215:VAL:O	1:E:218:LYS:HG2	2.09	0.52
1:F:145:TYR:HE1	1:F:149:LYS:HD3	1.65	0.52
1:D:56:SER:HA	1:D:59:ILE:HD12	1.90	0.52
1:B:276:LEU:O	1:B:283:ARG:HA	2.09	0.52
1:D:218:LYS:O	1:D:221:GLU:HB2	2.09	0.52
1:F:203:GLN:HG2	1:H:208:VAL:HG23	1.91	0.52
1:H:218:LYS:O	1:H:221:GLU:HB2	2.10	0.52
1:B:114:ILE:HD13	1:B:328:ALA:O	2.10	0.52
1:D:138:ASN:HD22	1:D:140:VAL:H	1.55	0.52
1:H:276:LEU:HD21	1:H:279:LEU:HB3	1.91	0.52
1:A:86:CYS:HB2	1:A:127:SER:CB	2.39	0.52
1:A:215:VAL:HG11	1:A:226:LEU:HD11	1.90	0.52
1:B:55:GLU:HB3	1:B:59:ILE:CD1	2.38	0.52
1:A:145:TYR:HE1	1:A:149:LYS:HD2	1.75	0.52
1:C:101:LYS:HZ3	1:C:101:LYS:HB3	1.72	0.52
1:E:161:SER:O	1:E:164:ILE:CG2	2.57	0.52
1:A:156:GLU:O	1:A:297:GLY:HA3	2.10	0.52
1:B:256:ALA:O	1:B:260:ARG:HG2	2.10	0.52
1:D:276:LEU:HD22	1:D:279:LEU:HB3	1.92	0.52
1:G:16:LYS:NZ	1:H:264:HIS:HB3	2.24	0.52
1:F:52:ASP:OD1	4:F:352:NAD:O2B	2.21	0.52
1:G:54:ASN:HD21	1:G:56:SER:HB2	1.75	0.52
1:C:145:TYR:CE1	1:C:329:PHE:HE2	2.27	0.52
1:D:39:LEU:HD22	1:D:44:ILE:CG2	2.39	0.52
1:D:71:PHE:HB3	5:D:368:HOH:O	2.09	0.52
1:C:250:GLY:N	5:C:355:HOH:O	2.41	0.52
1:B:71:PHE:HE2	5:C:356:HOH:O	1.93	0.52
1:F:149:LYS:HA	1:F:149:LYS:CE	2.39	0.52
1:B:94:ILE:CG2	1:B:117:PHE:CZ	2.92	0.52
1:F:86:CYS:O	1:F:129:PHE:HD1	1.93	0.52
1:A:75:PRO:HG3	1:B:266:GLU:HG3	1.92	0.52
1:H:94:ILE:HG22	1:H:117:PHE:CZ	2.45	0.52
1:B:243:LYS:HG3	1:C:56:SER:CB	2.40	0.52
1:A:145:TYR:CE1	1:A:149:LYS:HD2	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HD3	1:D:59:ILE:HG22	1.92	0.52
1:C:192:GLU:O	1:C:197:GLU:HB3	2.09	0.52
1:B:174:LEU:HB2	1:B:185:VAL:HG11	1.91	0.52
1:C:266:GLU:HG2	1:D:75:PRO:HG3	1.91	0.52
1:G:112:LYS:HA	1:G:112:LYS:CE	2.16	0.52
1:C:15:MET:HA	1:D:265:ASN:OD1	2.10	0.52
1:G:101:LYS:CB	1:G:102:PRO:CD	2.88	0.52
1:C:69:LYS:HA	1:C:72:ALA:HB2	1.92	0.52
1:G:54:ASN:C	1:G:54:ASN:ND2	2.63	0.52
1:C:209:MET:HE2	1:C:209:MET:HA	1.91	0.52
1:C:265:ASN:HD22	1:C:295:ARG:H	1.58	0.51
1:B:289:VAL:HG11	1:B:301:VAL:CG1	2.39	0.51
1:C:178:PHE:HZ	1:C:215:VAL:CG1	2.22	0.51
1:E:71:PHE:CD1	1:H:257:ARG:HG2	2.45	0.51
5:E:423:HOH:O	1:H:71:PHE:CE2	2.50	0.51
1:B:64:ASP:OD2	1:C:244:LYS:HE2	2.10	0.51
1:F:57:LYS:HG2	5:F:409:HOH:O	2.09	0.51
1:E:54:ASN:C	1:E:54:ASN:HD22	2.14	0.51
1:A:137:THR:HB	1:A:143:LEU:HD13	1.91	0.51
1:F:223:GLN:HG2	5:F:397:HOH:O	2.10	0.51
1:B:15:MET:C	1:B:17:ASN:N	2.62	0.51
1:H:125:MET:HA	1:H:125:MET:CE	2.37	0.51
1:C:116:ILE:HG23	1:C:120:ILE:HD12	1.92	0.51
1:D:187:ALA:HA	5:D:399:HOH:O	2.09	0.51
1:C:87:ARG:HH11	1:C:87:ARG:HB2	1.74	0.51
1:D:65:PHE:HB3	1:D:78:ILE:HD13	1.92	0.51
1:H:197:GLU:OE2	1:H:234:ARG:HA	2.11	0.51
1:E:199:PRO:HG3	1:E:230:PHE:CD1	2.46	0.51
1:F:198:LEU:CB	1:F:313:ARG:CD	2.84	0.51
1:F:215:VAL:HG23	1:F:215:VAL:O	2.10	0.51
5:A:422:HOH:O	1:D:70:VAL:HG22	2.08	0.51
1:E:69:LYS:C	1:E:71:PHE:H	2.12	0.51
1:F:213:LYS:CA	1:F:216:GLU:HB3	2.38	0.51
1:D:55:GLU:C	1:D:59:ILE:HD12	2.30	0.51
1:A:283:ARG:O	1:A:322:LYS:HE2	2.09	0.51
1:F:294:ASN:HD22	1:F:296:ASN:N	2.02	0.51
1:G:26:ILE:HG21	1:G:120:ILE:HG23	1.92	0.51
1:G:185:VAL:HG13	1:G:206:ILE:HD13	1.92	0.51
1:A:258:VAL:O	1:A:261:ALA:N	2.43	0.51
1:E:228:ARG:HH22	1:E:231:VAL:HG11	1.74	0.51
1:D:22:ARG:CG	1:D:89:ALA:CA	2.82	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:HG21	1:B:120:ILE:HG23	1.93	0.51
1:D:170:PHE:CD2	1:D:189:ILE:HD13	2.44	0.51
1:B:76:VAL:HG13	1:B:78:ILE:HD12	1.92	0.51
1:H:66:ASN:O	1:H:69:LYS:HG2	2.11	0.51
1:H:15:MET:HB3	1:H:17:ASN:H	1.75	0.51
1:B:15:MET:CB	1:B:19:GLY:HA3	2.41	0.51
1:G:228:ARG:HD3	1:G:228:ARG:C	2.30	0.51
1:H:251:ILE:HG12	4:H:352:NAD:C4N	2.39	0.51
1:E:153:LEU:HB3	1:E:154:PRO:HD2	1.93	0.51
1:B:87:ARG:CB	1:B:87:ARG:NH1	2.74	0.51
1:A:208:VAL:HB	1:C:203:GLN:HG3	1.92	0.51
1:C:132:LEU:HD12	1:C:157:ARG:HA	1.93	0.51
1:D:21:ALA:HB1	1:D:263:LEU:HD13	1.93	0.51
1:H:118:ARG:HG2	1:H:150:PHE:CZ	2.45	0.51
1:A:52:ASP:OD1	1:A:54:ASN:N	2.33	0.51
1:A:223:GLN:NE2	5:A:398:HOH:O	2.44	0.51
1:E:24:VAL:HG22	1:E:49:VAL:HB	1.91	0.51
1:G:187:ALA:HA	5:G:473:HOH:O	2.09	0.51
1:C:101:LYS:NZ	1:C:101:LYS:CB	2.73	0.51
1:C:112:LYS:HA	1:C:112:LYS:HE2	1.92	0.51
1:H:241:ILE:HG12	1:H:247:THR:HG22	1.91	0.51
1:H:215:VAL:HG23	5:H:406:HOH:O	2.10	0.51
1:C:260:ARG:NH2	1:D:75:PRO:HD2	2.25	0.51
1:C:280:TYR:OH	1:C:304:ILE:N	2.43	0.51
1:F:280:TYR:OH	1:F:302:ILE:O	2.19	0.51
1:A:208:VAL:HG22	1:C:188:TYR:CE2	2.46	0.51
1:H:116:ILE:HD12	1:H:116:ILE:N	2.25	0.51
1:E:264:HIS:O	1:E:265:ASN:C	2.49	0.51
1:E:203:GLN:NE2	1:G:209:MET:CE	2.74	0.50
1:C:117:PHE:O	1:C:121:VAL:CG2	2.54	0.50
1:G:55:GLU:O	1:G:58:ALA:HB3	2.11	0.50
1:E:24:VAL:HG13	1:E:51:ILE:HD12	1.93	0.50
1:A:145:TYR:CD1	1:A:329:PHE:CE2	2.97	0.50
1:D:36:VAL:HG21	1:D:50:LEU:HD21	1.92	0.50
1:F:118:ARG:NH1	1:F:118:ARG:HB3	2.12	0.50
1:G:101:LYS:CB	1:G:102:PRO:HD2	2.32	0.50
1:A:86:CYS:O	1:A:87:ARG:C	2.49	0.50
1:B:63:MET:CE	1:C:243:LYS:HD2	2.41	0.50
1:H:293:ILE:HD12	1:H:298:ILE:HG13	1.93	0.50
1:C:311:LYS:CA	5:C:402:HOH:O	2.59	0.50
1:B:24:VAL:CG1	1:B:51:ILE:CD1	2.88	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ILE:HG22	1:F:160:GLY:N	2.27	0.50
1:F:114:ILE:HG22	1:F:115:ALA:N	2.24	0.50
1:C:16:LYS:CA	1:C:77:ASP:HB2	2.41	0.50
1:D:265:ASN:HB2	1:D:295:ARG:CB	2.37	0.50
1:G:40:MET:HE3	1:G:69:LYS:HA	1.91	0.50
1:C:327:ARG:NH2	1:C:328:ALA:HB2	2.26	0.50
1:F:169:ARG:HG2	1:G:67:HIS:CD2	2.46	0.50
1:C:169:ARG:NH1	5:C:389:HOH:O	2.25	0.50
1:A:15:MET:SD	1:A:17:ASN:O	2.70	0.50
1:D:228:ARG:CB	1:D:228:ARG:NH1	2.75	0.50
1:G:265:ASN:HB2	1:H:15:MET:HA	1.87	0.50
1:E:69:LYS:HA	1:E:72:ALA:H	1.75	0.50
1:H:257:ARG:HD2	1:H:257:ARG:O	2.11	0.50
1:D:91:LEU:HD22	1:D:259:THR:HG23	1.93	0.50
1:F:172:PHE:HA	5:F:390:HOH:O	2.10	0.50
1:F:251:ILE:HG13	1:F:255:LEU:HD21	1.94	0.50
1:B:307:ASN:OD1	1:B:310:GLU:HG3	2.11	0.50
1:E:30:PHE:HB3	1:E:248:TYR:CG	2.46	0.50
1:H:221:GLU:OE1	1:H:221:GLU:CA	2.36	0.50
1:B:209:MET:CE	1:D:203:GLN:NE2	2.75	0.50
1:E:215:VAL:CB	1:E:222:ALA:HB1	2.26	0.50
1:F:145:TYR:CZ	1:F:149:LYS:HD3	2.46	0.50
1:A:295:ARG:HB3	1:B:15:MET:CE	2.42	0.50
1:A:320:THR:O	1:A:323:SER:HB2	2.11	0.50
1:C:40:MET:O	5:C:363:HOH:O	2.20	0.50
1:F:174:LEU:HD23	1:F:229:ILE:CD1	2.42	0.50
1:B:167:THR:O	1:B:171:ARG:HG3	2.12	0.50
1:B:23:VAL:CG1	1:B:91:LEU:HD23	2.42	0.50
1:F:189:ILE:HD13	1:F:199:PRO:HA	1.92	0.50
1:A:295:ARG:HD2	1:B:15:MET:HE3	1.93	0.50
1:E:266:GLU:HG3	1:F:75:PRO:HG3	1.91	0.50
1:C:178:PHE:HZ	1:C:215:VAL:HG12	1.77	0.50
1:E:164:ILE:HD11	1:E:254:GLY:O	2.11	0.50
1:D:228:ARG:NH1	1:D:228:ARG:O	2.45	0.50
1:A:31:VAL:HG22	1:A:251:ILE:HG21	1.93	0.50
1:A:132:LEU:N	1:A:132:LEU:HD22	2.27	0.50
1:H:90:ASP:HB3	1:H:295:ARG:HH22	1.76	0.50
1:D:287:ILE:HD13	1:D:314:PHE:CE1	2.47	0.50
1:G:207:GLY:HA3	5:G:478:HOH:O	2.10	0.50
1:G:148:TRP:HA	1:G:158:VAL:HG21	1.93	0.50
1:E:118:ARG:NE	1:E:330:THR:OG1	2.43	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLY:HA3	1:C:46:ASP:HB2	1.94	0.50
1:E:71:PHE:CD2	5:H:358:HOH:O	2.64	0.50
1:A:215:VAL:HB	1:A:222:ALA:HB1	1.94	0.50
1:B:59:ILE:CG2	1:C:243:LYS:HD3	2.42	0.50
1:E:146:ALA:HA	1:E:329:PHE:HZ	1.75	0.50
1:F:116:ILE:O	1:F:120:ILE:HG13	2.12	0.50
1:D:269:ILE:HD13	1:D:302:ILE:CD1	2.42	0.50
1:H:118:ARG:O	1:H:122:GLU:HB2	2.12	0.50
1:E:110:VAL:HG12	1:E:111:ASP:OD1	2.12	0.50
1:H:248:TYR:HA	1:H:251:ILE:HG22	1.93	0.50
1:A:162:GLY:CA	5:A:378:HOH:O	2.59	0.50
1:A:162:GLY:HA2	5:A:378:HOH:O	2.12	0.50
1:G:221:GLU:O	1:G:222:ALA:O	2.30	0.49
1:H:32:GLY:O	1:H:36:VAL:HG23	2.12	0.49
1:D:166:ASP:OD1	1:D:193:HIS:ND1	2.35	0.49
5:A:422:HOH:O	1:D:70:VAL:CG2	2.59	0.49
1:A:91:LEU:HA	1:A:132:LEU:O	2.12	0.49
1:E:61:ASP:O	1:E:65:PHE:CD2	2.65	0.49
1:D:116:ILE:HG22	1:D:120:ILE:HD11	1.95	0.49
1:G:148:TRP:CD1	1:G:148:TRP:O	2.65	0.49
1:G:169:ARG:NH1	5:G:468:HOH:O	2.44	0.49
1:H:272:VAL:O	1:H:288:GLY:HA2	2.12	0.49
1:G:112:LYS:HB2	5:G:456:HOH:O	2.13	0.49
1:B:186:HIS:N	1:B:205:TYR:O	2.40	0.49
1:C:241:ILE:HD13	5:C:374:HOH:O	2.13	0.49
1:F:304:ILE:HA	1:H:209:MET:HE3	1.90	0.49
1:E:265:ASN:HB2	1:E:295:ARG:CB	2.38	0.49
1:D:114:ILE:CG2	5:D:415:HOH:O	2.58	0.49
1:B:287:ILE:HG13	1:B:321:LEU:CD1	2.41	0.49
1:D:196:THR:HB	1:D:317:SER:HB2	1.92	0.49
1:A:15:MET:HG2	1:B:295:ARG:CG	2.43	0.49
1:G:22:ARG:HA	1:G:47:GLU:O	2.13	0.49
1:A:104:GLU:C	1:A:105:THR:HG22	2.31	0.49
1:E:265:ASN:OD1	1:F:16:LYS:N	2.45	0.49
1:F:35:TYR:CZ	1:F:39:LEU:HD11	2.48	0.49
1:A:26:ILE:HA	1:A:51:ILE:O	2.13	0.49
1:B:268:ALA:O	1:B:292:VAL:HA	2.12	0.49
1:A:206:ILE:CG1	1:A:211:ILE:HD11	2.42	0.49
1:B:18:ASN:HA	5:B:357:HOH:O	2.11	0.49
1:E:63:MET:O	1:E:67:HIS:CG	2.66	0.49
1:C:138:ASN:HA	1:C:140:VAL:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ILE:HG22	1:D:120:ILE:HD12	1.95	0.49
1:B:216:GLU:CG	1:B:217:SER:N	2.75	0.49
1:E:44:ILE:HD13	1:E:260:ARG:HB3	1.95	0.49
1:C:222:ALA:O	1:C:226:LEU:HG	2.12	0.49
1:D:164:ILE:CD1	1:D:270:LEU:HD22	2.41	0.49
1:G:299:ARG:C	1:G:300:GLU:HG3	2.32	0.49
1:H:178:PHE:CZ	1:H:211:ILE:HG23	2.47	0.49
1:G:317:SER:O	1:G:318:ALA:C	2.51	0.49
1:E:68:GLY:HA3	1:H:253:MET:HG3	1.95	0.49
1:A:174:LEU:HB2	1:A:185:VAL:HG11	1.94	0.49
1:E:94:ILE:HD13	1:E:120:ILE:HG21	1.94	0.49
1:H:175:GLY:HA2	1:H:185:VAL:HG21	1.94	0.49
1:A:22:ARG:HG2	1:A:24:VAL:HG23	1.95	0.49
1:G:193:HIS:CE1	3:G:351:OXM:O2	2.65	0.49
1:A:209:MET:HG2	1:A:214:LEU:CD2	2.43	0.49
1:H:124:VAL:CG2	1:H:129:PHE:CD2	2.95	0.49
1:G:190:ILE:CD1	1:G:200:VAL:CG2	2.86	0.49
1:E:40:MET:O	1:E:73:PRO:HD2	2.12	0.49
1:C:55:GLU:O	1:C:56:SER:C	2.51	0.49
1:C:22:ARG:HB3	1:C:89:ALA:HA	1.93	0.49
1:A:15:MET:N	5:A:419:HOH:O	2.45	0.49
1:C:261:ALA:HA	1:C:266:GLU:HB2	1.95	0.49
1:C:90:ASP:HB3	1:C:295:ARG:HH22	1.77	0.49
1:D:21:ALA:N	1:D:46:ASP:HB2	2.28	0.49
1:B:87:ARG:HG2	1:B:128:GLY:O	2.13	0.49
1:C:140:VAL:CG1	1:C:193:HIS:HB3	2.43	0.49
1:C:114:ILE:HD13	1:C:143:LEU:CD2	2.39	0.49
1:A:215:VAL:O	1:A:218:LYS:HG2	2.12	0.49
1:C:247:THR:CG2	3:C:351:OXM:O3	2.57	0.49
1:C:148:TRP:CD1	1:C:153:LEU:O	2.66	0.49
1:C:275:TYR:HB2	1:C:286:TYR:CE2	2.47	0.49
1:G:218:LYS:CD	1:G:222:ALA:HB2	2.42	0.49
1:G:24:VAL:HB	1:G:92:VAL:HG22	1.95	0.49
1:C:31:VAL:CG1	1:C:95:CYS:HB3	2.43	0.49
1:C:31:VAL:HG12	1:C:95:CYS:HB3	1.95	0.49
1:A:279:LEU:HD23	1:A:301:VAL:HG12	1.95	0.49
1:B:92:VAL:HG12	1:B:133:PHE:CD1	2.48	0.49
1:B:222:ALA:HB3	5:B:399:HOH:O	2.12	0.48
1:G:220:GLU:CA	1:G:223:GLN:HB2	2.43	0.48
1:E:212:ARG:HH12	1:E:226:LEU:CD1	2.25	0.48
1:C:15:MET:HE3	1:D:295:ARG:CB	2.43	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:289:VAL:CG2	1:H:290:PRO:HD2	2.42	0.48
1:F:192:GLU:O	1:F:197:GLU:HB3	2.13	0.48
1:A:83:TYR:O	1:A:127:SER:CB	2.61	0.48
1:E:170:PHE:O	1:E:174:LEU:HD12	2.13	0.48
1:C:213:LYS:HA	1:C:216:GLU:CB	2.42	0.48
1:A:206:ILE:HG13	1:A:214:LEU:HD13	1.94	0.48
1:G:40:MET:HE3	1:G:69:LYS:HB3	1.95	0.48
1:F:139:PRO:O	1:F:141:ASP:N	2.45	0.48
1:G:294:ASN:C	1:G:294:ASN:HD22	2.17	0.48
1:E:221:GLU:CA	5:E:416:HOH:O	2.49	0.48
1:E:145:TYR:CD1	1:E:329:PHE:HE2	2.31	0.48
1:G:240:ILE:HG22	1:G:244:LYS:CD	2.43	0.48
1:D:39:LEU:CD2	1:D:44:ILE:HB	2.44	0.48
1:H:16:LYS:O	1:H:77:ASP:OD2	2.30	0.48
1:C:90:ASP:HB3	1:C:295:ARG:NH2	2.29	0.48
1:F:112:LYS:CE	1:F:112:LYS:HA	2.41	0.48
1:F:161:SER:O	1:F:162:GLY:C	2.51	0.48
1:C:26:ILE:HA	1:C:51:ILE:O	2.12	0.48
1:A:236:ALA:O	1:A:240:ILE:HG13	2.12	0.48
1:F:262:ILE:O	1:F:264:HIS:N	2.46	0.48
1:B:212:ARG:HH11	1:B:226:LEU:HD12	1.78	0.48
1:D:117:PHE:O	1:D:121:VAL:HG23	2.13	0.48
1:A:67:HIS:CE1	1:D:240:ILE:HD11	2.49	0.48
1:B:23:VAL:HG13	1:B:91:LEU:HD23	1.94	0.48
1:C:264:HIS:ND1	1:D:74:LYS:HD3	2.28	0.48
1:D:15:MET:O	1:D:47:GLU:OE2	2.32	0.48
1:G:24:VAL:CG2	1:G:89:ALA:HB2	2.44	0.48
1:A:100:GLN:CG	1:A:105:THR:O	2.61	0.48
1:A:106:ARG:O	1:A:109:LEU:CG	2.59	0.48
1:B:166:ASP:OD2	1:B:197:GLU:OE1	2.32	0.48
1:H:278:GLY:N	1:H:282:GLU:O	2.44	0.48
1:H:164:ILE:HD12	1:H:258:VAL:CG2	2.43	0.48
1:G:141:ASP:HB3	1:G:286:TYR:O	2.13	0.48
1:F:182:PRO:HB2	1:G:70:VAL:CG1	2.43	0.48
1:D:165:LEU:C	1:D:165:LEU:HD12	2.31	0.48
1:D:293:ILE:CD1	1:D:298:ILE:HD13	2.43	0.48
1:A:122:GLU:O	1:A:126:ALA:HB2	2.14	0.48
1:C:26:ILE:HG12	1:C:51:ILE:HD12	1.94	0.48
1:A:241:ILE:O	1:A:245:GLY:HA2	2.13	0.48
1:E:175:GLY:O	1:E:179:SER:N	2.47	0.48
1:C:174:LEU:CD2	1:C:229:ILE:HD13	2.41	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:PRO:HG3	1:E:304:ILE:HG23	1.95	0.48
1:D:204:ALA:O	5:D:403:HOH:O	2.20	0.48
1:G:134:LEU:HA	1:G:159:ILE:O	2.13	0.48
1:G:26:ILE:HG21	1:G:120:ILE:HG21	1.95	0.48
1:G:260:ARG:HB3	1:G:260:ARG:HE	1.51	0.48
1:G:90:ASP:O	1:G:131:GLY:HA3	2.13	0.48
1:H:218:LYS:HB3	1:H:218:LYS:HE2	1.55	0.48
1:B:215:VAL:CB	1:B:222:ALA:CB	2.82	0.48
1:F:142:ILE:CD1	1:F:321:LEU:HD22	2.44	0.48
1:F:118:ARG:NE	1:F:330:THR:OG1	2.47	0.48
1:E:162:GLY:C	5:E:377:HOH:O	2.51	0.48
1:F:235:ASP:O	1:F:239:GLN:HG3	2.13	0.48
1:G:19:GLY:N	5:G:433:HOH:O	2.47	0.48
1:H:58:ALA:HB1	1:H:80:HIS:HD2	1.79	0.48
1:D:280:TYR:OH	1:D:303:GLU:HA	2.14	0.48
1:F:39:LEU:CD2	1:F:44:ILE:HD12	2.42	0.48
1:B:124:VAL:CG2	1:B:129:PHE:CB	2.92	0.48
1:G:307:ASN:O	1:G:311:LYS:HG3	2.13	0.48
1:G:167:THR:O	1:G:171:ARG:HG3	2.14	0.48
1:B:322:LYS:HE3	5:B:408:HOH:O	2.13	0.48
1:F:67:HIS:CD2	1:G:169:ARG:HG2	2.49	0.48
1:A:161:SER:OG	5:A:382:HOH:O	2.15	0.48
1:F:295:ARG:O	1:F:295:ARG:NH1	2.46	0.48
1:G:47:GLU:HB3	1:G:79:TRP:CH2	2.49	0.48
1:A:209:MET:CG	1:A:214:LEU:CD2	2.91	0.48
1:F:15:MET:HB2	1:F:19:GLY:N	2.28	0.48
1:C:15:MET:O	1:C:47:GLU:HG3	2.14	0.48
1:H:276:LEU:CD2	1:H:279:LEU:CB	2.92	0.48
1:H:144:THR:HG21	1:H:286:TYR:CD2	2.48	0.48
1:G:145:TYR:HE1	1:G:329:PHE:HE2	1.57	0.48
1:D:54:ASN:ND2	1:D:56:SER:HB2	2.27	0.48
1:F:146:ALA:CB	1:F:329:PHE:CZ	2.97	0.48
1:E:223:GLN:OE1	1:E:223:GLN:HA	2.10	0.48
1:B:138:ASN:HB2	4:B:352:NAD:HO2N	1.72	0.48
1:B:265:ASN:HA	1:B:295:ARG:H	1.79	0.47
1:C:220:GLU:O	1:C:221:GLU:C	2.52	0.47
1:E:193:HIS:HB2	5:E:377:HOH:O	2.13	0.47
1:C:16:LYS:NZ	1:D:264:HIS:CB	2.74	0.47
1:H:191:GLY:HA2	1:H:287:ILE:HD11	1.96	0.47
1:C:226:LEU:O	1:C:229:ILE:HB	2.13	0.47
1:H:228:ARG:C	1:H:228:ARG:HH11	2.17	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:PHE:HB3	1:E:78:ILE:HD13	1.96	0.47
1:A:122:GLU:O	1:A:126:ALA:CB	2.61	0.47
1:B:124:VAL:HG22	1:B:129:PHE:HB3	1.96	0.47
1:B:169:ARG:HG2	1:C:67:HIS:CG	2.49	0.47
1:G:44:ILE:HG22	1:G:263:LEU:HD12	1.97	0.47
1:C:257:ARG:O	1:C:260:ARG:HB2	2.14	0.47
1:B:118:ARG:NH2	1:B:330:THR:HG21	2.30	0.47
1:H:243:LYS:HB2	1:H:243:LYS:HZ2	1.77	0.47
1:A:125:MET:SD	1:A:153:LEU:HD11	2.54	0.47
1:A:41:ASN:HB2	1:D:41:ASN:HB3	1.96	0.47
1:D:198:LEU:HA	1:D:199:PRO:HD3	1.79	0.47
1:H:136:ALA:O	4:H:352:NAD:H2N	2.14	0.47
1:D:260:ARG:HD3	1:D:260:ARG:HH11	1.44	0.47
1:D:130:GLN:O	1:D:157:ARG:NH1	2.39	0.47
1:D:36:VAL:HG21	1:D:50:LEU:CD2	2.44	0.47
1:E:208:VAL:CG2	1:G:304:ILE:HG21	2.45	0.47
1:F:87:ARG:HD2	1:F:128:GLY:HA3	1.95	0.47
1:H:175:GLY:CA	1:H:185:VAL:HG21	2.45	0.47
1:G:325:LEU:HD22	1:G:329:PHE:CE2	2.49	0.47
1:A:83:TYR:O	1:A:86:CYS:HB2	2.14	0.47
1:A:198:LEU:HD22	1:A:313:ARG:HB2	1.95	0.47
1:G:159:ILE:HD11	1:G:297:GLY:HA2	1.96	0.47
1:C:324:VAL:O	1:C:328:ALA:N	2.46	0.47
1:A:48:ILE:O	1:A:78:ILE:HA	2.15	0.47
1:A:299:ARG:C	1:A:300:GLU:HG3	2.34	0.47
1:B:272:VAL:O	1:B:288:GLY:HA2	2.14	0.47
1:G:112:LYS:CA	1:G:112:LYS:CE	2.89	0.47
1:B:39:LEU:CD2	1:B:44:ILE:HD12	2.42	0.47
1:D:324:VAL:O	1:D:328:ALA:HB3	2.14	0.47
1:A:41:ASN:CB	1:D:41:ASN:HB3	2.44	0.47
1:D:189:ILE:HA	1:D:198:LEU:O	2.14	0.47
1:H:166:ASP:HB3	1:H:189:ILE:HG21	1.96	0.47
1:C:24:VAL:HG11	1:C:51:ILE:HD11	1.97	0.47
5:A:419:HOH:O	1:B:295:ARG:CD	2.58	0.47
1:F:205:TYR:CE2	1:H:205:TYR:CE2	3.02	0.47
1:B:15:MET:CB	1:B:19:GLY:CA	2.90	0.47
1:D:177:TYR:HD2	1:D:178:PHE:CZ	2.32	0.47
5:G:557:HOH:O	1:H:295:ARG:HG3	2.15	0.47
1:G:52:ASP:HB3	1:G:58:ALA:HB2	1.96	0.47
1:C:177:TYR:CE1	1:C:225:ASP:OD2	2.68	0.47
1:E:322:LYS:O	1:E:325:LEU:HB2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:SER:OG	1:G:310:GLU:OE1	2.32	0.47
1:G:295:ARG:CG	1:H:15:MET:HG3	2.43	0.47
1:H:150:PHE:CZ	1:H:330:THR:HB	2.49	0.47
1:F:87:ARG:CZ	1:F:87:ARG:HB3	2.44	0.47
1:H:65:PHE:O	1:H:67:HIS:N	2.48	0.47
1:H:279:LEU:HD22	5:H:407:HOH:O	2.14	0.47
1:E:55:GLU:O	1:E:59:ILE:HG13	2.15	0.47
1:B:305:GLU:OE1	1:D:213:LYS:HE2	2.15	0.47
1:G:86:CYS:O	1:G:89:ALA:N	2.41	0.47
1:F:200:VAL:HG11	1:F:304:ILE:CD1	2.45	0.47
1:H:313:ARG:O	1:H:314:PHE:C	2.53	0.47
1:C:35:TYR:CE1	1:C:255:LEU:HB3	2.50	0.47
1:B:203:GLN:HG3	1:D:208:VAL:O	2.15	0.47
1:D:170:PHE:CG	1:D:189:ILE:HD11	2.49	0.47
1:G:93:VAL:HG13	1:G:134:LEU:HG	1.96	0.47
1:G:93:VAL:HG13	1:G:134:LEU:O	2.14	0.47
1:E:164:ILE:CD1	1:E:258:VAL:HG23	2.45	0.47
1:G:279:LEU:CD2	1:G:301:VAL:HB	2.45	0.47
1:B:38:ALA:O	1:B:42:GLN:HG3	2.15	0.47
1:B:31:VAL:HG13	1:B:251:ILE:CG2	2.45	0.47
1:A:170:PHE:HE2	1:A:187:ALA:HB1	1.79	0.47
1:H:132:LEU:HD22	5:H:376:HOH:O	2.15	0.47
1:C:231:VAL:O	1:C:235:ASP:HB2	2.14	0.47
1:F:308:ASP:O	1:F:312:ASN:HB2	2.15	0.47
1:E:264:HIS:CA	1:F:16:LYS:HZ3	2.27	0.47
1:A:291:ALA:HB1	1:A:298:ILE:CG2	2.44	0.47
1:B:94:ILE:HG21	1:B:117:PHE:CE2	2.50	0.47
1:D:185:VAL:HG22	1:D:206:ILE:HD12	1.97	0.47
1:D:92:VAL:HG12	1:D:133:PHE:CD1	2.50	0.47
1:B:41:ASN:O	1:B:73:PRO:HG3	2.14	0.47
1:F:212:ARG:NH1	1:F:226:LEU:HD13	2.27	0.47
1:E:15:MET:CB	1:E:19:GLY:CA	2.77	0.47
1:H:215:VAL:CB	1:H:222:ALA:CB	2.69	0.47
1:E:218:LYS:HB3	1:E:218:LYS:HE2	1.55	0.47
1:C:220:GLU:O	1:C:221:GLU:O	2.31	0.47
1:B:16:LYS:HE3	1:B:75:PRO:O	2.15	0.47
5:F:422:HOH:O	1:G:75:PRO:HA	2.15	0.47
1:F:251:ILE:HG13	1:F:255:LEU:HD22	1.97	0.47
1:D:118:ARG:CG	1:D:118:ARG:NH1	2.77	0.47
1:D:145:TYR:CD1	1:D:329:PHE:HE2	2.32	0.47
1:A:327:ARG:NH2	1:A:328:ALA:HB2	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:TYR:CZ	1:G:303:GLU:HA	2.49	0.47
1:B:24:VAL:HB	1:B:92:VAL:HG22	1.95	0.47
1:F:247:THR:HG21	3:F:351:OXM:O3	2.15	0.47
1:F:215:VAL:HA	1:F:218:LYS:HE3	1.97	0.47
1:B:243:LYS:HD3	1:C:59:ILE:CG2	2.45	0.47
1:F:74:LYS:HB2	5:F:361:HOH:O	2.15	0.47
1:C:148:TRP:CZ3	1:C:275:TYR:CE2	3.03	0.47
1:H:248:TYR:C	1:H:251:ILE:HG22	2.35	0.47
1:D:118:ARG:HH11	1:D:118:ARG:HG2	1.80	0.47
1:G:229:ILE:O	1:G:233:VAL:HG23	2.14	0.47
1:A:109:LEU:O	1:A:113:ASN:ND2	2.48	0.46
1:B:110:VAL:HG12	1:B:114:ILE:CD1	2.45	0.46
1:C:15:MET:HA	1:D:265:ASN:CB	2.45	0.46
1:A:107:LEU:CD2	1:A:324:VAL:HG21	2.46	0.46
1:G:240:ILE:HB	1:G:247:THR:HG22	1.98	0.46
1:E:173:LEU:O	5:E:383:HOH:O	2.20	0.46
1:F:58:ALA:HB1	1:F:80:HIS:HD2	1.80	0.46
1:F:237:ALA:O	1:F:241:ILE:HD12	2.15	0.46
1:E:213:LYS:HG2	1:E:213:LYS:O	2.15	0.46
1:G:137:THR:HG22	1:G:143:LEU:HD13	1.96	0.46
1:C:15:MET:N	1:C:20:GLY:CA	2.78	0.46
1:E:109:LEU:CD2	5:E:374:HOH:O	2.62	0.46
1:E:173:LEU:HD12	1:E:233:VAL:HG23	1.97	0.46
1:A:174:LEU:HD23	1:A:229:ILE:HD13	1.97	0.46
1:D:228:ARG:HA	1:D:228:ARG:NH1	2.29	0.46
1:D:16:LYS:CE	1:D:75:PRO:O	2.63	0.46
1:G:24:VAL:HG21	1:G:89:ALA:HB2	1.97	0.46
1:F:18:ASN:N	1:F:47:GLU:OE2	2.47	0.46
1:H:276:LEU:HD22	1:H:279:LEU:CB	2.45	0.46
1:D:26:ILE:HD13	1:D:83:TYR:HE1	1.81	0.46
1:A:167:THR:O	1:A:168:ALA:C	2.53	0.46
1:D:30:PHE:HB3	1:D:248:TYR:CG	2.50	0.46
1:E:189:ILE:CG2	1:E:197:GLU:HB2	2.46	0.46
1:A:67:HIS:HE1	1:D:240:ILE:HD11	1.81	0.46
1:A:206:ILE:HG12	1:A:211:ILE:HG12	1.96	0.46
1:F:15:MET:O	1:F:47:GLU:OE2	2.33	0.46
1:D:136:ALA:O	4:D:352:NAD:H2N	2.16	0.46
1:B:174:LEU:HD23	1:B:229:ILE:HD13	1.96	0.46
1:H:26:ILE:HD11	1:H:92:VAL:HG13	1.97	0.46
1:C:219:GLY:O	1:C:221:GLU:N	2.48	0.46
1:A:83:TYR:HE2	1:A:124:VAL:HG12	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ILE:HG13	1:D:321:LEU:CD1	2.44	0.46
1:F:229:ILE:O	1:F:233:VAL:HG23	2.15	0.46
1:C:250:GLY:CA	5:C:355:HOH:O	2.62	0.46
1:F:21:ALA:HB1	1:F:263:LEU:HD22	1.96	0.46
1:G:262:ILE:O	1:G:265:ASN:N	2.45	0.46
1:A:265:ASN:HA	1:A:295:ARG:H	1.80	0.46
1:E:251:ILE:HD13	5:E:381:HOH:O	2.15	0.46
1:C:16:LYS:HE2	1:D:264:HIS:O	2.14	0.46
1:D:140:VAL:HG21	1:D:162:GLY:H	1.80	0.46
1:E:155:HIS:CD2	1:E:275:TYR:HB3	2.50	0.46
1:C:138:ASN:HB3	1:C:139:PRO:HA	1.96	0.46
1:C:166:ASP:OD2	1:C:193:HIS:ND1	2.37	0.46
1:G:107:LEU:HD23	1:G:107:LEU:N	2.29	0.46
1:H:267:ASN:ND2	1:H:294:ASN:CB	2.75	0.46
1:A:56:SER:HA	1:A:59:ILE:HD12	1.97	0.46
1:C:134:LEU:HA	1:C:159:ILE:O	2.16	0.46
1:B:275:TYR:CZ	1:B:284:ASP:HA	2.50	0.46
1:D:181:ALA:HB3	1:D:184:ASN:OD1	2.16	0.46
1:C:110:VAL:HG13	1:C:142:ILE:HG21	1.97	0.46
1:C:114:ILE:HD11	1:C:142:ILE:CG2	2.46	0.46
1:A:224:LYS:HB3	1:A:224:LYS:HE3	1.82	0.46
1:E:163:THR:HA	1:E:166:ASP:OD1	2.16	0.46
1:F:138:ASN:HA	1:F:140:VAL:N	2.31	0.46
1:B:244:LYS:NZ	1:C:61:ASP:OD1	2.45	0.46
1:A:36:VAL:HG13	1:A:48:ILE:HG21	1.97	0.46
1:H:178:PHE:HZ	1:H:211:ILE:HG23	1.81	0.46
1:B:216:GLU:HA	5:B:400:HOH:O	2.16	0.46
1:C:177:TYR:HE1	1:C:225:ASP:OD2	1.98	0.46
1:D:60:GLY:HA2	1:D:63:MET:HG3	1.97	0.46
1:D:295:ARG:HD3	1:D:295:ARG:C	2.34	0.46
1:D:137:THR:HG23	4:D:352:NAD:O3D	2.16	0.46
1:D:164:ILE:HD13	1:D:258:VAL:HG23	1.96	0.46
1:G:186:HIS:CD2	1:G:207:GLY:O	2.69	0.46
1:F:208:VAL:CG2	1:H:203:GLN:HG3	2.45	0.46
1:C:52:ASP:OD2	1:C:54:ASN:HB3	2.15	0.46
1:E:15:MET:SD	1:E:17:ASN:O	2.73	0.46
1:H:15:MET:HB2	1:H:19:GLY:CA	2.46	0.46
1:F:114:ILE:HG23	1:F:330:THR:HA	1.95	0.46
1:B:59:ILE:N	1:B:59:ILE:CD1	2.79	0.46
1:F:35:TYR:CE2	1:F:93:VAL:HG21	2.50	0.46
1:F:264:HIS:O	1:F:265:ASN:C	2.54	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ASP:OD2	1:H:244:LYS:CE	2.64	0.46
1:A:120:ILE:O	1:A:124:VAL:CG1	2.60	0.46
1:F:157:ARG:HD3	1:F:157:ARG:HH11	1.33	0.46
1:D:270:LEU:HD12	1:D:293:ILE:HG13	1.97	0.46
1:C:120:ILE:O	1:C:124:VAL:CG1	2.64	0.46
1:D:129:PHE:CG	1:D:130:GLN:N	2.83	0.46
1:H:249:TYR:O	1:H:253:MET:HG2	2.16	0.46
1:B:209:MET:HA	1:B:210:PRO:HD3	1.67	0.45
1:C:266:GLU:CG	1:D:75:PRO:HG3	2.47	0.45
1:F:110:VAL:HG21	1:F:324:VAL:CG1	2.46	0.45
1:E:295:ARG:CD	1:F:15:MET:HG3	2.39	0.45
1:D:138:ASN:CB	4:D:352:NAD:O2D	2.53	0.45
1:B:35:TYR:CZ	1:B:93:VAL:HG21	2.51	0.45
1:G:44:ILE:HD13	1:G:260:ARG:HG2	1.98	0.45
1:A:175:GLY:HA2	1:A:185:VAL:HG21	1.97	0.45
1:G:251:ILE:HG13	1:G:255:LEU:HD22	1.97	0.45
1:B:159:ILE:HD12	1:B:262:ILE:HD11	1.98	0.45
1:D:18:ASN:N	1:D:47:GLU:OE2	2.49	0.45
1:G:74:LYS:HB3	1:G:74:LYS:HE3	1.53	0.45
1:C:148:TRP:CE2	1:C:155:HIS:HB3	2.51	0.45
1:A:125:MET:CE	1:A:153:LEU:HD11	2.46	0.45
1:A:123:SER:O	1:A:126:ALA:HB3	2.16	0.45
1:F:208:VAL:HG23	1:F:208:VAL:O	2.15	0.45
1:F:275:TYR:CZ	1:F:284:ASP:HA	2.51	0.45
1:F:177:TYR:CE1	1:F:225:ASP:HB3	2.52	0.45
1:D:265:ASN:HD22	1:D:295:ARG:CB	2.24	0.45
1:C:99:ASN:HA	5:C:373:HOH:O	2.16	0.45
1:C:120:ILE:O	1:C:124:VAL:HG13	2.17	0.45
1:A:304:ILE:CB	1:C:209:MET:HE1	2.46	0.45
1:H:230:PHE:O	1:H:233:VAL:HB	2.17	0.45
1:H:149:LYS:HA	1:H:149:LYS:CE	2.45	0.45
1:A:327:ARG:HH21	1:A:328:ALA:HB2	1.81	0.45
1:C:164:ILE:HD12	1:C:258:VAL:HG23	1.97	0.45
1:E:244:LYS:HD2	1:H:60:GLY:CA	2.45	0.45
1:E:69:LYS:O	1:E:70:VAL:C	2.53	0.45
1:C:180:VAL:HG21	1:C:206:ILE:CG2	2.43	0.45
1:A:149:LYS:HE3	1:A:149:LYS:HA	1.98	0.45
1:B:299:ARG:CZ	1:B:300:GLU:OE2	2.64	0.45
1:A:175:GLY:CA	1:A:185:VAL:HG21	2.46	0.45
1:F:165:LEU:HA	5:F:424:HOH:O	2.15	0.45
1:C:276:LEU:HD11	1:C:287:ILE:CG2	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:GLN:O	1:E:243:LYS:HD2	2.16	0.45
1:A:37:PHE:HD1	1:A:37:PHE:HA	1.62	0.45
1:A:15:MET:HG3	1:B:295:ARG:HD3	1.98	0.45
1:H:112:LYS:CE	1:H:112:LYS:HA	2.47	0.45
1:F:16:LYS:HE3	1:F:46:ASP:HA	1.99	0.45
1:D:113:ASN:CB	1:D:143:LEU:HD11	2.47	0.45
1:A:304:ILE:HG22	1:C:209:MET:HE3	1.98	0.45
1:H:145:TYR:O	1:H:148:TRP:HB3	2.17	0.45
1:A:279:LEU:HB2	5:A:399:HOH:O	2.16	0.45
1:G:153:LEU:HB3	1:G:154:PRO:CD	2.46	0.45
1:G:180:VAL:HG23	1:G:181:ALA:O	2.17	0.45
1:F:101:LYS:O	1:F:104:GLU:HB2	2.16	0.45
1:C:15:MET:C	1:C:17:ASN:H	2.00	0.45
1:H:313:ARG:HA	1:H:316:HIS:HB3	1.98	0.45
1:H:313:ARG:HH11	1:H:313:ARG:HD2	1.43	0.45
1:A:151:SER:OG	1:A:153:LEU:HD12	2.16	0.45
1:C:101:LYS:HB2	1:C:104:GLU:OE1	2.17	0.45
1:G:36:VAL:HG21	1:G:50:LEU:CD2	2.46	0.45
1:C:299:ARG:O	1:C:300:GLU:HG3	2.16	0.45
1:D:220:GLU:HA	1:D:223:GLN:CB	2.36	0.45
1:A:196:THR:OG1	1:A:317:SER:CB	2.65	0.45
1:C:213:LYS:HA	1:C:216:GLU:HB3	1.99	0.45
1:E:142:ILE:CD1	1:E:142:ILE:N	2.78	0.45
1:A:244:LYS:O	1:A:244:LYS:HG2	2.17	0.45
1:D:138:ASN:HA	1:D:140:VAL:N	2.32	0.45
1:H:274:ALA:HB1	1:H:301:VAL:CG2	2.46	0.45
1:H:278:GLY:CA	1:H:282:GLU:O	2.65	0.45
1:C:189:ILE:CD1	1:C:230:PHE:HE1	2.19	0.45
1:A:110:VAL:HB	1:A:111:ASP:H	1.68	0.45
1:E:40:MET:HE2	1:E:72:ALA:HB2	1.98	0.45
1:B:57:LYS:NZ	1:B:61:ASP:OD2	2.49	0.45
1:E:290:PRO:HG3	1:E:304:ILE:HG21	1.99	0.45
1:F:148:TRP:HB2	1:F:158:VAL:CG2	2.46	0.45
1:B:240:ILE:O	1:B:241:ILE:C	2.54	0.45
1:F:22:ARG:HE	1:F:22:ARG:HB2	1.57	0.45
1:A:15:MET:CB	1:A:19:GLY:CA	2.62	0.45
1:F:159:ILE:HD12	1:F:262:ILE:HD11	1.99	0.45
1:C:264:HIS:O	1:D:16:LYS:HD3	2.16	0.45
1:E:208:VAL:HG22	1:G:188:TYR:CE2	2.52	0.45
1:C:15:MET:C	1:C:17:ASN:N	2.57	0.45
1:D:264:HIS:O	1:D:265:ASN:C	2.55	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:VAL:O	1:C:114:ILE:HG12	2.17	0.45
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.71	0.45
1:H:189:ILE:CD1	1:H:230:PHE:CE1	2.99	0.45
1:B:35:TYR:O	1:B:38:ALA:HB3	2.17	0.45
1:E:180:VAL:O	1:E:181:ALA:C	2.54	0.45
1:A:16:LYS:HE3	1:A:46:ASP:CB	2.47	0.45
1:C:257:ARG:NH1	1:C:257:ARG:O	2.49	0.45
1:F:329:PHE:CD1	1:F:329:PHE:C	2.89	0.45
1:A:265:ASN:HD22	1:A:265:ASN:HA	1.61	0.45
1:E:264:HIS:CA	1:F:16:LYS:NZ	2.80	0.45
1:G:74:LYS:HD2	1:G:75:PRO:CD	2.34	0.45
1:H:319:ALA:O	1:H:320:THR:C	2.54	0.45
1:A:107:LEU:HA	1:A:139:PRO:CG	2.46	0.45
1:B:243:LYS:HD2	1:C:59:ILE:HG22	1.98	0.45
1:G:291:ALA:HB1	1:G:298:ILE:CG2	2.44	0.45
1:A:242:GLU:O	1:A:242:GLU:HG3	2.17	0.45
1:B:49:VAL:HG22	1:B:79:TRP:CZ2	2.52	0.45
1:A:15:MET:CB	1:A:19:GLY:N	2.75	0.44
1:E:200:VAL:O	1:E:200:VAL:HG12	2.17	0.44
1:C:15:MET:N	1:C:20:GLY:N	2.65	0.44
1:H:27:GLY:O	1:H:32:GLY:HA3	2.16	0.44
1:H:280:TYR:HB3	1:H:314:PHE:CE2	2.52	0.44
1:B:30:PHE:N	4:B:352:NAD:O2N	2.49	0.44
1:E:280:TYR:OH	1:E:304:ILE:HG12	2.16	0.44
1:D:187:ALA:HB2	1:D:204:ALA:HB1	1.98	0.44
1:E:134:LEU:HD13	1:E:258:VAL:HG11	1.99	0.44
1:D:129:PHE:CE1	1:D:131:GLY:N	2.71	0.44
1:H:173:LEU:O	1:H:176:GLU:N	2.49	0.44
1:A:16:LYS:HA	1:A:16:LYS:HD3	1.42	0.44
1:D:221:GLU:OE1	5:D:425:HOH:O	2.20	0.44
1:G:220:GLU:N	1:G:223:GLN:HB2	2.32	0.44
1:F:145:TYR:CD1	1:F:145:TYR:C	2.90	0.44
1:A:264:HIS:HA	1:B:16:LYS:HZ3	1.81	0.44
1:F:16:LYS:HE2	1:F:75:PRO:O	2.18	0.44
1:A:132:LEU:N	1:A:132:LEU:CD2	2.80	0.44
1:F:139:PRO:O	1:F:140:VAL:C	2.56	0.44
1:D:170:PHE:CG	1:D:189:ILE:CD1	3.00	0.44
1:F:266:GLU:O	1:F:267:ASN:HB2	2.17	0.44
1:F:171:ARG:O	1:F:175:GLY:N	2.49	0.44
1:H:133:PHE:CD1	1:H:153:LEU:HD11	2.53	0.44
1:D:153:LEU:HB3	1:D:154:PRO:CD	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PHE:HB3	1:C:248:TYR:CG	2.52	0.44
1:H:112:LYS:CE	1:H:112:LYS:CA	2.95	0.44
1:B:100:GLN:HA	1:B:109:LEU:HD21	1.99	0.44
1:G:107:LEU:HD21	1:G:192:GLU:OE2	2.18	0.44
1:D:116:ILE:CG2	1:D:120:ILE:HD11	2.47	0.44
1:D:269:ILE:HG21	1:D:302:ILE:HD12	2.00	0.44
1:B:165:LEU:HD22	1:B:251:ILE:CA	2.47	0.44
1:D:235:ASP:O	1:D:236:ALA:C	2.56	0.44
1:A:80:HIS:NE2	5:A:359:HOH:O	2.19	0.44
1:A:90:ASP:HA	5:A:367:HOH:O	2.18	0.44
1:G:86:CYS:CB	1:G:124:VAL:HG23	2.47	0.44
1:C:16:LYS:HZ3	1:D:264:HIS:CA	2.31	0.44
1:A:54:ASN:ND2	1:A:54:ASN:O	2.49	0.44
1:A:160:GLY:HA3	1:A:273:SER:CB	2.48	0.44
1:H:165:LEU:HD12	1:H:165:LEU:O	2.17	0.44
1:G:66:ASN:ND2	5:G:442:HOH:O	2.50	0.44
1:E:92:VAL:HG23	1:E:129:PHE:CE1	2.53	0.44
1:H:159:ILE:HG12	1:H:298:ILE:HD12	1.99	0.44
1:F:148:TRP:CB	1:F:158:VAL:HG21	2.47	0.44
1:F:169:ARG:HD3	1:F:236:ALA:CB	2.47	0.44
1:D:100:GLN:NE2	1:D:241:ILE:HD11	2.33	0.44
1:G:16:LYS:HZ1	1:H:264:HIS:CA	2.29	0.44
1:E:240:ILE:HG23	1:E:244:LYS:HD3	1.99	0.44
1:E:67:HIS:CG	1:H:169:ARG:HG2	2.51	0.44
1:E:70:VAL:HG21	1:H:171:ARG:HB2	1.99	0.44
1:H:298:ILE:HG22	1:H:300:GLU:N	2.32	0.44
1:F:148:TRP:HA	1:F:158:VAL:HG21	1.99	0.44
1:C:209:MET:HG3	1:C:214:LEU:HD21	1.99	0.44
1:E:276:LEU:HA	1:E:276:LEU:HD23	1.80	0.44
1:G:280:TYR:CE1	1:G:289:VAL:CG2	3.00	0.44
1:A:171:ARG:HD2	1:A:185:VAL:O	2.17	0.44
1:A:206:ILE:CG1	1:A:211:ILE:CD1	2.96	0.44
1:A:52:ASP:OD2	4:A:352:NAD:H1B	2.17	0.44
1:A:215:VAL:HB	1:A:222:ALA:CB	2.47	0.44
1:D:274:ALA:HB1	1:D:301:VAL:HG22	2.00	0.44
1:D:274:ALA:HB3	1:D:289:VAL:HG12	2.00	0.44
1:D:280:TYR:CE1	1:D:289:VAL:HG21	2.53	0.44
1:H:189:ILE:HD13	1:H:230:PHE:CE1	2.50	0.44
1:H:248:TYR:HA	1:H:251:ILE:CG2	2.48	0.44
1:E:167:THR:O	1:E:171:ARG:HG3	2.17	0.44
1:H:155:HIS:CD2	1:H:275:TYR:HB3	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.67	0.44
1:G:218:LYS:HG3	1:G:222:ALA:CB	2.39	0.44
1:G:18:ASN:N	1:G:47:GLU:OE2	2.51	0.44
1:E:261:ALA:HA	1:E:266:GLU:HB2	2.00	0.44
1:E:209:MET:HA	1:E:210:PRO:HD3	1.86	0.44
1:C:15:MET:CG	1:C:19:GLY:CA	2.94	0.44
1:B:100:GLN:HE21	3:B:351:OXM:HN1	1.64	0.44
1:E:220:GLU:HA	1:E:223:GLN:CB	2.35	0.44
1:B:64:ASP:HB2	1:C:244:LYS:HE2	2.00	0.44
1:E:205:TYR:CZ	1:G:205:TYR:CE2	3.06	0.44
1:G:186:HIS:HB2	1:G:205:TYR:HB2	2.00	0.44
1:B:282:GLU:HG3	1:B:318:ALA:HB1	2.00	0.44
1:E:113:ASN:HB3	1:E:143:LEU:HD11	2.00	0.44
1:D:227:GLU:O	1:D:231:VAL:HG23	2.18	0.44
1:A:100:GLN:CB	1:A:109:LEU:HD11	2.47	0.44
1:F:94:ILE:HG21	1:F:117:PHE:CE2	2.52	0.44
1:B:19:GLY:N	5:B:357:HOH:O	2.51	0.44
1:G:70:VAL:HG22	5:G:440:HOH:O	2.17	0.44
1:G:299:ARG:CZ	1:G:300:GLU:OE2	2.66	0.44
1:A:56:SER:CA	1:A:59:ILE:HD12	2.48	0.44
1:E:21:ALA:HB1	1:E:263:LEU:HD13	2.00	0.44
1:D:275:TYR:HB2	1:D:286:TYR:CE1	2.53	0.44
1:C:267:ASN:HD22	1:C:292:VAL:HG12	1.83	0.44
1:H:16:LYS:O	1:H:77:ASP:CG	2.56	0.43
1:D:15:MET:N	1:D:20:GLY:HA3	2.32	0.43
1:F:110:VAL:O	1:F:114:ILE:HB	2.18	0.43
1:C:221:GLU:HB3	1:C:224:LYS:N	2.26	0.43
1:A:265:ASN:OD1	1:B:17:ASN:HB2	2.17	0.43
1:E:209:MET:HG2	1:G:304:ILE:HG22	2.00	0.43
1:B:25:VAL:HG21	1:B:36:VAL:CG2	2.48	0.43
1:G:145:TYR:HD1	1:G:329:PHE:CZ	2.36	0.43
1:F:172:PHE:CE2	1:F:173:LEU:HD23	2.53	0.43
1:H:325:LEU:HD23	1:H:325:LEU:HA	1.76	0.43
1:E:166:ASP:OD2	1:E:197:GLU:OE1	2.36	0.43
1:C:309:ASP:O	1:C:313:ARG:HG2	2.16	0.43
1:E:89:ALA:O	1:E:129:PHE:HE1	2.01	0.43
1:E:304:ILE:HG13	1:E:306:LEU:HD23	1.98	0.43
1:D:216:GLU:CD	1:G:327:ARG:HB2	2.38	0.43
1:H:201:TRP:HZ3	1:H:211:ILE:HD13	1.83	0.43
1:D:329:PHE:HD1	1:D:330:THR:H	1.65	0.43
1:D:124:VAL:O	1:D:127:SER:OG	2.20	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:SER:HA	1:G:287:ILE:O	2.18	0.43
1:A:272:VAL:O	1:A:288:GLY:HA2	2.18	0.43
1:F:279:LEU:HD12	1:F:279:LEU:HA	1.77	0.43
1:D:221:GLU:O	1:D:225:ASP:HB2	2.18	0.43
1:F:313:ARG:CG	1:F:313:ARG:NH1	2.68	0.43
1:B:101:LYS:CB	1:B:102:PRO:CD	2.92	0.43
1:A:220:GLU:CA	1:A:223:GLN:HB2	2.46	0.43
1:H:23:VAL:O	1:H:48:ILE:HA	2.19	0.43
1:E:75:PRO:CA	5:H:356:HOH:O	2.60	0.43
1:E:57:LYS:NZ	1:E:61:ASP:OD2	2.39	0.43
1:E:173:LEU:CB	1:E:229:ILE:HG23	2.48	0.43
1:B:92:VAL:HG12	1:B:133:PHE:CE1	2.53	0.43
1:H:96:ALA:O	1:H:137:THR:CG2	2.66	0.43
1:G:215:VAL:CG2	1:G:222:ALA:CB	2.96	0.43
1:D:18:ASN:N	1:D:18:ASN:OD1	2.50	0.43
1:H:118:ARG:HD2	1:H:330:THR:HG1	1.79	0.43
1:E:264:HIS:O	1:F:16:LYS:HD3	2.18	0.43
1:C:15:MET:CE	1:D:265:ASN:ND2	2.81	0.43
1:E:106:ARG:NH1	1:E:194:GLY:HA2	2.34	0.43
1:F:244:LYS:HE3	1:G:64:ASP:OD2	2.17	0.43
1:D:170:PHE:CD2	1:D:189:ILE:HD11	2.52	0.43
1:B:117:PHE:O	1:B:121:VAL:HB	2.18	0.43
1:C:299:ARG:HG2	1:C:300:GLU:HG3	1.99	0.43
1:G:219:GLY:C	1:G:221:GLU:N	2.69	0.43
1:A:265:ASN:CB	1:B:15:MET:HA	2.32	0.43
1:H:121:VAL:O	1:H:124:VAL:HG13	2.18	0.43
1:G:40:MET:HE3	1:G:69:LYS:CA	2.48	0.43
1:A:246:ALA:O	1:A:248:TYR:CD1	2.71	0.43
1:B:299:ARG:C	1:B:300:GLU:HG3	2.38	0.43
1:B:241:ILE:O	1:B:245:GLY:N	2.52	0.43
1:B:280:TYR:CZ	1:B:303:GLU:HA	2.54	0.43
1:D:299:ARG:C	1:D:300:GLU:HG3	2.37	0.43
1:C:117:PHE:HE2	1:C:135:VAL:HG13	1.83	0.43
1:F:31:VAL:HG23	4:F:352:NAD:PN	2.58	0.43
1:C:328:ALA:HB1	5:C:408:HOH:O	2.18	0.43
1:D:132:LEU:HD22	1:D:132:LEU:N	2.34	0.43
1:H:148:TRP:CD1	1:H:153:LEU:O	2.72	0.43
1:A:258:VAL:O	1:A:259:THR:C	2.56	0.43
1:C:112:LYS:HB2	5:C:377:HOH:O	2.18	0.43
1:B:309:ASP:O	1:B:313:ARG:HG3	2.17	0.43
1:B:145:TYR:CD1	1:B:145:TYR:C	2.92	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASN:HB2	1:D:143:LEU:HD11	2.01	0.43
1:H:314:PHE:O	1:H:317:SER:N	2.52	0.43
1:E:70:VAL:HG11	1:H:171:ARG:CZ	2.48	0.43
1:F:209:MET:HE1	1:H:304:ILE:HA	2.01	0.43
1:G:145:TYR:HA	1:G:286:TYR:CE1	2.53	0.43
1:A:218:LYS:HE2	1:A:218:LYS:HB3	1.85	0.43
1:B:203:GLN:NE2	1:B:305:GLU:O	2.52	0.43
1:H:46:ASP:C	1:H:47:GLU:HG3	2.38	0.43
1:B:124:VAL:HG23	1:B:129:PHE:HB2	2.00	0.43
1:A:137:THR:HB	1:A:143:LEU:CD1	2.48	0.43
1:D:57:LYS:NZ	1:D:61:ASP:OD2	2.41	0.43
1:D:237:ALA:HB2	3:D:351:OXM:C2	2.48	0.43
1:A:16:LYS:HZ3	1:B:264:HIS:HB3	1.83	0.43
1:E:294:ASN:ND2	1:E:295:ARG:N	2.65	0.43
1:E:52:ASP:OD1	4:E:352:NAD:H1B	2.18	0.43
1:H:279:LEU:HD12	1:H:279:LEU:HA	1.86	0.43
1:A:221:GLU:O	1:A:222:ALA:C	2.57	0.43
1:D:275:TYR:HB2	1:D:286:TYR:CD1	2.54	0.43
1:A:289:VAL:HA	1:A:290:PRO:HD2	1.91	0.43
1:E:292:VAL:N	1:E:300:GLU:O	2.50	0.43
1:G:23:VAL:O	1:G:48:ILE:HA	2.19	0.43
1:F:91:LEU:HD11	1:F:134:LEU:HB3	2.01	0.43
1:H:213:LYS:C	1:H:216:GLU:HB3	2.39	0.43
1:G:106:ARG:HG2	1:G:138:ASN:CG	2.39	0.43
1:H:280:TYR:CZ	1:H:303:GLU:HA	2.53	0.43
1:D:318:ALA:O	1:D:322:LYS:CG	2.56	0.43
1:B:177:TYR:CZ	1:B:225:ASP:HB3	2.54	0.43
1:B:182:PRO:C	1:B:184:ASN:N	2.72	0.43
1:B:168:ALA:HA	1:C:70:VAL:HG21	2.01	0.43
1:G:174:LEU:HB3	1:G:185:VAL:HG11	2.01	0.43
1:G:128:GLY:O	1:G:130:GLN:HG2	2.18	0.43
1:E:276:LEU:O	1:E:284:ASP:N	2.51	0.43
1:D:279:LEU:HD22	5:D:407:HOH:O	2.18	0.43
1:F:67:HIS:CG	1:G:169:ARG:HG2	2.54	0.43
1:F:177:TYR:HD2	1:F:178:PHE:CE2	2.37	0.43
1:H:28:ALA:N	1:H:52:ASP:OD2	2.49	0.43
1:E:212:ARG:O	1:E:213:LYS:CB	2.67	0.43
1:A:209:MET:HG2	1:A:214:LEU:HD21	2.01	0.43
1:C:290:PRO:HG3	1:C:304:ILE:HG21	2.01	0.43
1:H:327:ARG:NH2	1:H:328:ALA:HB2	2.33	0.43
1:E:240:ILE:CG1	1:H:63:MET:CE	2.91	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:HD11	1:D:134:LEU:HB2	2.01	0.43
1:A:83:TYR:CD2	1:A:124:VAL:HG12	2.54	0.43
1:G:15:MET:N	1:G:20:GLY:HA3	2.34	0.43
1:A:133:PHE:HE1	1:A:153:LEU:CD1	2.32	0.43
1:A:55:GLU:O	1:A:59:ILE:CD1	2.66	0.43
1:A:304:ILE:HA	1:C:209:MET:CE	2.48	0.43
1:A:253:MET:HB3	1:A:253:MET:HE3	1.76	0.43
1:B:265:ASN:HB2	1:B:295:ARG:HG2	2.00	0.43
1:H:15:MET:SD	1:H:17:ASN:O	2.77	0.43
1:E:212:ARG:O	1:E:213:LYS:HB2	2.19	0.43
1:E:218:LYS:O	1:E:219:GLY:O	2.36	0.43
1:A:209:MET:SD	1:A:213:LYS:CE	3.07	0.43
1:F:189:ILE:CD1	1:F:199:PRO:HA	2.48	0.43
1:A:264:HIS:CB	1:B:16:LYS:HZ1	2.24	0.43
1:C:275:TYR:CZ	1:C:284:ASP:HA	2.53	0.43
1:F:29:GLY:HA2	5:F:408:HOH:O	2.19	0.43
1:D:274:ALA:HB1	1:D:301:VAL:CG2	2.49	0.43
1:B:248:TYR:HA	1:B:251:ILE:CG2	2.49	0.43
1:B:248:TYR:HA	1:B:251:ILE:HG22	2.00	0.43
1:E:35:TYR:HA	1:E:252:ALA:HB1	2.00	0.43
1:B:213:LYS:HG2	1:B:214:LEU:HG	2.00	0.42
1:B:182:PRO:C	1:B:184:ASN:H	2.23	0.42
1:G:309:ASP:OD2	1:G:313:ARG:HD2	2.18	0.42
1:D:39:LEU:HD22	1:D:44:ILE:CB	2.49	0.42
1:B:251:ILE:O	1:B:255:LEU:HD22	2.19	0.42
1:A:141:ASP:OD1	1:A:273:SER:OG	2.30	0.42
1:A:15:MET:HB2	1:A:19:GLY:C	2.32	0.42
1:B:209:MET:HE3	1:B:209:MET:HB2	1.83	0.42
1:B:211:ILE:O	1:B:215:VAL:HG13	2.19	0.42
1:B:75:PRO:HA	5:B:364:HOH:O	2.19	0.42
1:F:182:PRO:HG3	5:F:390:HOH:O	2.18	0.42
1:B:60:GLY:HA3	1:C:244:LYS:HD2	2.00	0.42
1:A:145:TYR:CE1	1:A:329:PHE:HE2	2.35	0.42
1:H:148:TRP:CA	1:H:158:VAL:HG21	2.49	0.42
1:C:170:PHE:CE2	1:C:187:ALA:HB1	2.55	0.42
1:F:202:SER:HB3	1:F:310:GLU:OE2	2.19	0.42
1:G:125:MET:HE3	1:G:125:MET:HA	2.00	0.42
1:G:121:VAL:HA	1:G:124:VAL:HG12	2.01	0.42
1:B:87:ARG:CZ	1:B:87:ARG:CB	2.97	0.42
1:D:294:ASN:HD21	1:D:296:ASN:HB2	1.84	0.42
1:A:180:VAL:CG1	1:C:269:ILE:HD11	2.46	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:VAL:CG2	1:E:129:PHE:CZ	3.01	0.42
1:C:116:ILE:CG2	1:C:120:ILE:CD1	2.96	0.42
1:C:311:LYS:HA	5:C:402:HOH:O	2.19	0.42
1:A:16:LYS:NZ	1:B:264:HIS:HB3	2.34	0.42
1:B:210:PRO:O	1:B:213:LYS:HB3	2.20	0.42
1:F:198:LEU:HA	1:F:199:PRO:HD3	1.84	0.42
1:H:318:ALA:O	1:H:322:LYS:HG3	2.18	0.42
1:D:260:ARG:O	1:D:261:ALA:C	2.57	0.42
1:F:106:ARG:O	1:F:109:LEU:HD12	2.19	0.42
1:C:200:VAL:HG13	1:C:306:LEU:HD22	2.01	0.42
1:A:295:ARG:HH11	1:A:295:ARG:HG2	1.85	0.42
1:F:221:GLU:O	1:F:222:ALA:C	2.56	0.42
1:H:279:LEU:O	1:H:303:GLU:HG3	2.20	0.42
1:A:29:GLY:HA3	4:A:352:NAD:O5B	2.19	0.42
1:A:212:ARG:HH11	1:A:226:LEU:CD1	2.30	0.42
1:C:156:GLU:O	1:C:297:GLY:HA3	2.19	0.42
1:A:243:LYS:CD	1:D:59:ILE:HG22	2.49	0.42
1:A:271:THR:HG22	1:A:290:PRO:HD3	2.01	0.42
1:G:165:LEU:HD12	1:G:165:LEU:O	2.20	0.42
1:G:83:TYR:C	1:G:85:ASP:N	2.71	0.42
1:H:118:ARG:HA	1:H:150:PHE:CD2	2.54	0.42
1:H:113:ASN:C	1:H:115:ALA:N	2.72	0.42
1:H:124:VAL:O	1:H:127:SER:N	2.44	0.42
1:H:279:LEU:O	1:H:303:GLU:OE2	2.38	0.42
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.50	0.42
1:D:93:VAL:HA	1:D:134:LEU:O	2.19	0.42
1:D:164:ILE:HD13	1:D:258:VAL:CG2	2.49	0.42
1:E:24:VAL:HG11	1:E:86:CYS:SG	2.60	0.42
1:A:148:TRP:CD1	1:A:153:LEU:O	2.73	0.42
1:C:292:VAL:CG2	1:C:302:ILE:HD11	2.49	0.42
1:A:62:ALA:O	1:A:66:ASN:ND2	2.52	0.42
1:F:159:ILE:CD1	1:F:262:ILE:HD11	2.50	0.42
1:B:102:PRO:C	1:B:104:GLU:H	2.23	0.42
1:F:209:MET:HE3	1:H:304:ILE:HA	2.00	0.42
1:A:223:GLN:HG2	5:A:397:HOH:O	2.19	0.42
1:E:106:ARG:O	1:E:109:LEU:HD12	2.20	0.42
1:C:148:TRP:CD1	1:C:155:HIS:HA	2.55	0.42
1:C:275:TYR:HB2	1:C:286:TYR:CZ	2.55	0.42
1:F:140:VAL:O	1:F:144:THR:OG1	2.22	0.42
1:A:169:ARG:NH1	5:A:386:HOH:O	2.53	0.42
1:H:204:ALA:HB3	1:H:211:ILE:HD12	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:CD	5:D:363:HOH:O	2.57	0.42
1:H:124:VAL:HG22	1:H:125:MET:N	2.34	0.42
1:E:40:MET:HE3	1:E:72:ALA:HB2	2.01	0.42
1:B:203:GLN:NE2	1:D:209:MET:HE1	2.35	0.42
1:H:265:ASN:HB2	1:H:295:ARG:HB2	2.01	0.42
1:F:139:PRO:CD	1:F:143:LEU:HD12	2.49	0.42
1:E:145:TYR:O	1:E:148:TRP:HB3	2.20	0.42
1:C:279:LEU:HD12	1:C:279:LEU:HA	1.62	0.42
1:C:324:VAL:HG13	1:C:327:ARG:HH11	1.83	0.42
1:A:279:LEU:HD12	1:A:279:LEU:HA	1.29	0.42
1:C:280:TYR:CB	1:C:314:PHE:CE2	3.03	0.42
1:F:200:VAL:HG11	1:F:304:ILE:HD12	2.02	0.42
1:E:295:ARG:HG3	1:F:15:MET:HG3	2.00	0.42
1:F:217:SER:O	1:F:218:LYS:CB	2.68	0.42
1:D:56:SER:CA	1:D:59:ILE:HD12	2.50	0.42
1:H:148:TRP:CZ3	1:H:275:TYR:CE2	3.08	0.42
1:E:287:ILE:HD12	1:E:318:ALA:HA	2.02	0.42
1:D:215:VAL:HA	1:D:218:LYS:HG2	2.01	0.42
1:E:16:LYS:HB3	1:E:77:ASP:HB2	2.02	0.42
1:G:222:ALA:O	1:G:223:GLN:C	2.58	0.42
1:H:15:MET:C	1:H:17:ASN:H	2.05	0.42
1:A:113:ASN:O	1:A:117:PHE:HD1	2.03	0.42
1:D:107:LEU:HD23	1:D:107:LEU:N	2.35	0.42
1:A:172:PHE:HB2	5:A:422:HOH:O	2.20	0.42
1:G:40:MET:HE3	1:G:69:LYS:CB	2.50	0.42
1:A:248:TYR:HA	1:A:251:ILE:HG22	2.02	0.42
1:E:74:LYS:HE3	1:E:74:LYS:HB3	1.88	0.42
1:E:170:PHE:CE2	1:E:187:ALA:CB	2.99	0.42
1:D:56:SER:N	1:D:59:ILE:HD12	2.35	0.42
1:B:35:TYR:OH	1:B:93:VAL:HG21	2.20	0.42
1:C:24:VAL:HG23	1:C:89:ALA:HB2	2.01	0.42
1:E:153:LEU:HB3	1:E:154:PRO:CD	2.50	0.42
1:E:325:LEU:HD23	1:E:325:LEU:HA	1.81	0.42
1:F:36:VAL:HG13	1:F:48:ILE:HG21	2.02	0.42
1:F:290:PRO:HB2	1:F:302:ILE:HB	2.02	0.41
1:F:112:LYS:HB2	5:F:375:HOH:O	2.20	0.41
1:F:117:PHE:CZ	1:F:137:THR:HB	2.55	0.41
1:F:117:PHE:O	1:F:121:VAL:HG23	2.20	0.41
1:A:181:ALA:HA	1:A:182:PRO:HD3	1.96	0.41
1:E:120:ILE:O	1:E:121:VAL:C	2.58	0.41
1:H:274:ALA:HB1	1:H:301:VAL:HG21	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:HA	4:A:352:NAD:H3D	2.01	0.41
1:G:325:LEU:HA	1:G:325:LEU:HD23	1.63	0.41
1:D:293:ILE:HD13	1:D:298:ILE:HD13	2.02	0.41
1:E:74:LYS:HD2	1:E:75:PRO:CD	2.46	0.41
1:E:89:ALA:O	1:E:129:PHE:CE1	2.73	0.41
1:B:258:VAL:O	1:B:259:THR:C	2.58	0.41
1:B:287:ILE:HD13	1:B:287:ILE:HG21	1.85	0.41
1:C:323:SER:O	1:C:327:ARG:N	2.53	0.41
1:E:164:ILE:HD12	1:E:258:VAL:CG2	2.48	0.41
1:C:36:VAL:HG21	1:C:50:LEU:CD2	2.48	0.41
1:E:205:TYR:O	1:E:206:ILE:CD1	2.67	0.41
1:D:206:ILE:HD11	1:D:211:ILE:HD11	2.02	0.41
1:H:26:ILE:HD11	1:H:92:VAL:CG1	2.50	0.41
1:E:142:ILE:CD1	1:E:321:LEU:HD22	2.50	0.41
1:A:40:MET:HE1	1:A:69:LYS:HA	2.02	0.41
1:G:209:MET:HE3	1:G:209:MET:HB2	1.77	0.41
1:G:209:MET:O	1:G:214:LEU:HD11	2.20	0.41
1:H:111:ASP:O	1:H:112:LYS:C	2.58	0.41
1:C:114:ILE:HD11	1:C:142:ILE:HG23	2.03	0.41
1:A:72:ALA:HB1	1:A:73:PRO:HD2	2.01	0.41
4:H:352:NAD:H6N	5:H:377:HOH:O	2.19	0.41
1:D:118:ARG:O	1:D:122:GLU:HG3	2.19	0.41
1:E:139:PRO:HG2	1:E:142:ILE:HB	2.02	0.41
1:E:157:ARG:HD3	1:E:157:ARG:HH11	1.63	0.41
1:H:219:GLY:C	1:H:221:GLU:H	2.24	0.41
1:C:280:TYR:HB3	1:C:314:PHE:CE2	2.54	0.41
1:D:162:GLY:O	1:D:193:HIS:HB2	2.20	0.41
1:B:25:VAL:HG21	1:B:36:VAL:HG23	2.02	0.41
1:F:138:ASN:HB2	4:F:352:NAD:O2D	2.20	0.41
1:B:182:PRO:HB2	1:C:70:VAL:CG1	2.51	0.41
1:B:59:ILE:CB	1:C:243:LYS:HD3	2.50	0.41
1:C:87:ARG:CZ	1:C:87:ARG:HB2	2.50	0.41
1:D:98:ALA:O	1:D:109:LEU:HD13	2.20	0.41
1:D:196:THR:HB	1:D:317:SER:CB	2.50	0.41
1:A:164:ILE:HG12	1:A:164:ILE:O	2.20	0.41
1:H:223:GLN:HG2	5:H:405:HOH:O	2.20	0.41
1:F:198:LEU:HB2	1:F:313:ARG:CD	2.49	0.41
1:G:31:VAL:HG21	4:G:352:NAD:C6N	2.51	0.41
1:E:162:GLY:HA2	5:E:377:HOH:O	2.19	0.41
1:C:137:THR:HG22	1:C:138:ASN:N	2.34	0.41
1:A:192:GLU:H	1:A:317:SER:HG	1.68	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLU:HA	5:C:382:HOH:O	2.19	0.41
1:E:57:LYS:HG2	5:E:408:HOH:O	2.20	0.41
1:B:240:ILE:CG2	1:B:244:LYS:HD2	2.50	0.41
1:F:201:TRP:HZ3	1:F:211:ILE:HD13	1.86	0.41
1:H:16:LYS:CB	1:H:77:ASP:OD1	2.68	0.41
1:E:251:ILE:O	1:E:255:LEU:HB2	2.21	0.41
1:H:317:SER:O	1:H:320:THR:HB	2.20	0.41
1:G:145:TYR:HE1	1:G:329:PHE:CE2	2.34	0.41
1:A:116:ILE:HG23	1:A:120:ILE:HD11	2.01	0.41
1:A:317:SER:O	1:A:320:THR:HB	2.20	0.41
1:B:203:GLN:O	1:B:205:TYR:CE2	2.74	0.41
1:A:50:LEU:C	1:A:51:ILE:HG13	2.41	0.41
1:C:24:VAL:HG22	1:C:49:VAL:HB	2.02	0.41
1:H:173:LEU:O	1:H:174:LEU:C	2.59	0.41
1:D:93:VAL:HG13	1:D:134:LEU:HG	2.01	0.41
1:F:172:PHE:CE2	1:F:173:LEU:CD2	3.04	0.41
1:G:15:MET:HG2	1:H:265:ASN:HB2	2.01	0.41
1:E:132:LEU:H	1:E:132:LEU:CD2	2.32	0.41
1:C:262:ILE:HG22	1:C:263:LEU:N	2.35	0.41
1:G:216:GLU:HG3	1:G:217:SER:N	2.35	0.41
1:E:193:HIS:CE1	3:E:351:OXM:O2	2.73	0.41
1:H:313:ARG:HB3	1:H:313:ARG:HE	1.51	0.41
1:D:247:THR:C	1:D:248:TYR:CD1	2.94	0.41
1:H:325:LEU:O	1:H:326:ALA:C	2.58	0.41
1:B:172:PHE:CE1	1:C:69:LYS:NZ	2.85	0.41
1:A:129:PHE:HE2	1:A:133:PHE:CE1	2.38	0.41
1:D:55:GLU:O	1:D:59:ILE:CG1	2.69	0.41
1:B:173:LEU:HD12	1:B:233:VAL:HG23	2.03	0.41
1:H:308:ASP:OD1	1:H:311:LYS:HD2	2.21	0.41
1:G:174:LEU:CB	1:G:185:VAL:HG11	2.50	0.41
1:H:148:TRP:CH2	1:H:275:TYR:CE2	3.09	0.41
1:F:230:PHE:O	1:F:233:VAL:HB	2.21	0.41
1:C:165:LEU:O	1:C:169:ARG:HG3	2.21	0.41
1:G:144:THR:OG1	1:G:160:GLY:HA3	2.21	0.41
1:A:15:MET:CE	1:B:296:ASN:OD1	2.68	0.41
1:E:118:ARG:HG2	1:E:150:PHE:CE2	2.56	0.41
1:G:171:ARG:HD2	1:G:185:VAL:O	2.20	0.41
1:A:279:LEU:O	1:A:303:GLU:OE2	2.39	0.41
1:B:277:ASP:HA	1:B:283:ARG:HB3	2.01	0.41
1:C:165:LEU:HD21	1:C:169:ARG:NH2	2.35	0.41
1:H:181:ALA:HB3	1:H:184:ASN:OD1	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ILE:HD13	1:E:262:ILE:HG21	1.87	0.41
1:G:220:GLU:OE1	1:G:224:LYS:HD3	2.21	0.41
1:D:15:MET:HG3	1:D:19:GLY:CA	2.51	0.41
1:G:83:TYR:O	1:G:86:CYS:N	2.41	0.41
1:G:92:VAL:HG12	1:G:133:PHE:CD1	2.55	0.41
1:H:74:LYS:CG	1:H:75:PRO:HD2	2.51	0.41
1:H:125:MET:HA	1:H:125:MET:HE3	2.02	0.41
1:H:124:VAL:HG23	1:H:129:PHE:CD2	2.56	0.41
1:B:138:ASN:HA	1:B:140:VAL:N	2.36	0.41
1:G:172:PHE:HA	1:G:182:PRO:HB3	2.02	0.41
1:E:69:LYS:O	1:E:71:PHE:N	2.54	0.41
1:B:54:ASN:HD21	1:B:57:LYS:H	1.67	0.41
1:C:81:GLY:HA3	1:C:85:ASP:OD2	2.21	0.41
1:G:316:HIS:O	1:G:319:ALA:HB3	2.20	0.41
1:A:248:TYR:HA	1:A:251:ILE:CG2	2.51	0.41
1:A:212:ARG:HH12	1:A:226:LEU:HB2	1.81	0.41
1:A:63:MET:CE	1:D:243:LYS:CD	2.98	0.41
1:F:257:ARG:NH1	1:F:266:GLU:OE2	2.47	0.41
1:H:54:ASN:HD21	1:H:56:SER:HB2	1.86	0.41
1:H:241:ILE:HG23	1:H:245:GLY:O	2.21	0.41
1:G:35:TYR:CD1	1:G:255:LEU:HB3	2.56	0.41
1:A:76:VAL:HB	5:A:357:HOH:O	2.21	0.41
1:D:16:LYS:HE2	1:D:75:PRO:O	2.21	0.41
1:B:203:GLN:NE2	1:D:209:MET:CE	2.84	0.41
1:B:172:PHE:HA	1:B:182:PRO:HB3	2.03	0.41
1:C:40:MET:HG3	1:C:76:VAL:HG11	2.03	0.41
1:G:328:ALA:HB1	5:G:490:HOH:O	2.21	0.41
1:C:279:LEU:CD2	1:C:301:VAL:HB	2.46	0.41
1:G:230:PHE:CG	1:G:230:PHE:O	2.74	0.41
1:F:201:TRP:C	1:F:203:GLN:N	2.75	0.40
1:D:16:LYS:O	1:D:47:GLU:HG2	2.21	0.40
1:F:77:ASP:HB3	1:F:79:TRP:CZ3	2.53	0.40
1:H:72:ALA:C	1:H:74:LYS:N	2.75	0.40
1:E:29:GLY:HA3	4:E:352:NAD:PA	2.60	0.40
1:C:213:LYS:HA	1:C:216:GLU:HB2	2.02	0.40
1:G:38:ALA:O	1:G:42:GLN:HG3	2.21	0.40
1:G:264:HIS:HB3	1:H:16:LYS:CE	2.51	0.40
1:A:100:GLN:CA	1:A:109:LEU:HD21	2.52	0.40
1:F:110:VAL:HG13	1:F:142:ILE:HG21	2.03	0.40
1:E:265:ASN:CB	1:F:16:LYS:H	2.29	0.40
1:H:36:VAL:HG11	1:H:65:PHE:CE2	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD22	1:A:324:VAL:HG21	2.02	0.40
1:F:31:VAL:HG23	4:F:352:NAD:O5D	2.21	0.40
1:E:280:TYR:HE1	1:E:302:ILE:O	2.02	0.40
1:C:116:ILE:HG23	1:C:120:ILE:CD1	2.52	0.40
1:G:309:ASP:OD1	1:G:313:ARG:NH1	2.54	0.40
1:E:160:GLY:HA3	1:E:273:SER:HB2	2.03	0.40
1:H:306:LEU:C	1:H:307:ASN:O	2.58	0.40
1:F:109:LEU:HD23	5:F:376:HOH:O	2.20	0.40
1:D:58:ALA:HB1	1:D:80:HIS:CD2	2.56	0.40
1:G:16:LYS:HA	1:G:47:GLU:HG2	2.02	0.40
1:B:18:ASN:N	1:B:47:GLU:OE2	2.54	0.40
1:B:279:LEU:HA	1:B:279:LEU:HD12	1.64	0.40
1:F:154:PRO:HA	5:F:381:HOH:O	2.21	0.40
1:B:294:ASN:C	1:B:294:ASN:ND2	2.72	0.40
1:E:203:GLN:HG3	1:G:208:VAL:HB	2.04	0.40
1:H:16:LYS:HB2	1:H:77:ASP:OD1	2.21	0.40
1:B:15:MET:O	1:B:47:GLU:OE2	2.40	0.40
1:H:280:TYR:OH	1:H:303:GLU:HA	2.22	0.40
1:D:26:ILE:HD13	1:D:83:TYR:CE1	2.56	0.40
1:A:142:ILE:HG13	1:A:324:VAL:HG11	2.03	0.40
1:B:169:ARG:O	1:B:173:LEU:HG	2.21	0.40
1:D:145:TYR:HD2	1:D:286:TYR:HD1	1.69	0.40
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.57	0.40
1:G:230:PHE:CD1	1:G:230:PHE:O	2.75	0.40
1:F:41:ASN:O	1:F:73:PRO:HG3	2.20	0.40
1:H:198:LEU:HA	1:H:199:PRO:HD3	1.93	0.40
1:C:251:ILE:HA	1:C:251:ILE:HD12	1.74	0.40
1:C:264:HIS:O	1:C:265:ASN:C	2.59	0.40
1:A:100:GLN:HG3	1:A:105:THR:O	2.21	0.40
1:F:114:ILE:HG21	1:F:330:THR:CA	2.50	0.40
1:F:142:ILE:O	1:F:145:TYR:HB3	2.21	0.40
1:E:94:ILE:CG2	1:E:117:PHE:CE2	3.03	0.40
1:C:15:MET:HE2	1:D:265:ASN:ND2	2.37	0.40
1:A:237:ALA:HA	1:A:247:THR:HG21	2.04	0.40
1:A:247:THR:OG1	3:A:351:OXM:N1	2.54	0.40
1:D:280:TYR:HB3	1:D:314:PHE:CE2	2.57	0.40
1:G:156:GLU:O	1:G:297:GLY:HA3	2.21	0.40
1:D:125:MET:O	1:D:126:ALA:C	2.59	0.40
1:B:263:LEU:HA	1:B:263:LEU:HD23	1.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASN:OD1	5:B:384:HOH:O[2_645]	2.13	0.07
1:C:312:ASN:ND2	5:B:384:HOH:O[2_645]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/316 (99%)	255 (81%)	48 (15%)	11 (4%)	4	6
1	B	314/316 (99%)	266 (85%)	40 (13%)	8 (2%)	7	10
1	C	314/316 (99%)	273 (87%)	30 (10%)	11 (4%)	4	6
1	D	314/316 (99%)	273 (87%)	35 (11%)	6 (2%)	10	16
1	E	314/316 (99%)	271 (86%)	34 (11%)	9 (3%)	6	8
1	F	314/316 (99%)	268 (85%)	38 (12%)	8 (2%)	7	10
1	G	314/316 (99%)	269 (86%)	35 (11%)	10 (3%)	5	6
1	H	314/316 (99%)	258 (82%)	48 (15%)	8 (2%)	7	10
All	All	2512/2528 (99%)	2133 (85%)	308 (12%)	71 (3%)	6	9

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	B	110	VAL
1	C	213	LYS
1	C	220	GLU
1	C	221	GLU
1	E	213	LYS
1	E	220	GLU
1	F	140	VAL
1	F	213	LYS
1	F	218	LYS
1	G	213	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	219	GLY
1	G	220	GLU
1	G	262	ILE
1	G	263	LEU
1	H	213	LYS
1	A	110	VAL
1	A	295	ARG
1	B	162	GLY
1	B	213	LYS
1	B	219	GLY
1	D	87	ARG
1	D	213	LYS
1	D	248	TYR
1	E	110	VAL
1	E	219	GLY
1	F	248	TYR
1	F	263	LEU
1	G	110	VAL
1	H	66	ASN
1	H	265	ASN
1	A	140	VAL
1	A	218	LYS
1	A	219	GLY
1	A	248	TYR
1	B	248	TYR
1	C	55	GLU
1	C	140	VAL
1	C	183	GLN
1	D	19	GLY
1	E	248	TYR
1	H	219	GLY
1	H	325	LEU
1	A	19	GLY
1	B	295	ARG
1	C	19	GLY
1	C	248	TYR
1	E	19	GLY
1	E	87	ARG
1	G	197	GLU
1	G	265	ASN
1	H	223	GLN
1	A	112	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	328	ALA
1	C	149	LYS
1	D	221	GLU
1	E	121	VAL
1	F	219	GLY
1	H	112	LYS
1	A	217	SER
1	B	19	GLY
1	C	262	ILE
1	D	219	GLY
1	G	19	GLY
1	H	120	ILE
1	F	139	PRO
1	F	262	ILE
1	A	162	GLY
1	E	262	ILE
1	G	233	VAL
1	C	110	VAL

### 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	254/254 (100%)	213 (84%)	41 (16%)	3	5
1	B	254/254 (100%)	208 (82%)	46 (18%)	2	3
1	C	254/254 (100%)	219 (86%)	35 (14%)	4	8
1	D	254/254 (100%)	213 (84%)	41 (16%)	3	5
1	E	254/254 (100%)	210 (83%)	44 (17%)	2	4
1	F	254/254 (100%)	217 (85%)	37 (15%)	4	7
1	G	254/254 (100%)	214 (84%)	40 (16%)	3	5
1	H	254/254 (100%)	213 (84%)	41 (16%)	3	5
All	All	2032/2032 (100%)	1707 (84%)	325 (16%)	3	5

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	ASN
1	A	40	MET
1	A	54	ASN
1	A	56	SER
1	A	63	MET
1	A	70	VAL
1	A	77	ASP
1	A	95	CYS
1	A	100	GLN
1	A	105	THR
1	A	106	ARG
1	A	107	LEU
1	A	110	VAL
1	A	111	ASP
1	A	114	ILE
1	A	118	ARG
1	A	119	SER
1	A	132	LEU
1	A	134	LEU
1	A	149	LYS
1	A	153	LEU
1	A	179	SER
1	A	180	VAL
1	A	198	LEU
1	A	203	GLN
1	A	211	ILE
1	A	213	LYS
1	A	218	LYS
1	A	228	ARG
1	A	244	LYS
1	A	255	LEU
1	A	260	ARG
1	A	265	ASN
1	A	273	SER
1	A	294	ASN
1	A	300	GLU
1	A	312	ASN
1	A	327	ARG
1	A	329	PHE
1	A	330	THR
1	B	17	ASN
1	B	54	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	55	GLU
1	B	59	ILE
1	B	63	MET
1	B	74	LYS
1	B	77	ASP
1	B	87	ARG
1	B	92	VAL
1	B	100	GLN
1	B	105	THR
1	B	118	ARG
1	B	119	SER
1	B	122	GLU
1	B	124	VAL
1	B	132	LEU
1	B	139	PRO
1	B	149	LYS
1	B	179	SER
1	B	198	LEU
1	B	203	GLN
1	B	209	MET
1	B	213	LYS
1	B	215	VAL
1	B	217	SER
1	B	218	LYS
1	B	223	GLN
1	B	227	GLU
1	B	228	ARG
1	B	243	LYS
1	B	244	LYS
1	B	247	THR
1	B	255	LEU
1	B	260	ARG
1	B	279	LEU
1	B	282	GLU
1	B	283	ARG
1	B	286	TYR
1	B	289	VAL
1	B	294	ASN
1	B	295	ARG
1	B	298	ILE
1	B	300	GLU
1	B	312	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	327	ARG
1	B	330	THR
1	C	16	LYS
1	C	18	ASN
1	C	51	ILE
1	C	54	ASN
1	C	69	LYS
1	C	70	VAL
1	C	77	ASP
1	C	100	GLN
1	C	107	LEU
1	C	112	LYS
1	C	118	ARG
1	C	119	SER
1	C	124	VAL
1	C	127	SER
1	C	149	LYS
1	C	164	ILE
1	C	171	ARG
1	C	198	LEU
1	C	203	GLN
1	C	211	ILE
1	C	213	LYS
1	C	216	GLU
1	C	224	LYS
1	C	227	GLU
1	C	228	ARG
1	C	243	LYS
1	C	244	LYS
1	C	247	THR
1	C	255	LEU
1	C	283	ARG
1	C	294	ASN
1	C	295	ARG
1	C	300	GLU
1	C	313	ARG
1	C	329	PHE
1	D	17	ASN
1	D	18	ASN
1	D	22	ARG
1	D	70	VAL
1	D	77	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	87	ARG
1	D	92	VAL
1	D	100	GLN
1	D	114	ILE
1	D	118	ARG
1	D	124	VAL
1	D	132	LEU
1	D	134	LEU
1	D	142	ILE
1	D	165	LEU
1	D	189	ILE
1	D	196	THR
1	D	198	LEU
1	D	203	GLN
1	D	209	MET
1	D	213	LYS
1	D	216	GLU
1	D	218	LYS
1	D	220	GLU
1	D	227	GLU
1	D	228	ARG
1	D	243	LYS
1	D	244	LYS
1	D	260	ARG
1	D	273	SER
1	D	275	TYR
1	D	279	LEU
1	D	287	ILE
1	D	294	ASN
1	D	295	ARG
1	D	300	GLU
1	D	313	ARG
1	D	323	SER
1	D	327	ARG
1	D	329	PHE
1	D	330	THR
1	E	16	LYS
1	E	17	ASN
1	E	18	ASN
1	E	26	ILE
1	E	54	ASN
1	E	56	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	74	LYS
1	E	77	ASP
1	E	85	ASP
1	E	100	GLN
1	E	101	LYS
1	E	105	THR
1	E	111	ASP
1	E	114	ILE
1	E	118	ARG
1	E	123	SER
1	E	125	MET
1	E	127	SER
1	E	132	LEU
1	E	142	ILE
1	E	149	LYS
1	E	164	ILE
1	E	174	LEU
1	E	179	SER
1	E	198	LEU
1	E	203	GLN
1	E	216	GLU
1	E	218	LYS
1	E	224	LYS
1	E	227	GLU
1	E	228	ARG
1	E	243	LYS
1	E	247	THR
1	E	273	SER
1	E	283	ARG
1	E	289	VAL
1	E	294	ASN
1	E	295	ARG
1	E	300	GLU
1	E	312	ASN
1	E	313	ARG
1	E	323	SER
1	E	329	PHE
1	E	330	THR
1	F	54	ASN
1	F	70	VAL
1	F	77	ASP
1	F	111	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	112	LYS
1	F	114	ILE
1	F	118	ARG
1	F	124	VAL
1	F	130	GLN
1	F	132	LEU
1	F	148	TRP
1	F	149	LYS
1	F	157	ARG
1	F	164	ILE
1	F	171	ARG
1	F	198	LEU
1	F	203	GLN
1	F	212	ARG
1	F	213	LYS
1	F	216	GLU
1	F	217	SER
1	F	218	LYS
1	F	223	GLN
1	F	227	GLU
1	F	228	ARG
1	F	243	LYS
1	F	244	LYS
1	F	255	LEU
1	F	260	ARG
1	F	273	SER
1	F	289	VAL
1	F	294	ASN
1	F	295	ARG
1	F	300	GLU
1	F	312	ASN
1	F	327	ARG
1	F	329	PHE
1	G	16	LYS
1	G	17	ASN
1	G	18	ASN
1	G	22	ARG
1	G	39	LEU
1	G	54	ASN
1	G	70	VAL
1	G	74	LYS
1	G	77	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	100	GLN
1	G	101	LYS
1	G	109	LEU
1	G	111	ASP
1	G	112	LYS
1	G	116	ILE
1	G	119	SER
1	G	130	GLN
1	G	132	LEU
1	G	149	LYS
1	G	159	ILE
1	G	190	ILE
1	G	203	GLN
1	G	209	MET
1	G	213	LYS
1	G	227	GLU
1	G	228	ARG
1	G	240	ILE
1	G	244	LYS
1	G	247	THR
1	G	248	TYR
1	G	255	LEU
1	G	269	ILE
1	G	294	ASN
1	G	295	ARG
1	G	298	ILE
1	G	300	GLU
1	G	312	ASN
1	G	313	ARG
1	G	327	ARG
1	G	329	PHE
1	H	16	LYS
1	H	17	ASN
1	H	54	ASN
1	H	70	VAL
1	H	74	LYS
1	H	77	ASP
1	H	100	GLN
1	H	112	LYS
1	H	118	ARG
1	H	119	SER
1	H	124	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	127	SER
1	H	130	GLN
1	H	132	LEU
1	H	149	LYS
1	H	161	SER
1	H	164	ILE
1	H	189	ILE
1	H	198	LEU
1	H	203	GLN
1	H	205	TYR
1	H	216	GLU
1	H	218	LYS
1	H	224	LYS
1	H	227	GLU
1	H	228	ARG
1	H	241	ILE
1	H	243	LYS
1	H	244	LYS
1	H	247	THR
1	H	251	ILE
1	H	260	ARG
1	H	283	ARG
1	H	294	ASN
1	H	295	ARG
1	H	302	ILE
1	H	312	ASN
1	H	313	ARG
1	H	327	ARG
1	H	329	PHE
1	H	330	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	223	GLN
1	A	267	ASN
1	A	294	ASN
1	A	316	HIS
1	B	54	ASN
1	B	130	GLN
1	B	203	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	316	HIS
1	C	54	ASN
1	C	138	ASN
1	C	264	HIS
1	C	267	ASN
1	C	294	ASN
1	D	17	ASN
1	D	54	ASN
1	D	138	ASN
1	D	155	HIS
1	D	203	GLN
1	D	267	ASN
1	D	294	ASN
1	D	316	HIS
1	E	54	ASN
1	E	138	ASN
1	E	155	HIS
1	E	203	GLN
1	E	267	ASN
1	E	294	ASN
1	F	41	ASN
1	F	54	ASN
1	F	138	ASN
1	F	203	GLN
1	F	223	GLN
1	F	267	ASN
1	F	294	ASN
1	G	54	ASN
1	G	138	ASN
1	G	203	GLN
1	G	223	GLN
1	G	264	HIS
1	G	267	ASN
1	G	294	ASN
1	G	316	HIS
1	H	41	ASN
1	H	54	ASN
1	H	138	ASN
1	H	155	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	H	267	ASN
1	H	294	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 ⓘ

24 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$
3	OXM	A	351	-	2,5,5	0.32	0	2,6,6	2.21	1 (50%)
4	NAD	A	352	-	38,48,48	1.16	5 (13%)	47,73,73	2.19	15 (31%)
2	FBP	A	353[A]	-	18,20,20	0.78	0	21,32,32	0.95	1 (4%)
2	FBP	A	353[C]	-	18,20,20	0.78	0	21,32,32	0.99	1 (4%)
3	OXM	B	351	-	2,5,5	0.68	0	2,6,6	0.93	0
4	NAD	B	352	-	38,48,48	1.18	4 (10%)	47,73,73	2.05	12 (25%)
2	FBP	B	353[B]	-	18,20,20	0.79	0	21,32,32	0.99	1 (4%)
2	FBP	B	353[D]	-	18,20,20	0.78	0	21,32,32	0.99	1 (4%)
3	OXM	C	351	-	2,5,5	0.59	0	2,6,6	0.66	0
4	NAD	C	352	-	38,48,48	1.14	2 (5%)	47,73,73	2.45	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OXM	D	351	-	2,5,5	0.24	0	2,6,6	1.23	0
4	NAD	D	352	-	38,48,48	0.95	3 (7%)	47,73,73	2.18	13 (27%)
3	OXM	E	351	-	2,5,5	0.43	0	2,6,6	3.94	2 (100%)
4	NAD	E	352	-	38,48,48	1.06	4 (10%)	47,73,73	1.86	9 (19%)
2	FBP	E	353[E]	-	18,20,20	0.78	0	21,32,32	0.99	1 (4%)
2	FBP	E	353[G]	-	18,20,20	0.79	0	21,32,32	0.99	1 (4%)
3	OXM	F	351	-	2,5,5	0.38	0	2,6,6	1.96	1 (50%)
4	NAD	F	352	-	38,48,48	1.23	4 (10%)	47,73,73	2.42	12 (25%)
2	FBP	F	353[F]	-	18,20,20	0.77	0	21,32,32	0.99	1 (4%)
2	FBP	F	353[H]	-	18,20,20	0.78	0	21,32,32	0.99	1 (4%)
3	OXM	G	351	-	2,5,5	0.41	0	2,6,6	3.27	1 (50%)
4	NAD	G	352	-	38,48,48	0.96	1 (2%)	47,73,73	2.23	11 (23%)
3	OXM	H	351	-	2,5,5	0.21	0	2,6,6	3.32	2 (100%)
4	NAD	H	352	-	38,48,48	1.23	4 (10%)	47,73,73	2.70	15 (31%)

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
3	OXM	A	351	-	-	0/0/4/4	0/0/0/0
4	NAD	A	352	-	-	0/22/62/62	0/5/5/5
2	FBP	A	353[A]	-	-	0/13/32/32	0/1/1/1
2	FBP	A	353[C]	-	-	0/13/32/32	0/1/1/1
3	OXM	B	351	-	-	0/0/4/4	0/0/0/0
4	NAD	B	352	-	-	0/22/62/62	0/5/5/5
2	FBP	B	353[B]	-	-	0/13/32/32	0/1/1/1
2	FBP	B	353[D]	-	-	0/13/32/32	0/1/1/1
3	OXM	C	351	-	-	0/0/4/4	0/0/0/0
4	NAD	C	352	-	-	0/22/62/62	0/5/5/5
3	OXM	D	351	-	-	0/0/4/4	0/0/0/0
4	NAD	D	352	-	-	0/22/62/62	0/5/5/5
3	OXM	E	351	-	-	0/0/4/4	0/0/0/0
4	NAD	E	352	-	-	0/22/62/62	0/5/5/5
2	FBP	E	353[E]	-	-	0/13/32/32	0/1/1/1
2	FBP	E	353[G]	-	-	0/13/32/32	0/1/1/1
3	OXM	F	351	-	-	0/0/4/4	0/0/0/0
4	NAD	F	352	-	-	0/22/62/62	0/5/5/5
2	FBP	F	353[F]	-	-	0/13/32/32	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	F	353[H]	-	-	0/13/32/32	0/1/1/1
3	OXM	G	351	-	-	0/0/4/4	0/0/0/0
4	NAD	G	352	-	-	0/22/62/62	0/5/5/5
3	OXM	H	351	-	-	0/0/4/4	0/0/0/0
4	NAD	H	352	-	-	0/22/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	352	NAD	O7N-C7N	-2.84	1.18	1.24
4	E	352	NAD	O4B-C1B	2.01	1.43	1.41
4	F	352	NAD	C6N-N1N	2.03	1.40	1.35
4	D	352	NAD	C6N-N1N	2.05	1.41	1.35
4	E	352	NAD	C2A-N1A	2.06	1.37	1.33
4	D	352	NAD	C2A-N1A	2.08	1.37	1.33
4	F	352	NAD	C4N-C3N	2.10	1.42	1.39
4	H	352	NAD	O4B-C1B	2.13	1.43	1.41
4	A	352	NAD	C2A-N1A	2.18	1.38	1.33
4	E	352	NAD	C6N-N1N	2.20	1.41	1.35
4	C	352	NAD	C6N-N1N	2.21	1.41	1.35
4	B	352	NAD	O4B-C1B	2.31	1.44	1.41
4	H	352	NAD	C6N-N1N	2.33	1.41	1.35
4	A	352	NAD	O4B-C1B	2.35	1.44	1.41
4	A	352	NAD	C6N-N1N	2.37	1.41	1.35
4	A	352	NAD	O4D-C1D	2.39	1.44	1.41
4	B	352	NAD	C6N-N1N	2.55	1.42	1.35
4	B	352	NAD	C2A-N1A	2.63	1.38	1.33
4	G	352	NAD	C3N-C7N	3.36	1.55	1.50
4	D	352	NAD	C3N-C7N	3.72	1.56	1.50
4	H	352	NAD	C3N-C7N	3.73	1.56	1.50
4	A	352	NAD	C3N-C7N	3.74	1.56	1.50
4	H	352	NAD	O7N-C7N	3.77	1.32	1.24
4	E	352	NAD	C3N-C7N	3.79	1.56	1.50
4	B	352	NAD	C3N-C7N	3.81	1.56	1.50
4	C	352	NAD	C3N-C7N	4.04	1.56	1.50
4	F	352	NAD	C3N-C7N	4.29	1.57	1.50

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	352	NAD	O7N-C7N-C3N	-7.90	110.96	119.59
4	A	352	NAD	C5N-C4N-C3N	-6.89	111.67	120.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	352	NAD	C5N-C4N-C3N	-6.86	111.71	120.33
4	H	352	NAD	C3N-C7N-N7N	-6.59	110.61	117.82
4	F	352	NAD	C5N-C4N-C3N	-6.54	112.11	120.33
4	D	352	NAD	C5N-C4N-C3N	-6.20	112.54	120.33
4	G	352	NAD	C4D-O4D-C1D	-5.95	103.19	109.72
4	E	352	NAD	C5N-C4N-C3N	-5.79	113.05	120.33
4	B	352	NAD	C4B-O4B-C1B	-5.74	103.41	109.72
4	G	352	NAD	C5N-C4N-C3N	-5.52	113.40	120.33
4	B	352	NAD	C5N-C4N-C3N	-5.13	113.88	120.33
4	C	352	NAD	C5N-C4N-C3N	-5.05	113.98	120.33
4	G	352	NAD	O4D-C1D-N1N	-4.88	102.77	108.13
4	C	352	NAD	C5N-C6N-N1N	-4.74	112.27	120.47
4	G	352	NAD	PN-O3-PA	-4.67	119.63	132.73
4	H	352	NAD	C4B-O4B-C1B	-4.66	104.59	109.72
4	D	352	NAD	C5N-C6N-N1N	-4.49	112.71	120.47
4	F	352	NAD	C4B-O4B-C1B	-4.34	104.95	109.72
4	A	352	NAD	C3N-C7N-N7N	-4.32	113.09	117.82
3	E	351	OXM	O1-C1-N1	-4.29	116.56	122.59
4	A	352	NAD	C4D-O4D-C1D	-4.26	105.04	109.72
4	D	352	NAD	C3N-C7N-N7N	-4.25	113.17	117.82
4	D	352	NAD	C4D-O4D-C1D	-4.16	105.15	109.72
4	B	352	NAD	C5N-C6N-N1N	-4.13	113.33	120.47
4	G	352	NAD	C5N-C6N-N1N	-3.99	113.58	120.47
4	F	352	NAD	C4N-C3N-C7N	-3.88	110.83	121.09
4	H	352	NAD	C5N-C6N-N1N	-3.86	113.80	120.47
4	H	352	NAD	C4D-O4D-C1D	-3.84	105.50	109.72
4	F	352	NAD	C4D-O4D-C1D	-3.69	105.67	109.72
4	F	352	NAD	C5N-C6N-N1N	-3.63	114.19	120.47
4	E	352	NAD	O4B-C1B-N9A	-3.63	100.50	108.10
4	D	352	NAD	C2B-C1B-N9A	-3.34	109.19	114.29
4	H	352	NAD	O7N-C7N-C3N	-3.33	115.95	119.59
4	E	352	NAD	C5N-C6N-N1N	-3.31	114.75	120.47
3	H	351	OXM	O1-C1-N1	-3.30	117.95	122.59
4	A	352	NAD	C5N-C6N-N1N	-3.29	114.78	120.47
4	C	352	NAD	C4D-O4D-C1D	-3.24	106.16	109.72
4	C	352	NAD	C1B-N9A-C4A	-3.23	122.06	126.94
4	E	352	NAD	C4N-C3N-C7N	-3.23	112.57	121.09
4	F	352	NAD	O7N-C7N-C3N	-3.17	116.13	119.59
4	B	352	NAD	C4N-C3N-C7N	-3.13	112.81	121.09
4	G	352	NAD	O3-PA-O5B	-2.93	95.15	102.94
4	C	352	NAD	PN-O3-PA	-2.93	124.51	132.73
4	A	352	NAD	C1B-N9A-C4A	-2.86	122.62	126.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	352	NAD	C4B-O4B-C1B	-2.84	106.60	109.72
4	B	352	NAD	O7N-C7N-C3N	-2.80	116.53	119.59
4	B	352	NAD	O4D-C1D-N1N	-2.74	105.12	108.13
4	H	352	NAD	O3-PA-O5B	-2.70	95.77	102.94
4	D	352	NAD	C4N-C3N-C7N	-2.63	114.14	121.09
4	B	352	NAD	C4D-O4D-C1D	-2.54	106.93	109.72
4	H	352	NAD	C4N-C3N-C7N	-2.43	114.66	121.09
4	A	352	NAD	C4N-C3N-C7N	-2.40	114.73	121.09
4	A	352	NAD	O4D-C1D-N1N	-2.34	105.56	108.13
4	D	352	NAD	PN-O3-PA	-2.33	126.18	132.73
4	E	352	NAD	O7N-C7N-C3N	-2.31	117.06	119.59
4	H	352	NAD	PN-O3-PA	-2.31	126.25	132.73
4	E	352	NAD	PN-O3-PA	-2.28	126.33	132.73
4	G	352	NAD	O5D-C5D-C4D	-2.27	100.76	109.12
4	C	352	NAD	C4B-O4B-C1B	-2.23	107.27	109.72
4	C	352	NAD	C4N-C3N-C7N	-2.10	115.54	121.09
4	C	352	NAD	O3-PA-O5B	-2.08	97.41	102.94
4	A	352	NAD	O3D-C3D-C4D	-2.03	104.95	111.05
4	F	352	NAD	C1B-N9A-C4A	-2.00	123.92	126.94
4	B	352	NAD	C2N-C3N-C7N	2.02	125.18	119.31
4	A	352	NAD	O3D-C3D-C2D	2.04	118.47	111.83
4	D	352	NAD	O2A-PA-O3	2.12	114.69	105.09
4	D	352	NAD	C4A-C5A-N7A	2.28	111.58	109.48
4	A	352	NAD	O7N-C7N-N7N	2.33	125.87	122.59
4	A	352	NAD	C4A-C5A-N7A	2.37	111.66	109.48
4	F	352	NAD	C2N-C3N-C7N	2.41	126.30	119.31
4	H	352	NAD	O3-PN-O5D	2.41	109.33	102.94
4	H	352	NAD	N3A-C2A-N1A	2.49	130.80	128.89
2	F	353[H]	FBP	O2P-P1-O1P	2.56	118.82	110.58
2	B	353[D]	FBP	O2P-P1-O1P	2.56	118.82	110.58
2	F	353[F]	FBP	O2P-P1-O1P	2.56	118.82	110.58
2	B	353[B]	FBP	O2P-P1-O1P	2.56	118.83	110.58
2	A	353[A]	FBP	O2P-P1-O1P	2.56	118.84	110.58
2	E	353[E]	FBP	O2P-P1-O1P	2.57	118.84	110.58
2	E	353[G]	FBP	O2P-P1-O1P	2.57	118.85	110.58
2	A	353[C]	FBP	O2P-P1-O1P	2.57	118.86	110.58
4	G	352	NAD	C4A-C5A-N7A	2.58	111.85	109.48
4	C	352	NAD	O2A-PA-O3	2.59	116.85	105.09
4	G	352	NAD	O2A-PA-O3	2.60	116.89	105.09
4	D	352	NAD	O7N-C7N-C3N	2.65	122.48	119.59
3	A	351	OXM	O1-C1-N1	2.67	126.36	122.59
3	F	351	OXM	O1-C1-N1	2.72	126.42	122.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	352	NAD	C2B-C1B-N9A	2.73	118.46	114.29
4	E	352	NAD	C2B-C1B-N9A	2.95	118.80	114.29
4	B	352	NAD	N6A-C6A-N1A	2.96	125.55	119.20
4	F	352	NAD	O7N-C7N-N7N	3.33	127.28	122.59
3	H	351	OXM	C2-C1-N1	3.33	121.61	115.90
4	B	352	NAD	C2N-C3N-C4N	3.34	122.01	118.29
4	B	352	NAD	C4A-C5A-N7A	3.36	112.57	109.48
3	E	351	OXM	C2-C1-N1	3.55	121.97	115.90
4	C	352	NAD	O4D-C1D-N1N	3.70	112.20	108.13
4	G	352	NAD	C2N-C3N-C4N	3.74	122.46	118.29
4	E	352	NAD	C2N-C3N-C4N	3.84	122.57	118.29
4	D	352	NAD	O4D-C1D-N1N	3.86	112.38	108.13
4	D	352	NAD	C2N-C3N-C4N	4.04	122.79	118.29
4	H	352	NAD	O4D-C1D-N1N	4.08	112.62	108.13
4	F	352	NAD	C2N-C3N-C4N	4.11	122.86	118.29
3	G	351	OXM	C2-C1-N1	4.41	123.45	115.90
4	A	352	NAD	C2N-C3N-C4N	4.64	123.46	118.29
4	H	352	NAD	C2N-C3N-C4N	5.04	123.91	118.29
4	B	352	NAD	C6N-C5N-C4N	5.32	127.48	119.44
4	E	352	NAD	C6N-C5N-C4N	5.39	127.58	119.44
4	G	352	NAD	C6N-C5N-C4N	5.49	127.74	119.44
4	A	352	NAD	C6N-C5N-C4N	6.03	128.56	119.44
4	F	352	NAD	C6N-C5N-C4N	6.09	128.64	119.44
4	H	352	NAD	C6N-C5N-C4N	6.23	128.85	119.44
4	C	352	NAD	C6N-C5N-C4N	6.33	129.01	119.44
4	D	352	NAD	C6N-C5N-C4N	6.38	129.09	119.44
4	C	352	NAD	O7N-C7N-N7N	6.45	131.67	122.59
4	F	352	NAD	O4D-C1D-N1N	7.18	116.02	108.13
4	H	352	NAD	O7N-C7N-N7N	7.62	133.32	122.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	OXM	2	0
4	A	352	NAD	7	0
3	B	351	OXM	2	0
4	B	352	NAD	9	0
3	C	351	OXM	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	352	NAD	3	0
3	D	351	OXM	1	0
4	D	352	NAD	6	0
3	E	351	OXM	2	0
4	E	352	NAD	9	0
3	F	351	OXM	1	0
4	F	352	NAD	6	0
3	G	351	OXM	1	0
4	G	352	NAD	9	0
4	H	352	NAD	4	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	316/316 (100%)	-0.46	13 (4%) 41 46	9, 25, 44, 56	0
1	B	316/316 (100%)	-0.55	7 (2%) 65 69	10, 23, 39, 56	0
1	C	316/316 (100%)	-0.58	9 (2%) 56 61	8, 23, 39, 51	0
1	D	316/316 (100%)	-0.52	5 (1%) 74 78	9, 24, 42, 50	0
1	E	316/316 (100%)	-0.60	6 (1%) 70 73	10, 26, 41, 51	0
1	F	316/316 (100%)	-0.62	8 (2%) 61 65	9, 23, 40, 54	0
1	G	316/316 (100%)	-0.61	4 (1%) 79 82	12, 24, 40, 53	0
1	H	316/316 (100%)	-0.45	7 (2%) 65 69	13, 25, 43, 52	0
All	All	2528/2528 (100%)	-0.55	59 (2%) 64 67	8, 24, 41, 56	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	MET	8.5
1	H	15	MET	4.8
1	H	18	ASN	4.2
1	H	222	ALA	4.0
1	A	330	THR	3.9
1	A	17	ASN	3.8
1	B	222	ALA	3.7
1	F	222	ALA	3.7
1	H	16	LYS	3.6
1	F	17	ASN	3.5
1	B	15	MET	3.5
1	E	222	ALA	3.4
1	B	16	LYS	3.4
1	B	17	ASN	3.3
1	C	17	ASN	3.3
1	A	16	LYS	3.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	16	LYS	3.2
1	B	18	ASN	3.2
1	A	222	ALA	3.1
1	E	15	MET	3.1
1	A	101	LYS	3.1
1	G	215	VAL	2.9
1	F	18	ASN	2.9
1	C	18	ASN	2.8
1	A	109	LEU	2.8
1	E	17	ASN	2.7
1	H	17	ASN	2.7
1	A	18	ASN	2.6
1	A	328	ALA	2.6
1	C	161	SER	2.5
1	D	18	ASN	2.5
1	B	215	VAL	2.5
1	C	19	GLY	2.4
1	C	103	GLY	2.4
1	F	330	THR	2.4
1	E	219	GLY	2.4
1	F	219	GLY	2.4
1	E	18	ASN	2.3
1	D	330	THR	2.3
1	A	15	MET	2.3
1	D	329	PHE	2.3
1	A	107	LEU	2.3
1	F	15	MET	2.3
1	C	127	SER	2.3
1	A	219	GLY	2.2
1	C	134	LEU	2.2
1	D	163	THR	2.2
1	F	215	VAL	2.2
1	G	103	GLY	2.2
1	B	251	ILE	2.2
1	A	221	GLU	2.2
1	F	16	LYS	2.1
1	G	15	MET	2.1
1	C	16	LYS	2.1
1	H	87	ARG	2.1
1	H	19	GLY	2.1
1	A	215	VAL	2.0
1	G	161	SER	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	255	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FBP	E	353[G]	20/20	0.92	0.19	3.86	22,39,52,52	20
2	FBP	E	353[E]	20/20	0.92	0.19	3.83	23,40,50,52	20
2	FBP	B	353[D]	20/20	0.94	0.16	2.15	24,39,49,52	20
2	FBP	B	353[B]	20/20	0.94	0.16	1.98	25,41,49,53	20
2	FBP	F	353[F]	20/20	0.95	0.13	1.19	22,40,50,54	20
2	FBP	F	353[H]	20/20	0.95	0.13	1.18	24,39,48,50	20
3	OXM	D	351	6/6	0.97	0.18	0.60	28,32,38,45	0
3	OXM	G	351	6/6	0.99	0.13	0.18	15,20,27,34	0
3	OXM	F	351	6/6	0.99	0.13	0.12	18,25,34,35	0
3	OXM	B	351	6/6	0.97	0.12	-0.38	22,32,41,53	0
4	NAD	B	352	44/44	0.97	0.11	-0.42	6,26,43,65	0
2	FBP	A	353[A]	20/20	0.97	0.10	-0.46	24,38,54,57	20
4	NAD	D	352	44/44	0.96	0.12	-0.46	8,27,44,51	0
2	FBP	A	353[C]	20/20	0.97	0.10	-0.46	25,39,52,59	20
3	OXM	A	351	6/6	0.98	0.12	-0.49	20,41,43,68	0
3	OXM	C	351	6/6	0.97	0.11	-0.51	9,23,27,50	0
4	NAD	A	352	44/44	0.98	0.08	-0.86	8,31,48,58	0
4	NAD	E	352	44/44	0.98	0.09	-0.87	7,29,38,52	0
4	NAD	G	352	44/44	0.97	0.10	-0.87	0,25,36,60	0
3	OXM	H	351	6/6	0.99	0.09	-0.89	21,24,32,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAD	C	352	44/44	0.98	0.08	-0.91	5,23,41,48	0
4	NAD	F	352	44/44	0.98	0.07	-1.01	13,27,44,52	0
3	OXM	E	351	6/6	0.99	0.12	-1.10	19,32,42,48	0
4	NAD	H	352	44/44	0.98	0.09	-1.12	14,31,55,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.