Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:04 PM UTC

PDB ID	:	1XFW / pdb_00001xfw
Title	:	Crystal structure of anthrax edema factor (EF) in complex with calmodulin and 3'5' cyclic AMP (cAMP)
Authors	:	Shen, Y.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on	:	2004-09-15
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

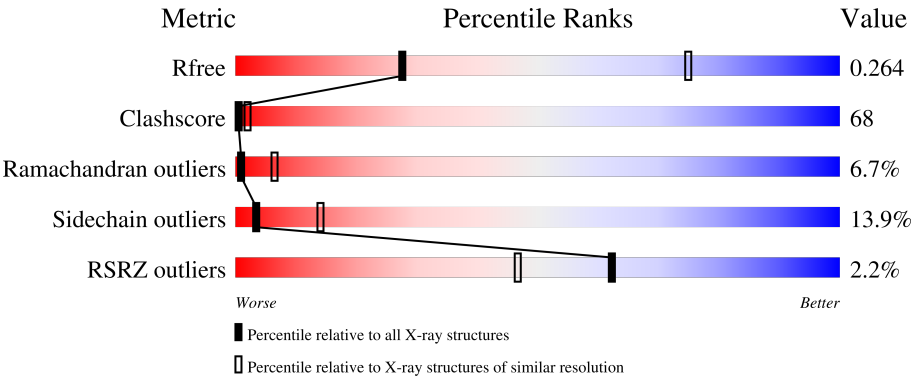
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



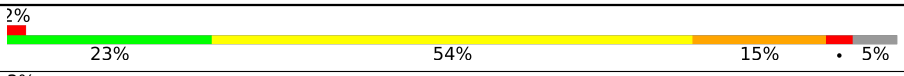
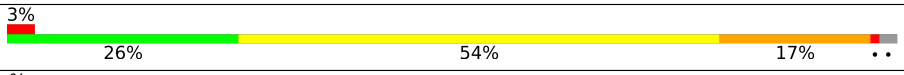
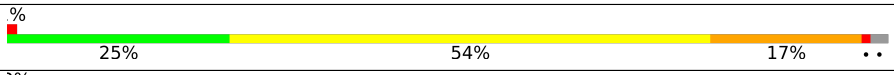
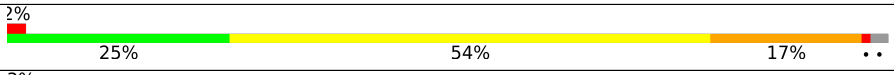
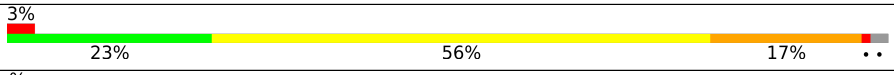
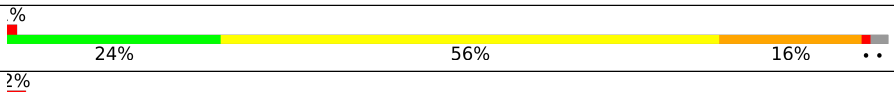
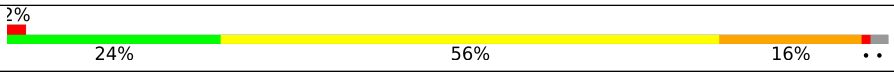
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	777	2% 23% 55% 14% • 5%
1	B	777	2% 23% 54% 15% • 5%
1	C	777	2% 23% 55% 15% • 5%
1	D	777	3% 23% 54% 15% • 5%
1	E	777	2% 23% 55% 15% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	777	
2	O	149	
2	P	149	
2	Q	149	
2	R	149	
2	S	149	
2	T	149	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 42990 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 Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	B	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	C	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	D	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	E	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	F	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P40136
A	25	HIS	-	expression tag	UNP P40136
A	26	HIS	-	expression tag	UNP P40136
A	27	HIS	-	expression tag	UNP P40136
A	28	HIS	-	expression tag	UNP P40136
A	29	HIS	-	expression tag	UNP P40136
A	30	HIS	-	expression tag	UNP P40136
A	31	ALA	-	cloning artifact	UNP P40136
A	32	ALA	-	cloning artifact	UNP P40136
B	24	MET	-	initiating methionine	UNP P40136
B	25	HIS	-	expression tag	UNP P40136
B	26	HIS	-	expression tag	UNP P40136
B	27	HIS	-	expression tag	UNP P40136
B	28	HIS	-	expression tag	UNP P40136
B	29	HIS	-	expression tag	UNP P40136
B	30	HIS	-	expression tag	UNP P40136
B	31	ALA	-	cloning artifact	UNP P40136

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	-	cloning artifact	UNP P40136
C	24	MET	-	initiating methionine	UNP P40136
C	25	HIS	-	expression tag	UNP P40136
C	26	HIS	-	expression tag	UNP P40136
C	27	HIS	-	expression tag	UNP P40136
C	28	HIS	-	expression tag	UNP P40136
C	29	HIS	-	expression tag	UNP P40136
C	30	HIS	-	expression tag	UNP P40136
C	31	ALA	-	cloning artifact	UNP P40136
C	32	ALA	-	cloning artifact	UNP P40136
D	24	MET	-	initiating methionine	UNP P40136
D	25	HIS	-	expression tag	UNP P40136
D	26	HIS	-	expression tag	UNP P40136
D	27	HIS	-	expression tag	UNP P40136
D	28	HIS	-	expression tag	UNP P40136
D	29	HIS	-	expression tag	UNP P40136
D	30	HIS	-	expression tag	UNP P40136
D	31	ALA	-	cloning artifact	UNP P40136
D	32	ALA	-	cloning artifact	UNP P40136
E	24	MET	-	initiating methionine	UNP P40136
E	25	HIS	-	expression tag	UNP P40136
E	26	HIS	-	expression tag	UNP P40136
E	27	HIS	-	expression tag	UNP P40136
E	28	HIS	-	expression tag	UNP P40136
E	29	HIS	-	expression tag	UNP P40136
E	30	HIS	-	expression tag	UNP P40136
E	31	ALA	-	cloning artifact	UNP P40136
E	32	ALA	-	cloning artifact	UNP P40136
F	24	MET	-	initiating methionine	UNP P40136
F	25	HIS	-	expression tag	UNP P40136
F	26	HIS	-	expression tag	UNP P40136
F	27	HIS	-	expression tag	UNP P40136
F	28	HIS	-	expression tag	UNP P40136
F	29	HIS	-	expression tag	UNP P40136
F	30	HIS	-	expression tag	UNP P40136
F	31	ALA	-	cloning artifact	UNP P40136
F	32	ALA	-	cloning artifact	UNP P40136

- Molecule 2 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

Continued on next page...

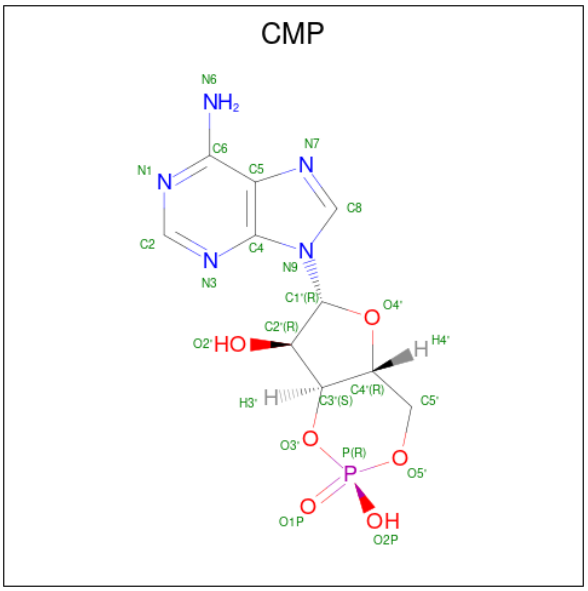
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	Q	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	R	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	S	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			
2	T	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	3	Total	Ca	0	0
			3	3		
5	P	3	Total	Ca	0	0
			3	3		
5	Q	3	Total	Ca	0	0
			3	3		
5	R	3	Total	Ca	0	0
			3	3		
5	S	3	Total	Ca	0	0
			3	3		
5	T	3	Total	Ca	0	0
			3	3		

- Molecule 6 is water.

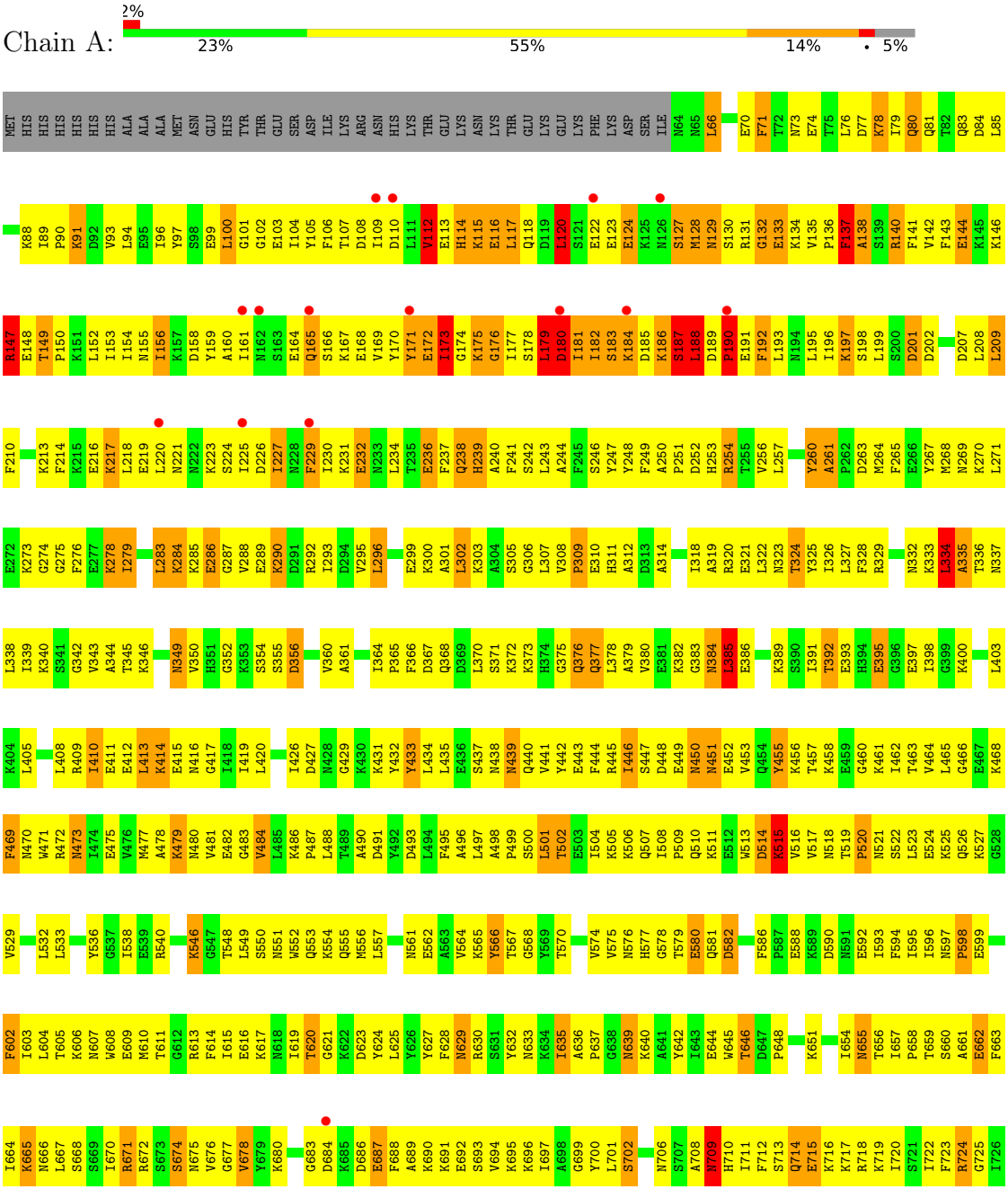
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	D	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	F	1	Total O 1 1	0	0

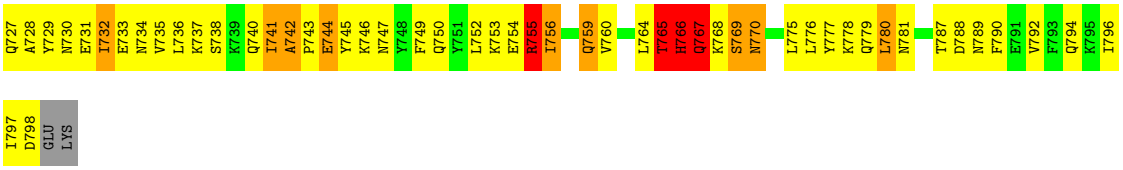
3 Residue-property plots (i)

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

- Molecule 1: Calmodulin-sensitive adenylate cyclase

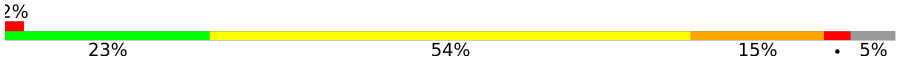
Chain A:

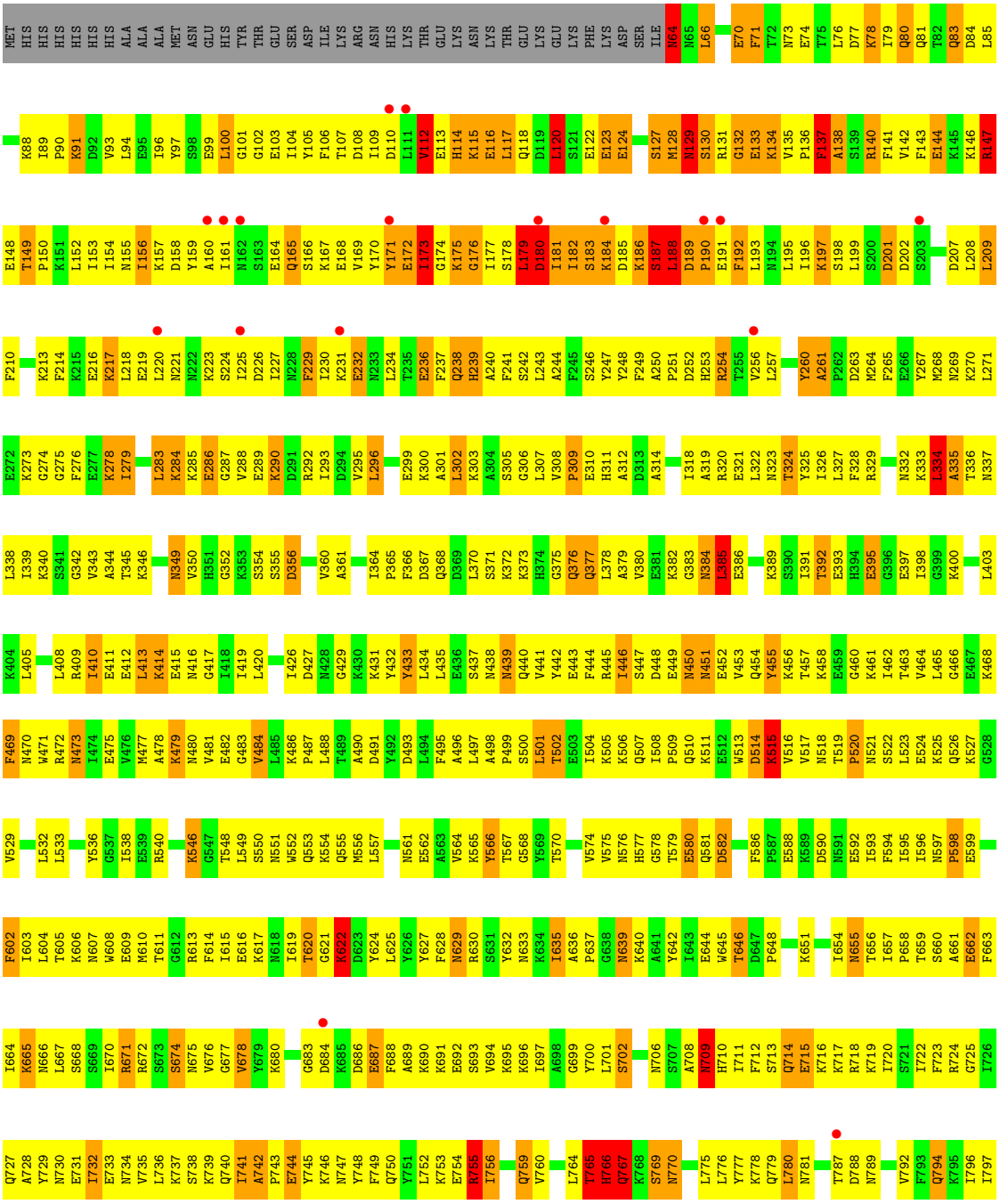




• Molecule 1: Calmodulin-sensitive adenylate cyclase

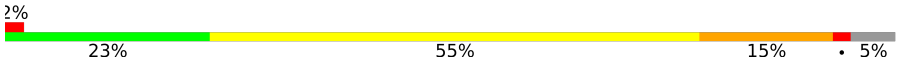
Chain B:

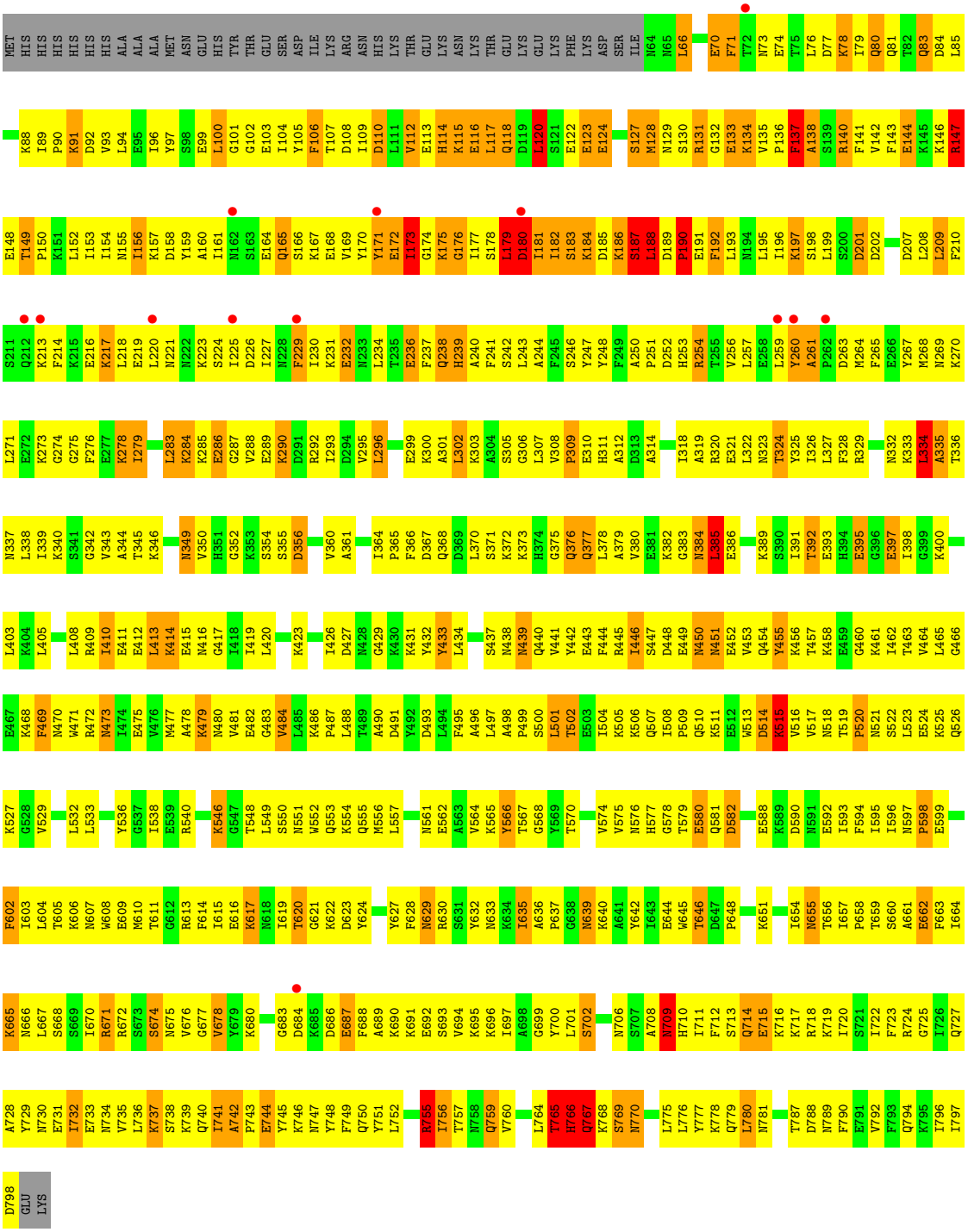




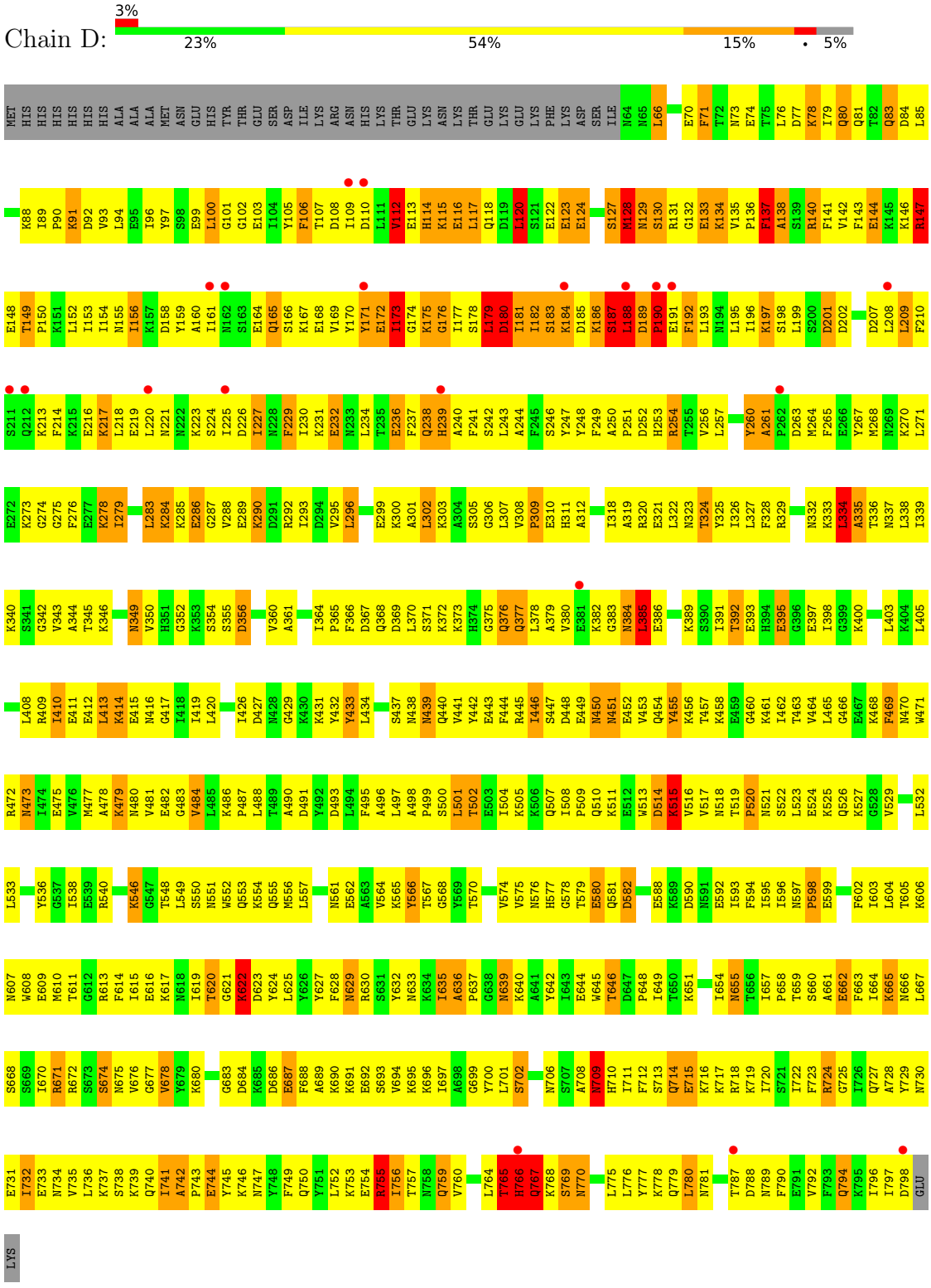
• Molecule 1: Calmodulin-sensitive adenylate cyclase

Chain C:

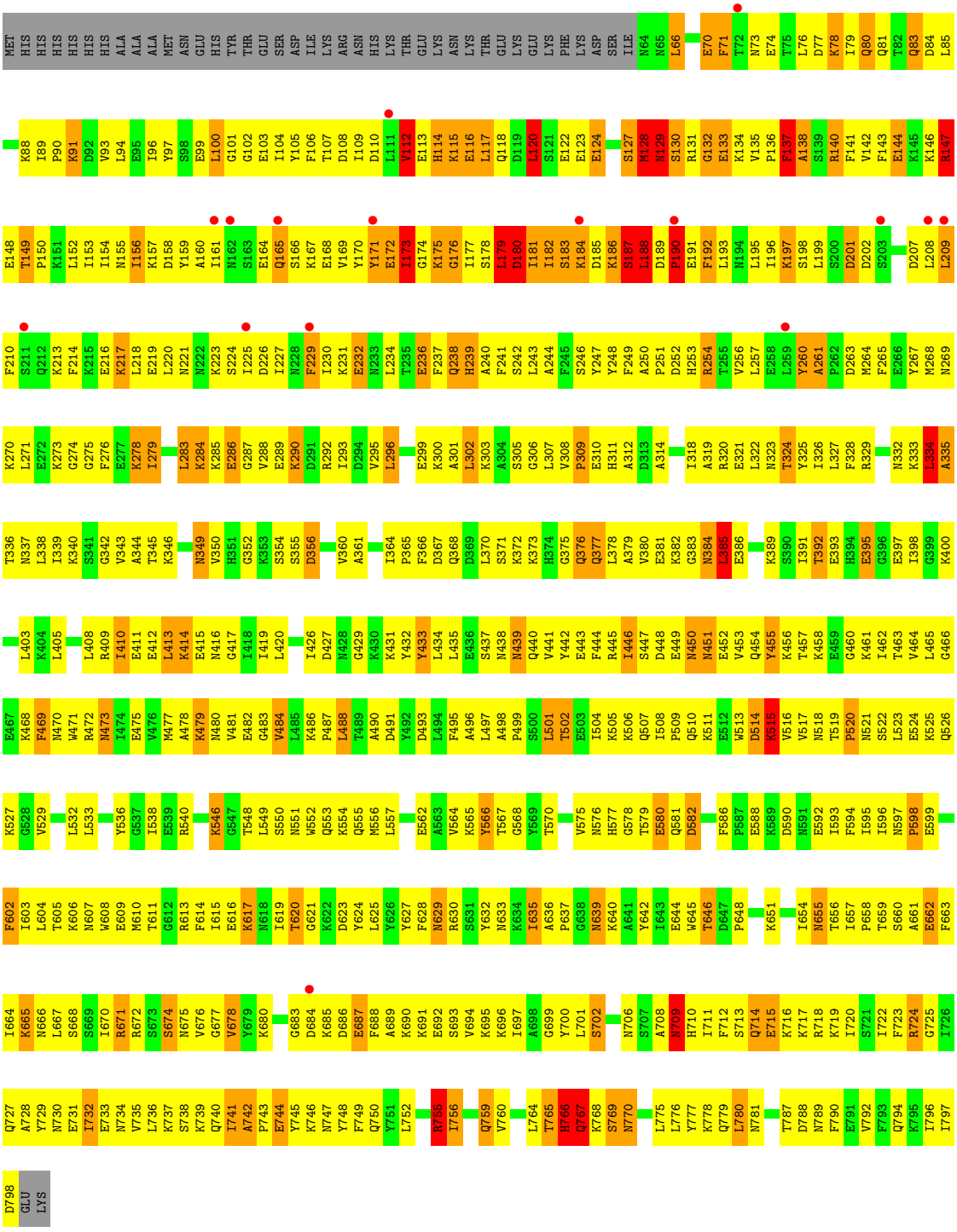




• Molecule 1: Calmodulin-sensitive adenylate cyclase

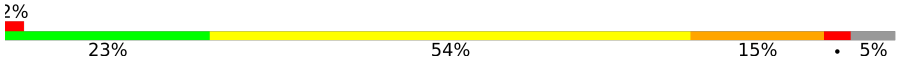


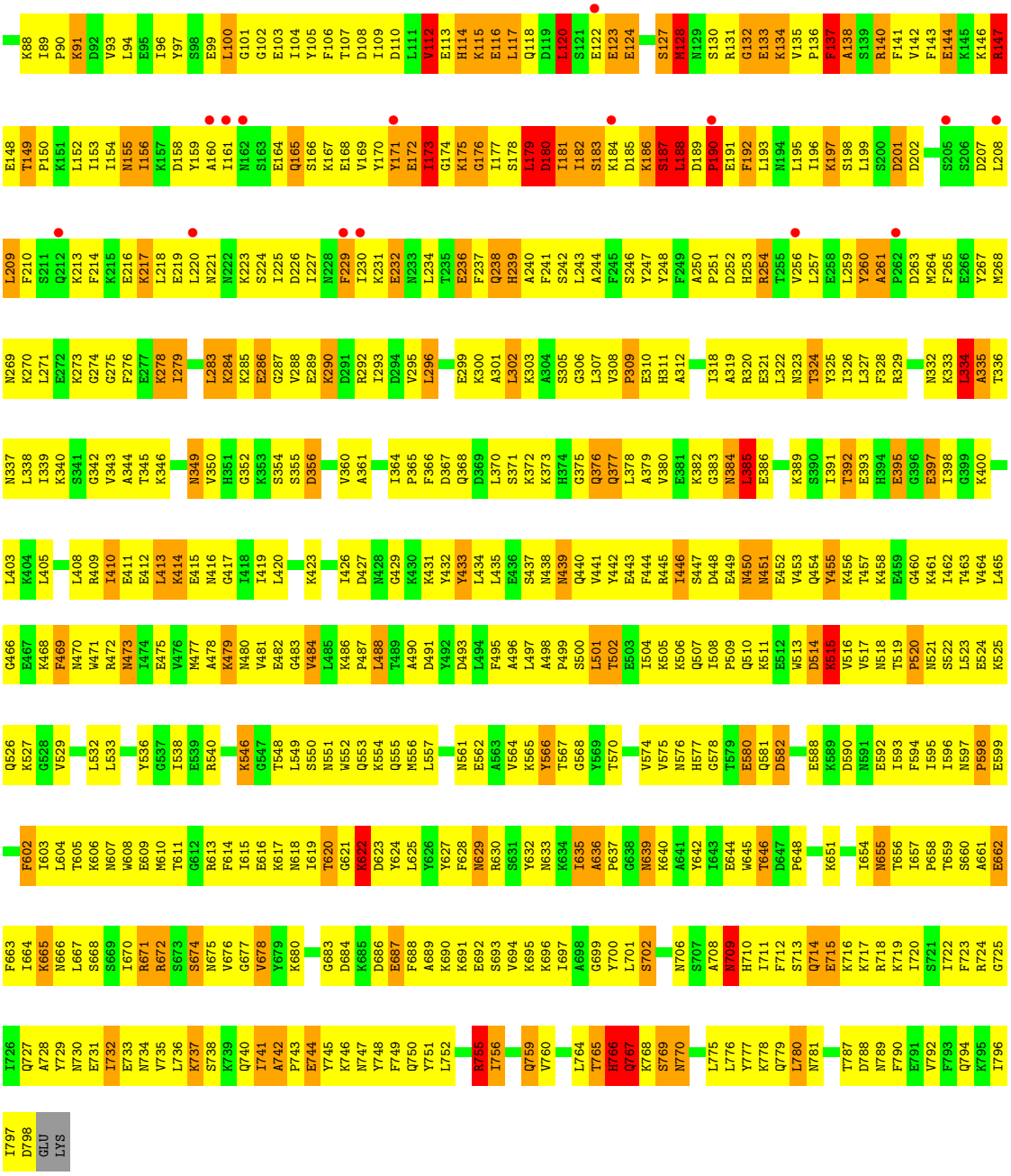
• Molecule 1: Calmodulin-sensitive adenylate cyclase



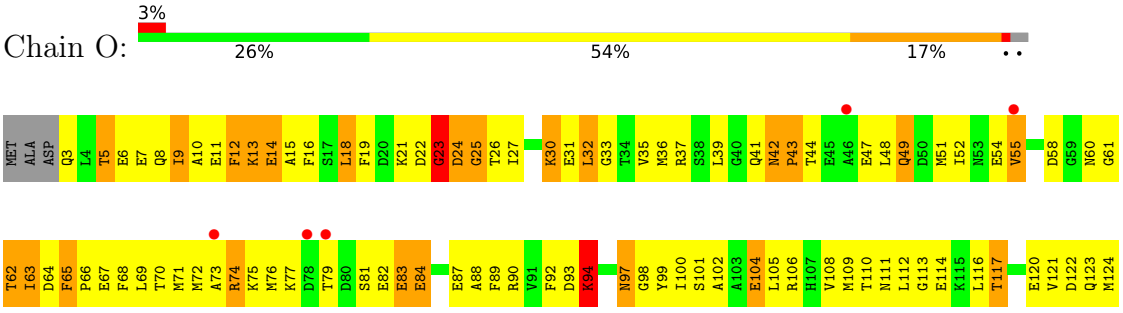
• Molecule 1: Calmodulin-sensitive adenylate cyclase

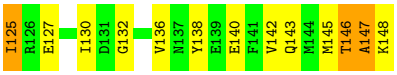
Chain F:





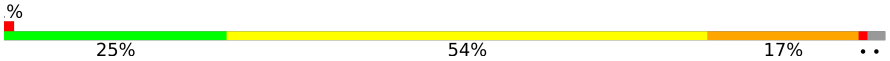
• Molecule 2: Calmodulin 2

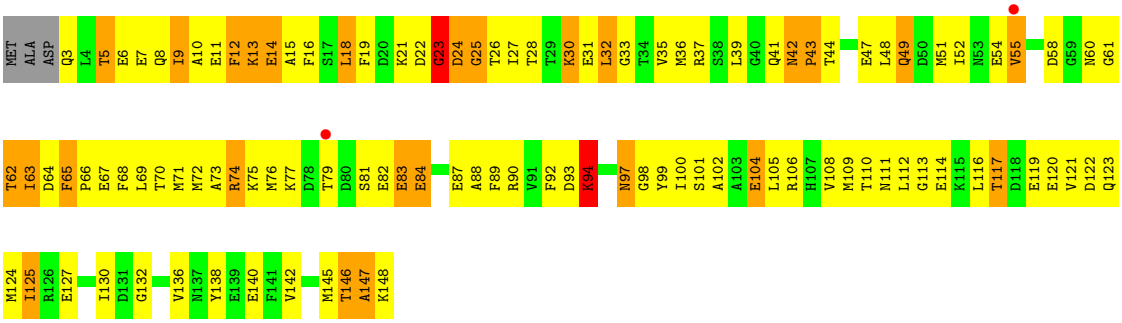




• Molecule 2: Calmodulin 2

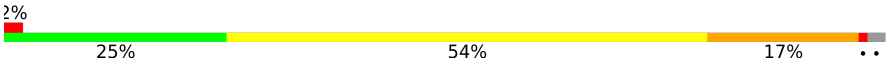
Chain P:

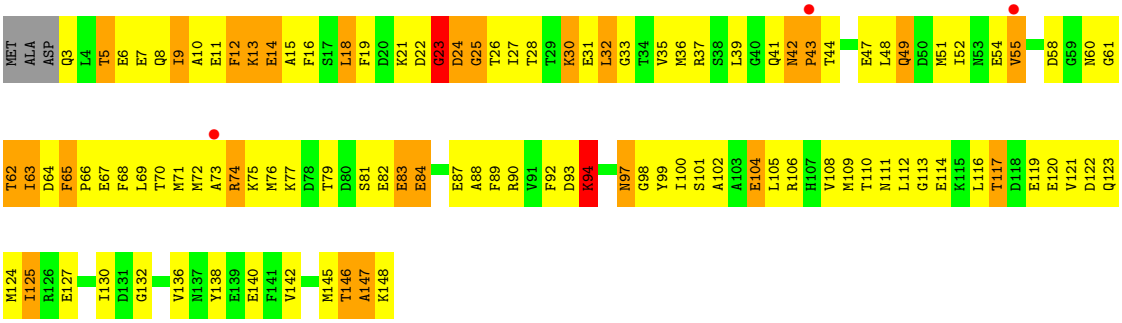




• Molecule 2: Calmodulin 2

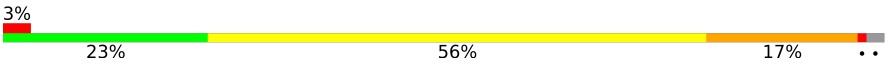
Chain Q:

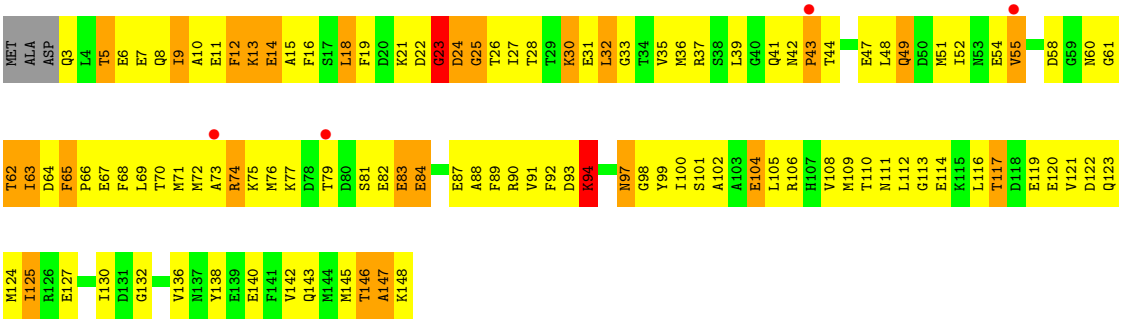




• Molecule 2: Calmodulin 2

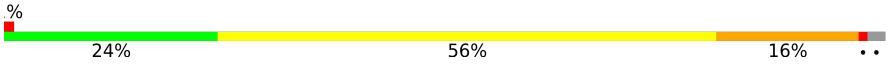
Chain R:

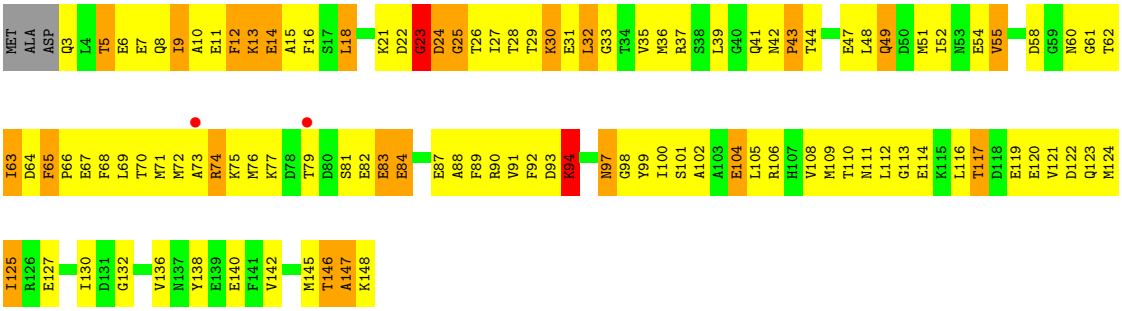




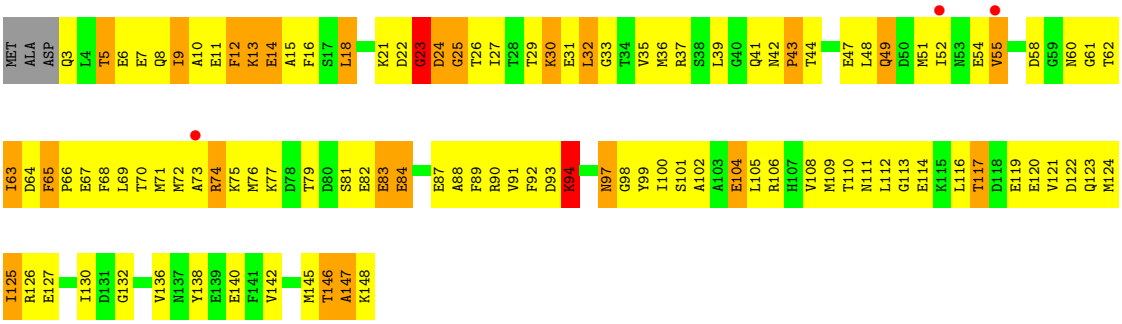
• Molecule 2: Calmodulin 2

Chain S:





• Molecule 2: Calmodulin 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	320.50Å 185.04Å 142.45Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	29.68 – 3.40 29.68 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.68-3.40) 93.5 (29.68-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.283 0.248 , 0.264	Depositor DCC
R_{free} test set	6075 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	92.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.449 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.438 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.440 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.440 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	42990	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CMP, MG, CA

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	0.69	6/6104 (0.1%)	1.26	83/8208 (1.0%)
1	B	0.71	9/6104 (0.1%)	1.29	88/8208 (1.1%)
1	C	0.76	14/6104 (0.2%)	1.27	82/8208 (1.0%)
1	D	0.72	8/6104 (0.1%)	1.30	87/8208 (1.1%)
1	E	0.70	6/6104 (0.1%)	1.26	83/8208 (1.0%)
1	F	0.73	10/6104 (0.2%)	1.28	82/8208 (1.0%)
2	O	0.79	1/1158 (0.1%)	1.18	8/1553 (0.5%)
2	P	0.80	1/1158 (0.1%)	1.19	8/1553 (0.5%)
2	Q	0.80	1/1158 (0.1%)	1.18	8/1553 (0.5%)
2	R	0.79	1/1158 (0.1%)	1.18	8/1553 (0.5%)
2	S	0.81	1/1158 (0.1%)	1.19	8/1553 (0.5%)
2	T	0.80	1/1158 (0.1%)	1.19	8/1553 (0.5%)
All	All	0.73	59/43572 (0.1%)	1.26	553/58566 (0.9%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	LYS	C-N	11.70	1.46	1.33
1	C	123	GLU	C-N	-10.17	1.19	1.33
1	F	737	LYS	C-N	-8.47	1.25	1.33
1	D	765	THR	C-N	-8.11	1.22	1.33
1	C	737	LYS	C-N	-7.96	1.25	1.33
2	S	42	ASN	N-CA	-7.75	1.35	1.46
2	T	42	ASN	N-CA	-7.72	1.35	1.46
2	P	42	ASN	N-CA	-7.71	1.35	1.46
2	O	42	ASN	N-CA	-7.65	1.35	1.46
2	Q	42	ASN	N-CA	-7.64	1.35	1.46
2	R	42	ASN	N-CA	-7.63	1.35	1.46
1	D	134	LYS	C-N	7.34	1.41	1.33
1	C	765	THR	C-N	-7.16	1.24	1.33
1	D	123	GLU	C-N	-6.82	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	PHE	C-N	6.58	1.42	1.33
1	F	134	LYS	C-N	6.53	1.40	1.33
1	F	740	GLN	C-N	-6.26	1.26	1.33
1	B	160	ALA	N-CA	6.20	1.53	1.46
1	C	160	ALA	N-CA	6.16	1.53	1.46
1	D	160	ALA	N-CA	6.14	1.53	1.46
1	A	160	ALA	N-CA	6.14	1.53	1.46
1	C	740	GLN	C-N	-6.14	1.26	1.33
1	F	160	ALA	N-CA	6.13	1.53	1.46
1	E	160	ALA	N-CA	6.09	1.53	1.46
1	E	70	GLU	C-N	-5.97	1.23	1.33
1	B	767	GLN	CA-C	5.94	1.58	1.52
1	D	767	GLN	CA-C	5.93	1.58	1.52
1	E	767	GLN	CA-C	5.92	1.58	1.52
1	A	767	GLN	CA-C	5.91	1.58	1.52
1	F	767	GLN	CA-C	5.90	1.58	1.52
1	C	767	GLN	CA-C	5.85	1.58	1.52
1	F	123	GLU	C-N	-5.74	1.25	1.33
1	B	134	LYS	C-N	-5.70	1.26	1.33
1	D	106	PHE	C-N	5.68	1.41	1.33
1	F	769	SER	N-CA	5.55	1.53	1.46
1	C	180	ASP	C-N	-5.54	1.26	1.33
1	C	769	SER	N-CA	5.50	1.53	1.46
1	A	190	PRO	N-CA	-5.50	1.40	1.47
1	A	769	SER	N-CA	5.50	1.53	1.46
1	B	769	SER	N-CA	5.49	1.53	1.46
1	E	769	SER	N-CA	5.46	1.53	1.46
1	D	769	SER	N-CA	5.45	1.53	1.46
1	C	118	GLN	C-N	-5.45	1.24	1.33
1	F	672	ARG	C-N	5.43	1.41	1.33
1	B	190	PRO	N-CA	-5.41	1.40	1.47
1	C	259	LEU	C-N	5.30	1.41	1.33
1	B	109	ILE	C-N	-5.29	1.26	1.33
1	C	109	ILE	C-N	-5.28	1.26	1.33
1	E	109	ILE	C-N	-5.28	1.26	1.33
1	B	622	LYS	C-N	-5.27	1.27	1.33
1	A	109	ILE	C-N	-5.24	1.26	1.33
1	F	109	ILE	C-N	-5.24	1.26	1.33
1	D	109	ILE	C-N	-5.23	1.26	1.33
1	B	70	GLU	C-N	-5.22	1.25	1.33
1	B	123	GLU	C-N	5.19	1.40	1.33
1	F	259	LEU	C-N	5.16	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	765	THR	C-N	-5.09	1.26	1.33
1	C	70	GLU	C-N	5.09	1.42	1.33
1	E	180	ASP	C-N	-5.01	1.26	1.33

All (553) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	ARG	N-CA-C	16.00	131.37	111.69
1	E	147	ARG	N-CA-C	15.98	131.35	111.69
1	D	147	ARG	N-CA-C	15.98	131.34	111.69
1	F	147	ARG	N-CA-C	15.98	131.34	111.69
1	F	188	LEU	N-CA-C	-15.81	89.94	110.33
1	D	188	LEU	N-CA-C	-15.80	89.95	110.33
1	A	188	LEU	N-CA-C	-15.79	89.96	110.33
1	C	188	LEU	N-CA-C	-15.79	89.97	110.33
1	E	188	LEU	N-CA-C	-15.78	89.98	110.33
1	B	188	LEU	N-CA-C	-15.76	90.00	110.33
1	D	622	LYS	CA-C-N	-13.89	102.75	122.06
1	D	622	LYS	C-N-CA	-13.89	102.75	122.06
1	A	147	ARG	N-CA-C	13.60	131.36	112.45
1	B	147	ARG	N-CA-C	13.59	131.34	112.45
1	B	622	LYS	CA-C-N	-13.24	105.05	122.79
1	B	622	LYS	C-N-CA	-13.24	105.05	122.79
1	F	160	ALA	N-CA-C	12.37	130.75	108.48
1	D	160	ALA	N-CA-C	12.36	130.73	108.48
1	A	160	ALA	N-CA-C	12.36	130.73	108.48
1	E	160	ALA	N-CA-C	12.36	130.73	108.48
1	B	160	ALA	N-CA-C	12.36	130.72	108.48
1	C	160	ALA	N-CA-C	12.35	130.72	108.48
1	F	219	GLU	N-CA-C	-12.18	98.40	113.02
1	D	219	GLU	N-CA-C	-12.15	98.43	113.02
1	A	219	GLU	N-CA-C	-12.12	98.47	113.02
1	B	219	GLU	N-CA-C	-12.06	98.55	113.02
1	E	219	GLU	N-CA-C	-12.05	98.56	113.02
1	C	219	GLU	N-CA-C	-11.99	98.64	113.02
1	F	146	LYS	N-CA-C	11.17	124.56	111.71
1	E	146	LYS	N-CA-C	11.13	124.52	111.71
1	C	146	LYS	N-CA-C	11.01	124.37	111.71
1	D	146	LYS	N-CA-C	10.96	124.31	111.71
2	S	122	ASP	N-CA-C	-10.62	100.26	113.01
2	T	122	ASP	N-CA-C	-10.62	100.27	113.01
2	P	122	ASP	N-CA-C	-10.60	100.29	113.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	122	ASP	N-CA-C	-10.56	100.34	113.01
2	O	122	ASP	N-CA-C	-10.55	100.35	113.01
2	R	122	ASP	N-CA-C	-10.48	100.43	113.01
1	D	622	LYS	N-CA-C	-10.36	94.46	109.18
1	A	146	LYS	N-CA-C	9.95	124.52	112.38
1	B	767	GLN	OE1-CD-NE2	-9.89	112.71	122.60
1	A	767	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	B	146	LYS	N-CA-C	9.87	124.42	112.38
1	D	767	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	F	767	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	C	767	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	E	767	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	C	740	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	F	740	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	740	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	B	740	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	D	740	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	E	740	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	F	120	LEU	N-CA-C	9.43	124.94	108.52
1	C	120	LEU	N-CA-C	9.43	124.92	108.52
1	A	120	LEU	N-CA-C	9.43	124.92	108.52
1	D	120	LEU	N-CA-C	9.42	124.91	108.52
1	E	120	LEU	N-CA-C	9.41	124.89	108.52
1	B	120	LEU	N-CA-C	9.40	124.88	108.52
1	F	159	TYR	CA-C-N	-9.01	106.21	121.89
1	F	159	TYR	C-N-CA	-9.01	106.21	121.89
1	B	159	TYR	CA-C-N	-9.01	106.22	121.89
1	B	159	TYR	C-N-CA	-9.01	106.22	121.89
1	E	159	TYR	CA-C-N	-9.01	106.22	121.89
1	E	159	TYR	C-N-CA	-9.01	106.22	121.89
1	A	159	TYR	CA-C-N	-9.00	106.23	121.89
1	A	159	TYR	C-N-CA	-9.00	106.23	121.89
1	C	159	TYR	CA-C-N	-8.99	106.24	121.89
1	C	159	TYR	C-N-CA	-8.99	106.24	121.89
1	D	159	TYR	CA-C-N	-8.98	106.27	121.89
1	D	159	TYR	C-N-CA	-8.98	106.27	121.89
1	A	366	PHE	N-CA-C	-8.90	101.02	112.23
1	D	366	PHE	N-CA-C	-8.85	101.08	112.23
1	D	260	TYR	N-CA-C	8.82	122.16	111.40
1	D	238	GLN	N-CA-C	-8.81	102.44	113.55
1	E	238	GLN	N-CA-C	-8.81	102.45	113.55
1	F	260	TYR	N-CA-C	8.80	122.14	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	TYR	N-CA-C	8.79	122.13	111.40
1	B	238	GLN	N-CA-C	-8.76	102.51	113.55
1	C	260	TYR	N-CA-C	8.76	122.09	111.40
1	F	366	PHE	N-CA-C	-8.76	101.19	112.23
1	A	238	GLN	N-CA-C	-8.75	102.53	113.55
1	B	366	PHE	N-CA-C	-8.69	101.28	112.23
1	F	238	GLN	N-CA-C	-8.67	102.62	113.55
1	C	238	GLN	N-CA-C	-8.62	102.69	113.55
1	C	366	PHE	N-CA-C	-8.60	101.40	112.23
1	E	366	PHE	N-CA-C	-8.51	101.51	112.23
1	B	766	HIS	N-CA-C	-8.32	103.26	113.41
1	F	766	HIS	N-CA-C	-8.32	103.26	113.41
1	C	766	HIS	N-CA-C	-8.32	103.26	113.41
1	A	766	HIS	N-CA-C	-8.32	103.26	113.41
1	E	766	HIS	N-CA-C	-8.32	103.26	113.41
1	D	766	HIS	N-CA-C	-8.30	103.28	113.41
1	D	674	SER	N-CA-C	-8.27	97.55	109.96
1	E	674	SER	N-CA-C	-8.27	97.56	109.96
1	A	674	SER	N-CA-C	-8.25	97.58	109.96
1	B	674	SER	N-CA-C	-8.25	97.59	109.96
1	C	674	SER	N-CA-C	-8.24	97.59	109.96
1	D	201	ASP	N-CA-C	-8.23	102.00	110.97
1	E	128	MET	N-CA-C	-8.22	93.59	107.80
1	F	674	SER	N-CA-C	-8.21	97.64	109.96
1	A	201	ASP	N-CA-C	-8.18	102.05	110.97
1	E	201	ASP	N-CA-C	-8.18	102.06	110.97
1	B	201	ASP	N-CA-C	-8.17	102.07	110.97
1	C	201	ASP	N-CA-C	-8.17	102.07	110.97
1	F	201	ASP	N-CA-C	-8.16	102.07	110.97
1	F	190	PRO	CA-C-N	-8.16	110.02	122.09
1	F	190	PRO	C-N-CA	-8.16	110.02	122.09
1	D	608	TRP	N-CA-C	-8.13	101.98	112.23
1	F	160	ALA	CA-C-N	8.11	133.27	121.02
1	F	160	ALA	C-N-CA	8.11	133.27	121.02
1	B	160	ALA	CA-C-N	8.10	133.25	121.02
1	B	160	ALA	C-N-CA	8.10	133.25	121.02
1	D	160	ALA	CA-C-N	8.09	133.24	121.02
1	D	160	ALA	C-N-CA	8.09	133.24	121.02
1	A	160	ALA	CA-C-N	8.09	133.23	121.02
1	A	160	ALA	C-N-CA	8.09	133.23	121.02
1	C	160	ALA	CA-C-N	8.06	133.19	121.02
1	C	160	ALA	C-N-CA	8.06	133.19	121.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	180	ASP	CA-CB-CG	-8.02	104.58	112.60
1	D	180	ASP	CA-CB-CG	-8.01	104.59	112.60
1	F	159	TYR	CA-C-O	-8.00	111.96	120.92
1	A	180	ASP	CA-CB-CG	-8.00	104.60	112.60
1	B	180	ASP	CA-CB-CG	-8.00	104.60	112.60
1	C	180	ASP	CA-CB-CG	-7.99	104.61	112.60
1	A	159	TYR	CA-C-O	-7.97	111.99	120.92
1	C	159	TYR	CA-C-O	-7.97	111.99	120.92
1	B	159	TYR	CA-C-O	-7.96	112.00	120.92
1	D	159	TYR	CA-C-O	-7.96	112.00	120.92
1	F	180	ASP	CA-CB-CG	-7.96	104.64	112.60
1	E	159	TYR	CA-C-O	-7.94	112.03	120.92
1	A	608	TRP	N-CA-C	-7.93	102.24	112.23
1	B	608	TRP	N-CA-C	-7.92	102.25	112.23
1	F	608	TRP	N-CA-C	-7.91	102.27	112.23
1	C	576	ASN	N-CA-C	7.86	123.05	113.38
1	C	608	TRP	N-CA-C	-7.84	102.36	112.23
1	B	576	ASN	N-CA-C	7.82	123.00	113.38
1	B	64	ASN	CA-C-N	-7.77	112.00	122.72
1	B	64	ASN	C-N-CA	-7.77	112.00	122.72
1	A	576	ASN	N-CA-C	7.77	122.93	113.38
1	E	576	ASN	N-CA-C	7.76	122.93	113.38
1	D	576	ASN	N-CA-C	7.67	122.82	113.38
1	E	608	TRP	N-CA-C	-7.67	102.57	112.23
1	A	171	TYR	N-CA-C	-7.58	104.02	113.20
1	F	576	ASN	N-CA-C	7.58	122.70	113.38
1	C	171	TYR	N-CA-C	-7.58	104.03	113.20
1	F	171	TYR	N-CA-C	-7.55	104.06	113.20
1	D	171	TYR	N-CA-C	-7.55	104.07	113.20
1	B	171	TYR	N-CA-C	-7.52	104.10	113.20
1	A	190	PRO	CA-C-N	-7.51	109.87	122.64
1	A	190	PRO	C-N-CA	-7.51	109.87	122.64
1	E	160	ALA	CA-C-N	7.51	133.21	121.35
1	E	160	ALA	C-N-CA	7.51	133.21	121.35
1	B	335	ALA	N-CA-C	-7.50	105.30	114.75
1	C	335	ALA	N-CA-C	-7.50	105.30	114.75
1	F	335	ALA	N-CA-C	-7.47	105.33	114.75
1	A	335	ALA	N-CA-C	-7.46	105.35	114.75
1	E	171	TYR	N-CA-C	-7.45	104.18	113.20
1	C	384	ASN	N-CA-C	-7.44	103.11	111.07
1	D	335	ALA	N-CA-C	-7.44	105.38	114.75
1	A	384	ASN	N-CA-C	-7.44	103.11	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	384	ASN	N-CA-C	-7.41	103.14	111.07
1	D	66	LEU	N-CA-C	7.41	119.14	111.14
1	F	384	ASN	N-CA-C	-7.38	103.17	111.07
1	D	384	ASN	N-CA-C	-7.35	103.21	111.07
1	C	732	ILE	N-CA-C	-7.28	103.75	110.82
1	E	335	ALA	N-CA-C	-7.28	105.57	114.75
1	B	384	ASN	N-CA-C	-7.28	103.28	111.07
1	F	546	LYS	N-CA-C	7.28	120.69	112.97
1	B	622	LYS	N-CA-C	-7.22	95.29	108.65
1	B	732	ILE	N-CA-C	-7.22	103.82	110.82
1	A	732	ILE	N-CA-C	-7.20	103.83	110.82
1	E	184	LYS	N-CA-C	-7.20	105.68	114.75
1	B	546	LYS	N-CA-C	7.19	120.59	112.97
1	C	546	LYS	N-CA-C	7.18	120.58	112.97
1	F	732	ILE	N-CA-C	-7.15	103.89	110.82
1	A	687	GLU	N-CA-C	-7.08	103.50	111.07
1	D	546	LYS	N-CA-C	7.07	120.46	112.97
1	E	379	ALA	N-CA-C	-7.06	103.63	111.82
2	T	88	ALA	N-CA-C	-7.06	103.58	111.28
1	A	546	LYS	N-CA-C	7.06	120.45	112.97
1	D	732	ILE	N-CA-C	-7.04	104.00	110.82
1	E	546	LYS	N-CA-C	7.02	120.41	112.97
1	E	260	TYR	N-CA-C	7.02	122.15	112.04
1	B	184	LYS	N-CA-C	-7.02	105.65	114.56
1	C	184	LYS	N-CA-C	-7.01	105.65	114.56
1	B	379	ALA	N-CA-C	-7.01	103.69	111.82
1	A	184	LYS	N-CA-C	-7.00	105.68	114.56
1	D	687	GLU	N-CA-C	-7.00	103.58	111.07
1	B	260	TYR	N-CA-C	6.99	122.11	112.04
1	D	184	LYS	N-CA-C	-6.98	105.69	114.56
1	E	732	ILE	N-CA-C	-6.94	104.08	110.82
1	F	379	ALA	N-CA-C	-6.93	103.74	111.71
1	A	129	ASN	N-CA-C	6.91	121.53	111.02
1	F	687	GLU	N-CA-C	-6.91	103.67	111.07
1	C	379	ALA	N-CA-C	-6.90	103.77	111.71
1	E	687	GLU	N-CA-C	-6.90	103.69	111.07
1	C	416	ASN	N-CA-C	-6.84	104.75	113.23
1	C	687	GLU	N-CA-C	-6.84	103.75	111.07
1	F	622	LYS	N-CA-C	-6.82	99.18	109.96
1	F	662	GLU	N-CA-C	-6.82	103.91	111.82
1	C	128	MET	N-CA-C	-6.82	95.84	107.23
1	F	416	ASN	N-CA-C	-6.79	104.81	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ALA	N-CA-C	-6.77	103.92	111.71
1	F	622	LYS	CA-C-N	-6.77	110.57	122.62
1	F	622	LYS	C-N-CA	-6.77	110.57	122.62
1	D	709	ASN	N-CA-C	-6.76	105.02	113.20
1	B	687	GLU	N-CA-C	-6.74	103.86	111.07
1	D	379	ALA	N-CA-C	-6.74	103.96	111.71
1	B	66	LEU	N-CA-C	6.72	118.40	111.14
1	C	173	ILE	N-CA-C	-6.72	104.21	110.53
1	A	416	ASN	N-CA-C	-6.71	104.91	113.23
1	C	662	GLU	N-CA-C	-6.71	104.04	111.82
1	D	416	ASN	N-CA-C	-6.67	104.95	113.23
1	D	662	GLU	N-CA-C	-6.67	104.08	111.82
1	B	709	ASN	N-CA-C	-6.66	105.14	113.20
1	E	709	ASN	N-CA-C	-6.66	105.14	113.20
1	E	662	GLU	N-CA-C	-6.65	104.10	111.82
2	T	9	ILE	N-CA-C	-6.62	106.53	111.90
2	R	88	ALA	N-CA-C	-6.62	104.06	111.28
1	B	416	ASN	N-CA-C	-6.62	105.02	113.23
1	A	709	ASN	N-CA-C	-6.61	105.20	113.20
1	D	128	MET	N-CA-C	-6.60	96.21	107.23
1	F	709	ASN	N-CA-C	-6.58	105.23	113.20
1	E	416	ASN	N-CA-C	-6.58	105.08	113.23
1	B	173	ILE	N-CA-C	-6.57	104.36	110.53
1	E	382	LYS	N-CA-C	-6.55	103.70	112.94
1	D	173	ILE	N-CA-C	-6.55	104.37	110.53
1	F	132	GLY	CA-C-N	-6.55	111.33	122.33
1	F	132	GLY	C-N-CA	-6.55	111.33	122.33
2	P	9	ILE	N-CA-C	-6.55	106.59	111.90
1	A	382	LYS	N-CA-C	-6.55	103.71	112.94
1	C	382	LYS	N-CA-C	-6.54	103.71	112.94
1	D	132	GLY	CA-C-N	-6.54	111.34	122.33
1	D	132	GLY	C-N-CA	-6.54	111.34	122.33
1	A	662	GLU	N-CA-C	-6.54	104.23	111.82
1	E	173	ILE	N-CA-C	-6.54	104.39	110.53
1	A	132	GLY	CA-C-N	-6.53	111.36	122.33
1	A	132	GLY	C-N-CA	-6.53	111.36	122.33
2	S	88	ALA	N-CA-C	-6.53	104.16	111.28
1	C	709	ASN	N-CA-C	-6.52	105.31	113.20
1	C	132	GLY	CA-C-N	-6.52	111.38	122.33
1	C	132	GLY	C-N-CA	-6.52	111.38	122.33
1	E	132	GLY	CA-C-N	-6.52	111.38	122.33
1	E	132	GLY	C-N-CA	-6.52	111.38	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	770	ASN	N-CA-C	-6.51	105.25	113.72
1	C	770	ASN	N-CA-C	-6.51	105.25	113.72
1	B	132	GLY	CA-C-N	-6.51	111.40	122.33
1	B	132	GLY	C-N-CA	-6.51	111.40	122.33
1	B	662	GLU	N-CA-C	-6.51	104.27	111.82
1	F	173	ILE	N-CA-C	-6.50	104.42	110.53
1	A	770	ASN	N-CA-C	-6.49	105.28	113.72
1	D	770	ASN	N-CA-C	-6.49	105.28	113.72
1	C	179	LEU	N-CA-C	6.49	121.20	113.16
1	F	770	ASN	N-CA-C	-6.49	105.29	113.72
1	D	179	LEU	N-CA-C	6.48	121.20	113.16
1	A	179	LEU	N-CA-C	6.48	121.19	113.16
1	E	770	ASN	N-CA-C	-6.47	105.30	113.72
2	O	9	ILE	N-CA-C	-6.47	106.66	111.90
1	B	179	LEU	N-CA-C	6.47	121.18	113.16
1	F	179	LEU	N-CA-C	6.46	121.18	113.16
1	E	179	LEU	N-CA-C	6.46	121.17	113.16
1	A	173	ILE	N-CA-C	-6.46	104.46	110.53
1	F	767	GLN	CG-CD-NE2	6.46	126.08	116.40
1	F	382	LYS	N-CA-C	-6.45	103.84	112.94
1	A	767	GLN	CG-CD-NE2	6.45	126.07	116.40
1	C	767	GLN	CG-CD-NE2	6.45	126.07	116.40
1	F	671	ARG	N-CA-C	-6.44	103.95	110.97
1	D	382	LYS	N-CA-C	-6.44	103.87	112.94
2	P	88	ALA	N-CA-C	-6.43	104.27	111.28
1	B	767	GLN	CG-CD-NE2	6.43	126.05	116.40
1	D	767	GLN	CG-CD-NE2	6.43	126.05	116.40
1	B	382	LYS	N-CA-C	-6.42	103.88	112.94
1	B	261	ALA	N-CA-C	-6.42	99.28	109.04
1	D	261	ALA	N-CA-C	-6.42	99.28	109.04
1	A	261	ALA	N-CA-C	-6.42	99.29	109.04
1	F	261	ALA	N-CA-C	-6.42	99.29	109.04
2	Q	88	ALA	N-CA-C	-6.42	104.29	111.28
1	A	190	PRO	N-CA-C	-6.42	99.25	112.47
1	E	767	GLN	CG-CD-NE2	6.42	126.02	116.40
1	B	671	ARG	N-CA-C	-6.41	103.98	110.97
1	E	261	ALA	N-CA-C	-6.41	99.30	109.04
1	C	261	ALA	N-CA-C	-6.41	99.31	109.04
1	B	667	LEU	N-CA-C	-6.40	103.92	111.03
2	Q	9	ILE	N-CA-C	-6.40	106.72	111.90
1	D	127	SER	N-CA-C	6.35	119.92	108.17
1	A	190	PRO	CB-CA-C	6.32	121.98	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	159	TYR	O-C-N	-6.31	114.85	122.11
1	C	159	TYR	O-C-N	-6.30	114.86	122.11
1	E	159	TYR	O-C-N	-6.30	114.87	122.11
1	E	667	LEU	N-CA-C	-6.30	104.04	111.03
1	A	159	TYR	O-C-N	-6.29	114.88	122.11
1	B	159	TYR	O-C-N	-6.28	114.89	122.11
1	E	671	ARG	N-CA-C	-6.28	104.13	110.97
1	C	671	ARG	N-CA-C	-6.27	104.14	110.97
1	B	132	GLY	N-CA-C	-6.26	103.53	112.55
1	F	140	ARG	N-CA-C	6.26	118.64	110.43
1	A	667	LEU	N-CA-C	-6.26	104.15	110.97
1	F	159	TYR	O-C-N	-6.26	114.92	122.11
1	A	132	GLY	N-CA-C	-6.25	103.55	112.55
1	E	132	GLY	N-CA-C	-6.25	103.55	112.55
1	D	667	LEU	N-CA-C	-6.25	104.09	111.03
1	D	671	ARG	N-CA-C	-6.25	104.16	110.97
1	B	128	MET	N-CA-C	-6.23	96.82	107.23
1	E	140	ARG	N-CA-C	6.22	118.58	110.43
1	D	190	PRO	CA-C-N	-6.18	111.50	122.07
1	D	190	PRO	C-N-CA	-6.18	111.50	122.07
1	F	64	ASN	CA-C-N	-6.18	112.67	121.50
1	F	64	ASN	C-N-CA	-6.18	112.67	121.50
1	B	140	ARG	N-CA-C	6.16	118.50	110.43
1	B	189	ASP	CA-C-N	-6.16	112.15	119.84
1	B	189	ASP	C-N-CA	-6.16	112.15	119.84
1	C	140	ARG	N-CA-C	6.15	118.49	110.43
1	A	671	ARG	N-CA-C	-6.15	104.26	110.97
1	A	128	MET	N-CA-C	-6.14	95.59	107.44
1	A	140	ARG	N-CA-C	6.13	118.46	110.43
1	F	667	LEU	N-CA-C	-6.10	104.26	111.03
1	E	188	LEU	N-CA-CB	6.06	118.53	110.29
1	D	188	LEU	N-CA-CB	6.04	118.51	110.29
1	A	188	LEU	N-CA-CB	6.04	118.50	110.29
1	D	140	ARG	N-CA-C	6.03	118.33	110.43
1	C	188	LEU	N-CA-CB	6.03	118.49	110.29
1	F	740	GLN	CG-CD-NE2	6.03	125.44	116.40
1	B	188	LEU	N-CA-CB	6.03	118.49	110.29
1	C	667	LEU	N-CA-C	-6.03	104.40	110.97
1	F	188	LEU	N-CA-CB	6.02	118.48	110.29
1	D	198	SER	N-CA-C	-6.02	104.65	112.23
2	O	88	ALA	N-CA-C	-6.01	104.73	111.28
1	D	740	GLN	CG-CD-NE2	6.01	125.41	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	740	GLN	CG-CD-NE2	6.00	125.41	116.40
1	A	740	GLN	CG-CD-NE2	6.00	125.40	116.40
1	B	740	GLN	CG-CD-NE2	5.99	125.38	116.40
1	C	770	ASN	CA-C-N	5.99	132.08	122.50
1	C	770	ASN	C-N-CA	5.99	132.08	122.50
1	E	740	GLN	CG-CD-NE2	5.98	125.37	116.40
2	T	32	LEU	N-CA-C	-5.96	104.70	111.07
1	A	198	SER	N-CA-C	-5.94	104.74	112.23
1	B	198	SER	N-CA-C	-5.93	104.75	112.23
1	A	66	LEU	N-CA-C	5.93	118.89	111.24
1	C	198	SER	N-CA-C	-5.93	104.76	112.23
1	F	198	SER	N-CA-C	-5.93	104.76	112.23
2	Q	32	LEU	N-CA-C	-5.92	104.73	111.07
1	E	190	PRO	CA-C-N	-5.92	111.56	121.39
1	E	190	PRO	C-N-CA	-5.92	111.56	121.39
2	R	94	LYS	N-CA-C	5.92	118.49	111.33
2	R	32	LEU	N-CA-C	-5.91	104.74	111.07
2	S	9	ILE	N-CA-C	-5.90	106.74	111.81
1	E	198	SER	N-CA-C	-5.89	104.81	112.23
1	C	159	TYR	N-CA-C	5.88	121.07	111.37
1	B	159	TYR	N-CA-C	5.88	121.07	111.37
1	D	159	TYR	N-CA-C	5.87	121.06	111.37
1	A	159	TYR	N-CA-C	5.87	121.06	111.37
1	C	190	PRO	CA-C-N	-5.87	112.03	122.07
1	C	190	PRO	C-N-CA	-5.87	112.03	122.07
1	F	770	ASN	CA-C-N	5.87	131.89	122.50
1	F	770	ASN	C-N-CA	5.87	131.89	122.50
2	R	9	ILE	N-CA-C	-5.87	106.76	111.81
1	C	190	PRO	N-CA-C	-5.86	100.39	112.47
1	E	159	TYR	N-CA-C	5.86	121.05	111.37
1	C	190	PRO	CB-CA-C	5.86	121.23	111.56
2	S	32	LEU	N-CA-C	-5.86	104.80	111.07
1	F	159	TYR	N-CA-C	5.85	121.03	111.37
2	T	94	LYS	N-CA-C	5.85	118.41	111.33
1	E	128	MET	CA-C-N	-5.85	110.37	121.54
1	E	128	MET	C-N-CA	-5.85	110.37	121.54
2	P	32	LEU	N-CA-C	-5.84	104.82	111.07
1	D	622	LYS	CA-C-O	-5.83	114.73	121.49
2	Q	94	LYS	N-CA-C	5.80	118.35	111.33
1	C	260	TYR	CB-CA-C	-5.80	101.05	110.79
1	A	260	TYR	CB-CA-C	-5.79	101.05	110.79
1	D	260	TYR	CB-CA-C	-5.79	101.06	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	260	TYR	CB-CA-C	-5.78	101.08	110.79
1	E	127	SER	N-CA-C	5.77	118.85	108.17
1	E	439	ASN	N-CA-C	-5.72	102.30	110.59
2	P	94	LYS	N-CA-C	5.69	118.21	111.33
2	O	94	LYS	N-CA-C	5.67	118.20	111.33
1	F	128	MET	N-CA-C	-5.66	97.24	107.60
1	D	439	ASN	N-CA-C	-5.66	102.38	110.59
2	O	32	LEU	N-CA-C	-5.66	105.02	111.07
1	B	765	THR	CA-C-N	-5.64	112.00	122.09
1	B	765	THR	C-N-CA	-5.64	112.00	122.09
1	F	439	ASN	N-CA-C	-5.64	102.42	110.59
1	B	127	SER	N-CA-C	5.61	118.55	108.17
1	F	286	GLU	N-CA-C	-5.59	106.78	113.21
1	C	439	ASN	N-CA-C	-5.56	102.53	110.59
2	R	132	GLY	N-CA-C	5.55	123.29	115.30
2	S	94	LYS	N-CA-C	5.55	118.05	111.33
1	F	127	SER	N-CA-C	5.55	118.43	108.17
1	B	439	ASN	N-CA-C	-5.54	102.55	110.59
1	D	190	PRO	CB-CA-C	5.53	120.69	111.56
1	D	227	ILE	CA-C-N	-5.53	112.44	120.29
1	D	227	ILE	C-N-CA	-5.53	112.44	120.29
1	B	433	TYR	N-CA-C	-5.51	101.49	110.20
1	B	129	ASN	N-CA-C	5.50	119.38	111.02
1	B	566	TYR	N-CA-C	-5.50	106.60	113.15
1	D	450	ASN	N-CA-C	-5.50	100.28	109.24
1	A	439	ASN	N-CA-C	-5.49	102.62	110.59
1	B	146	LYS	O-C-N	-5.49	115.25	122.39
2	O	132	GLY	N-CA-C	5.48	123.19	115.30
2	Q	132	GLY	N-CA-C	5.47	123.18	115.30
2	T	132	GLY	N-CA-C	5.47	123.17	115.30
1	B	190	PRO	CA-C-N	-5.46	112.73	122.07
1	B	190	PRO	C-N-CA	-5.46	112.73	122.07
1	C	741	ILE	N-CA-C	-5.46	101.56	108.93
1	B	450	ASN	N-CA-C	-5.45	100.36	109.24
2	P	132	GLY	N-CA-C	5.44	123.13	115.30
1	C	283	LEU	N-CA-C	-5.42	105.80	112.90
1	A	227	ILE	CA-C-N	-5.42	112.59	120.29
1	A	227	ILE	C-N-CA	-5.42	112.59	120.29
1	A	765	THR	CA-C-N	-5.42	112.39	122.09
1	A	765	THR	C-N-CA	-5.42	112.39	122.09
1	F	109	ILE	CB-CA-C	-5.42	102.41	111.29
1	A	450	ASN	N-CA-C	-5.42	100.41	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	TYR	N-CA-C	-5.41	101.65	110.20
2	S	132	GLY	N-CA-C	5.41	123.09	115.30
1	A	109	ILE	CB-CA-C	-5.41	102.42	111.29
1	E	109	ILE	CB-CA-C	-5.41	102.43	111.29
1	E	187	SER	CA-C-N	-5.40	111.33	120.95
1	E	187	SER	C-N-CA	-5.40	111.33	120.95
1	E	433	TYR	N-CA-C	-5.40	101.66	110.20
1	C	127	SER	N-CA-C	5.40	118.16	108.17
1	D	433	TYR	N-CA-C	-5.40	101.67	110.20
1	F	187	SER	CA-C-N	-5.40	111.34	120.95
1	F	187	SER	C-N-CA	-5.40	111.34	120.95
1	B	187	SER	CA-C-N	-5.39	111.35	120.95
1	B	187	SER	C-N-CA	-5.39	111.35	120.95
1	D	109	ILE	CB-CA-C	-5.39	102.44	111.29
1	C	187	SER	CA-C-N	-5.39	111.36	120.95
1	C	187	SER	C-N-CA	-5.39	111.36	120.95
1	C	450	ASN	N-CA-C	-5.39	100.45	109.24
1	A	187	SER	CA-C-N	-5.39	111.36	120.95
1	A	187	SER	C-N-CA	-5.39	111.36	120.95
1	C	286	GLU	N-CA-C	-5.39	107.01	113.21
1	B	109	ILE	CB-CA-C	-5.39	102.45	111.29
1	C	109	ILE	CB-CA-C	-5.39	102.46	111.29
1	E	741	ILE	N-CA-C	-5.39	101.73	108.84
1	D	187	SER	CA-C-N	-5.38	111.36	120.95
1	D	187	SER	C-N-CA	-5.38	111.36	120.95
1	E	286	GLU	N-CA-C	-5.38	107.03	113.21
1	D	286	GLU	N-CA-C	-5.37	107.03	113.21
1	F	566	TYR	N-CA-C	-5.37	106.77	113.15
1	E	450	ASN	N-CA-C	-5.36	100.50	109.24
1	A	286	GLU	N-CA-C	-5.36	107.04	113.21
1	B	286	GLU	N-CA-C	-5.36	107.05	113.21
1	D	741	ILE	N-CA-C	-5.36	101.77	108.84
1	E	129	ASN	CA-CB-CG	5.36	117.96	112.60
1	C	566	TYR	N-CA-C	-5.36	106.78	113.15
1	F	283	LEU	N-CA-C	-5.36	105.88	112.90
1	A	283	LEU	N-CA-C	-5.35	105.89	112.90
1	B	283	LEU	N-CA-C	-5.35	105.90	112.90
1	D	566	TYR	N-CA-C	-5.34	106.79	113.15
1	F	450	ASN	N-CA-C	-5.34	100.53	109.24
1	B	769	SER	N-CA-C	5.34	122.17	110.80
1	D	769	SER	N-CA-C	5.33	122.15	110.80
1	A	769	SER	N-CA-C	5.33	122.14	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	433	TYR	N-CA-C	-5.33	101.79	110.20
1	D	189	ASP	CA-C-N	-5.32	113.19	119.84
1	D	189	ASP	C-N-CA	-5.32	113.19	119.84
1	E	769	SER	N-CA-C	5.32	122.13	110.80
1	C	433	TYR	N-CA-C	-5.32	101.80	110.20
1	F	769	SER	N-CA-C	5.32	122.12	110.80
1	A	741	ILE	N-CA-C	-5.31	101.83	108.84
1	D	190	PRO	N-CA-C	-5.31	101.52	112.47
1	E	740	GLN	N-CA-C	5.31	118.93	110.70
1	A	566	TYR	N-CA-C	-5.31	106.83	113.15
1	B	740	GLN	N-CA-C	5.30	118.92	110.70
1	A	740	GLN	N-CA-C	5.30	118.91	110.70
1	B	741	ILE	N-CA-C	-5.30	101.84	108.84
1	C	83	GLN	N-CA-C	-5.30	105.15	111.03
1	D	132	GLY	N-CA-C	-5.30	103.55	112.77
1	F	83	GLN	N-CA-C	-5.30	105.15	111.03
1	D	83	GLN	N-CA-C	-5.30	105.15	111.03
1	F	132	GLY	N-CA-C	-5.30	103.55	112.77
1	E	566	TYR	N-CA-C	-5.30	106.85	113.15
1	C	769	SER	N-CA-C	5.29	122.08	110.80
1	D	740	GLN	N-CA-C	5.29	118.91	110.70
1	C	66	LEU	N-CA-C	5.29	118.07	111.24
1	C	132	GLY	N-CA-C	-5.28	103.58	112.77
1	F	741	ILE	N-CA-C	-5.28	101.80	108.93
1	B	695	LYS	N-CA-C	-5.28	105.94	112.38
1	E	283	LEU	N-CA-C	-5.28	105.99	112.90
1	A	127	SER	N-CA-C	5.27	117.93	108.17
1	B	190	PRO	CB-CA-C	5.27	120.26	111.56
1	F	629	ASN	N-CA-C	5.26	118.43	110.64
1	E	790	PHE	N-CA-C	-5.25	105.63	111.36
1	D	724	ARG	N-CA-C	-5.24	104.82	111.11
1	B	469	PHE	N-CA-C	5.24	116.76	108.96
1	D	239	HIS	N-CA-C	-5.24	106.58	112.87
1	B	190	PRO	N-CA-C	-5.23	101.69	112.47
1	C	695	LYS	N-CA-C	-5.23	106.00	112.38
1	E	260	TYR	CB-CA-C	-5.21	101.03	110.56
1	A	724	ARG	N-CA-C	-5.21	104.86	111.11
1	A	469	PHE	N-CA-C	5.20	116.71	108.96
1	B	260	TYR	CB-CA-C	-5.20	101.05	110.56
1	D	283	LEU	N-CA-C	-5.19	106.10	112.90
1	F	790	PHE	N-CA-C	-5.19	105.70	111.36
1	E	66	LEU	N-CA-C	5.19	117.93	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	239	HIS	N-CA-C	-5.18	106.65	112.87
1	B	83	GLN	N-CA-C	-5.17	105.29	111.03
2	S	43	PRO	N-CA-C	-5.17	103.05	111.68
1	E	83	GLN	N-CA-C	-5.17	105.30	111.03
1	D	629	ASN	N-CA-C	5.16	118.28	110.64
2	P	43	PRO	N-CA-C	-5.16	103.06	111.68
2	T	43	PRO	N-CA-C	-5.16	103.06	111.68
2	O	43	PRO	N-CA-C	-5.15	103.08	111.68
2	S	23	GLY	N-CA-C	5.15	125.38	113.18
1	D	636	ALA	CA-C-N	5.14	126.27	119.84
1	D	636	ALA	C-N-CA	5.14	126.27	119.84
2	Q	23	GLY	N-CA-C	5.14	125.36	113.18
1	C	469	PHE	N-CA-C	5.14	116.88	109.07
1	F	190	PRO	CB-CA-C	5.13	120.03	111.56
1	F	469	PHE	N-CA-C	5.13	116.87	109.07
1	D	695	LYS	N-CA-C	-5.13	106.12	112.38
2	R	43	PRO	N-CA-C	-5.13	103.11	111.68
2	P	23	GLY	N-CA-C	5.12	125.32	113.18
1	C	146	LYS	CA-C-N	-5.12	111.82	120.58
1	C	146	LYS	C-N-CA	-5.12	111.82	120.58
2	T	23	GLY	N-CA-C	5.12	125.31	113.18
1	E	239	HIS	N-CA-C	-5.12	106.73	112.87
1	B	239	HIS	N-CA-C	-5.11	106.74	112.87
2	O	23	GLY	N-CA-C	5.11	125.28	113.18
1	B	586	PHE	CA-C-N	5.10	125.02	119.76
1	B	586	PHE	C-N-CA	5.10	125.02	119.76
1	E	180	ASP	O-C-N	5.09	129.36	122.59
2	R	23	GLY	N-CA-C	5.09	125.24	113.18
2	Q	43	PRO	N-CA-C	-5.08	103.19	111.68
1	B	629	ASN	N-CA-C	5.08	118.16	110.64
1	F	695	LYS	N-CA-C	-5.07	106.19	112.38
1	A	790	PHE	N-CA-C	-5.07	105.83	111.36
1	E	629	ASN	N-CA-C	5.06	118.14	110.64
1	E	695	LYS	N-CA-C	-5.06	106.21	112.38
1	C	629	ASN	N-CA-C	5.05	118.12	110.64
1	F	636	ALA	CA-C-N	5.05	126.15	119.84
1	F	636	ALA	C-N-CA	5.05	126.15	119.84
1	E	469	PHE	N-CA-C	5.05	116.48	108.96
1	C	239	HIS	N-CA-C	-5.05	106.81	112.87
1	C	110	ASP	CA-C-N	-5.04	114.60	122.42
1	C	110	ASP	C-N-CA	-5.04	114.60	122.42
1	A	586	PHE	CA-C-N	5.04	124.95	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	586	PHE	C-N-CA	5.04	124.95	119.76
1	E	617	LYS	N-CA-C	5.04	116.58	111.14
1	D	469	PHE	N-CA-C	5.03	116.72	109.07
1	D	790	PHE	N-CA-C	-5.03	105.88	111.36
1	F	488	LEU	N-CA-C	5.03	117.69	109.59
1	E	586	PHE	CA-C-N	5.02	124.93	119.76
1	E	586	PHE	C-N-CA	5.02	124.93	119.76
1	A	629	ASN	N-CA-C	5.01	118.06	110.64
1	E	488	LEU	N-CA-C	5.01	117.66	109.59
1	E	724	ARG	N-CA-C	-5.01	105.10	111.11
1	C	790	PHE	N-CA-C	-5.01	105.90	111.36
1	A	239	HIS	N-CA-C	-5.01	106.86	112.87
1	A	695	LYS	N-CA-C	-5.00	106.27	112.38
1	C	617	LYS	N-CA-C	5.00	116.54	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5992	0	6010	831	0
1	B	5992	0	6010	841	0
1	C	5992	0	6010	832	0
1	D	5992	0	6010	833	0
1	E	5992	0	6010	836	0
1	F	5992	0	6010	826	0
2	O	1146	0	1071	153	0
2	P	1146	0	1071	159	0
2	Q	1146	0	1071	163	0
2	R	1146	0	1071	161	0
2	S	1146	0	1071	162	0
2	T	1146	0	1071	161	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	22	0	11	4	0
4	B	22	0	11	4	0
4	C	22	0	11	4	0
4	D	22	0	11	4	0
4	E	22	0	11	4	0
4	F	22	0	11	4	0
5	O	3	0	0	0	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	42990	0	42552	5779	0

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 68.

All (5779) 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)
4:A:901:CMP:C2	4:A:901:CMP:H2	0.97	1.49
4:D:904:CMP:H2	4:D:904:CMP:C2	0.97	1.49
4:B:902:CMP:H2	4:B:902:CMP:C2	0.97	1.48
4:C:903:CMP:H2	4:C:903:CMP:C2	0.97	1.48
4:F:906:CMP:H2	4:F:906:CMP:C2	0.97	1.47
4:E:905:CMP:H2	4:E:905:CMP:C2	0.97	1.47
1:A:179:LEU:O	1:A:183:SER:CB	1.67	1.42
1:B:179:LEU:O	1:B:183:SER:CB	1.66	1.40
1:D:179:LEU:O	1:D:183:SER:CB	1.71	1.39
1:E:179:LEU:O	1:E:183:SER:CB	1.69	1.39
1:C:179:LEU:O	1:C:183:SER:CB	1.73	1.35
1:B:179:LEU:O	1:B:183:SER:HB2	1.14	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:O	1:A:183:SER:HB2	1.12	1.30
1:D:179:LEU:O	1:D:183:SER:HB2	1.12	1.29
1:C:179:LEU:O	1:C:183:SER:HB2	1.14	1.28
1:E:179:LEU:O	1:E:183:SER:HB2	1.18	1.28
1:D:186:LYS:HA	1:D:190:PRO:HD3	1.20	1.17
1:A:186:LYS:HA	1:A:190:PRO:HD3	1.21	1.15
1:B:186:LYS:HA	1:B:190:PRO:HD3	1.20	1.13
1:C:296:LEU:HD23	1:C:296:LEU:N	1.64	1.12
1:E:186:LYS:CA	1:E:190:PRO:HD3	1.80	1.12
1:D:296:LEU:HD23	1:D:296:LEU:N	1.64	1.12
1:E:186:LYS:HA	1:E:190:PRO:HD3	1.11	1.10
1:E:296:LEU:H	1:E:296:LEU:CD2	1.60	1.10
1:F:296:LEU:H	1:F:296:LEU:CD2	1.59	1.10
1:C:296:LEU:H	1:C:296:LEU:CD2	1.59	1.10
1:B:296:LEU:H	1:B:296:LEU:CD2	1.60	1.09
1:E:296:LEU:HD23	1:E:296:LEU:N	1.64	1.09
1:A:296:LEU:H	1:A:296:LEU:CD2	1.60	1.09
1:D:296:LEU:H	1:D:296:LEU:CD2	1.60	1.09
1:A:296:LEU:HD23	1:A:296:LEU:N	1.64	1.09
1:C:186:LYS:HA	1:C:190:PRO:HD3	1.29	1.08
1:B:134:LYS:HG2	1:B:136:PRO:HD3	1.35	1.08
1:B:186:LYS:CA	1:B:190:PRO:HD3	1.83	1.07
1:B:296:LEU:HD23	1:B:296:LEU:N	1.64	1.06
1:B:179:LEU:O	1:B:183:SER:CA	2.04	1.05
1:E:179:LEU:O	1:E:183:SER:CA	2.05	1.05
1:F:296:LEU:HD23	1:F:296:LEU:N	1.64	1.05
1:E:134:LYS:HG2	1:E:136:PRO:HD3	1.38	1.05
1:A:296:LEU:HD22	1:A:606:LYS:HE2	1.35	1.04
1:D:186:LYS:CA	1:D:190:PRO:HD3	1.87	1.04
1:F:161:ILE:HA	1:F:167:LYS:HD2	1.38	1.04
1:A:186:LYS:CA	1:A:190:PRO:HD3	1.88	1.04
1:F:191:GLU:O	1:F:193:LEU:N	1.92	1.03
1:F:186:LYS:HA	1:F:190:PRO:HD3	1.41	1.03
1:C:161:ILE:HA	1:C:167:LYS:HD2	1.40	1.03
1:D:161:ILE:HA	1:D:167:LYS:HD2	1.40	1.02
1:E:180:ASP:OD1	1:E:180:ASP:N	1.91	1.02
1:A:161:ILE:HA	1:A:167:LYS:HD2	1.41	1.02
1:B:746:LYS:O	1:B:750:GLN:HG2	1.59	1.02
1:F:89:ILE:HD13	1:F:175:LYS:HE2	1.39	1.02
1:B:64:ASN:HD22	1:B:64:ASN:N	1.47	1.02
1:B:188:LEU:HD23	1:B:188:LEU:H	1.22	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ILE:HD13	1:C:175:LYS:HE2	1.39	1.02
1:C:188:LEU:HD23	1:C:188:LEU:H	1.22	1.02
1:D:188:LEU:H	1:D:188:LEU:HD23	1.22	1.02
1:A:89:ILE:HD13	1:A:175:LYS:HE2	1.38	1.01
1:A:134:LYS:HG2	1:A:136:PRO:HD3	1.41	1.01
1:B:296:LEU:HD22	1:B:606:LYS:HE2	1.38	1.01
1:D:296:LEU:HD22	1:D:606:LYS:HE2	1.39	1.01
1:E:89:ILE:HD13	1:E:175:LYS:HE2	1.39	1.01
1:B:161:ILE:HA	1:B:167:LYS:HD2	1.40	1.01
1:C:746:LYS:O	1:C:750:GLN:HG2	1.60	1.01
1:E:161:ILE:HA	1:E:167:LYS:HD2	1.38	1.01
2:Q:36:MET:HE3	2:Q:43:PRO:HG3	1.42	1.01
1:A:188:LEU:HD23	1:A:188:LEU:H	1.22	1.01
1:E:668:SER:HA	2:S:14:GLU:HG3	1.43	1.01
1:A:179:LEU:O	1:A:183:SER:CA	2.08	1.00
1:E:179:LEU:O	1:E:183:SER:N	1.92	1.00
1:E:188:LEU:HD23	1:E:188:LEU:H	1.22	1.00
1:B:134:LYS:HG2	1:B:136:PRO:CD	1.92	1.00
1:B:180:ASP:OD1	1:B:180:ASP:N	1.91	1.00
1:C:548:THR:H	4:C:903:CMP:HN61	1.09	0.99
1:B:179:LEU:O	1:B:183:SER:N	1.94	0.99
1:F:188:LEU:HD23	1:F:188:LEU:H	1.22	0.99
1:C:180:ASP:N	1:C:180:ASP:OD1	1.91	0.99
1:E:746:LYS:O	1:E:750:GLN:HG2	1.60	0.99
1:F:548:THR:H	4:F:906:CMP:HN61	1.08	0.99
2:T:36:MET:HE3	2:T:43:PRO:HG3	1.43	0.99
2:P:37:ARG:HA	2:P:41:GLN:O	1.63	0.99
1:A:746:LYS:O	1:A:750:GLN:HG2	1.62	0.99
1:E:296:LEU:HD22	1:E:606:LYS:HE2	1.42	0.99
1:A:180:ASP:OD1	1:A:180:ASP:N	1.91	0.99
2:R:36:MET:HE3	2:R:43:PRO:HG3	1.44	0.99
1:D:89:ILE:HD13	1:D:175:LYS:HE2	1.42	0.99
1:B:89:ILE:HD13	1:B:175:LYS:HE2	1.41	0.98
1:D:746:LYS:O	1:D:750:GLN:HG2	1.61	0.98
2:Q:13:LYS:HZ3	2:Q:65:PHE:HB3	1.26	0.98
1:C:296:LEU:HD22	1:C:606:LYS:HE2	1.42	0.98
1:F:296:LEU:HD22	1:F:606:LYS:HE2	1.43	0.98
2:O:36:MET:HE3	2:O:43:PRO:HG3	1.43	0.98
1:E:186:LYS:C	1:E:188:LEU:O	2.07	0.97
1:F:668:SER:HA	2:T:14:GLU:HG3	1.46	0.97
2:O:37:ARG:HA	2:O:41:GLN:O	1.65	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:36:MET:HE3	2:S:43:PRO:HG3	1.44	0.97
1:F:746:LYS:O	1:F:750:GLN:HG2	1.62	0.97
1:A:186:LYS:C	1:A:188:LEU:O	2.07	0.97
1:D:180:ASP:OD1	1:D:180:ASP:N	1.91	0.96
1:D:548:THR:H	4:D:904:CMP:HN61	1.07	0.96
1:C:173:ILE:HG13	1:C:242:SER:HB3	1.44	0.96
1:C:188:LEU:H	1:C:188:LEU:CD2	1.78	0.96
1:D:173:ILE:HG13	1:D:242:SER:HB3	1.45	0.96
1:F:186:LYS:C	1:F:188:LEU:O	2.07	0.96
1:D:188:LEU:H	1:D:188:LEU:CD2	1.78	0.96
1:B:173:ILE:HG13	1:B:242:SER:HB3	1.46	0.96
1:F:173:ILE:HG13	1:F:242:SER:HB3	1.45	0.96
1:E:329:ARG:HD2	1:E:590:ASP:OD2	1.66	0.96
1:F:188:LEU:H	1:F:188:LEU:CD2	1.78	0.96
2:T:13:LYS:HZ3	2:T:65:PHE:HB3	1.31	0.96
1:C:296:LEU:HD23	1:C:296:LEU:H	0.79	0.95
2:P:36:MET:HE3	2:P:43:PRO:HG3	1.44	0.95
2:S:37:ARG:HA	2:S:41:GLN:O	1.65	0.95
1:D:296:LEU:HD23	1:D:296:LEU:H	0.79	0.95
1:E:134:LYS:HG2	1:E:136:PRO:CD	1.95	0.95
1:A:188:LEU:H	1:A:188:LEU:CD2	1.78	0.95
1:B:668:SER:HA	2:P:14:GLU:HG3	1.47	0.95
1:B:329:ARG:HD2	1:B:590:ASP:OD2	1.66	0.95
1:C:186:LYS:C	1:C:188:LEU:O	2.09	0.95
2:R:37:ARG:HA	2:R:41:GLN:O	1.66	0.95
1:D:186:LYS:C	1:D:188:LEU:O	2.10	0.95
1:F:296:LEU:H	1:F:296:LEU:HD23	0.79	0.95
1:A:173:ILE:HG13	1:A:242:SER:HB3	1.47	0.95
1:A:548:THR:H	4:A:901:CMP:HN61	1.07	0.95
1:C:329:ARG:HD2	1:C:590:ASP:OD2	1.66	0.95
1:F:180:ASP:OD1	1:F:180:ASP:N	1.91	0.95
1:C:179:LEU:O	1:C:183:SER:CA	2.14	0.95
1:E:548:THR:H	4:E:905:CMP:HN61	1.07	0.95
1:D:179:LEU:O	1:D:183:SER:CA	2.13	0.95
1:A:128:MET:HE2	1:A:239:HIS:NE2	1.83	0.94
1:A:179:LEU:O	1:A:183:SER:N	1.99	0.94
1:B:188:LEU:H	1:B:188:LEU:CD2	1.78	0.94
1:E:188:LEU:H	1:E:188:LEU:CD2	1.78	0.94
2:S:13:LYS:HZ3	2:S:65:PHE:HB3	1.30	0.94
1:A:296:LEU:H	1:A:296:LEU:HD23	0.79	0.94
1:E:173:ILE:HG13	1:E:242:SER:HB3	1.46	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:HG2	1:A:136:PRO:CD	1.98	0.94
1:B:186:LYS:C	1:B:188:LEU:O	2.09	0.94
1:F:697:ILE:HD13	1:F:732:ILE:HD13	1.50	0.94
1:A:329:ARG:HD2	1:A:590:ASP:OD2	1.67	0.94
1:A:697:ILE:HD13	1:A:732:ILE:HD13	1.49	0.94
1:E:697:ILE:HD13	1:E:732:ILE:HD13	1.49	0.94
1:E:296:LEU:H	1:E:296:LEU:HD23	0.79	0.94
1:C:668:SER:HA	2:Q:14:GLU:HG3	1.50	0.94
1:D:668:SER:HA	2:R:14:GLU:HG3	1.50	0.94
1:A:668:SER:HA	2:O:14:GLU:HG3	1.49	0.93
1:C:186:LYS:CA	1:C:190:PRO:HD3	1.96	0.93
1:F:134:LYS:HG2	1:F:136:PRO:HD3	1.47	0.93
2:Q:37:ARG:HA	2:Q:41:GLN:O	1.68	0.93
1:B:697:ILE:HD13	1:B:732:ILE:HD13	1.49	0.93
1:D:697:ILE:HD13	1:D:732:ILE:HD13	1.51	0.93
2:P:13:LYS:HZ3	2:P:65:PHE:HB3	1.32	0.93
2:T:37:ARG:HA	2:T:41:GLN:O	1.67	0.93
1:D:308:VAL:HB	1:D:311:HIS:ND1	1.83	0.93
1:F:329:ARG:HD2	1:F:590:ASP:OD2	1.67	0.93
2:O:65:PHE:HB2	2:O:66:PRO:HD3	1.50	0.93
1:C:697:ILE:HD13	1:C:732:ILE:HD13	1.50	0.93
1:A:308:VAL:HB	1:A:311:HIS:ND1	1.83	0.93
1:D:329:ARG:HD2	1:D:590:ASP:OD2	1.67	0.92
1:D:134:LYS:HG2	1:D:136:PRO:HD3	1.48	0.92
1:C:131:ARG:H	1:C:170:TYR:HE2	1.14	0.92
1:E:187:SER:C	1:E:188:LEU:O	2.04	0.92
1:B:296:LEU:H	1:B:296:LEU:HD23	0.79	0.92
1:C:179:LEU:O	1:C:183:SER:N	2.03	0.92
1:F:308:VAL:HB	1:F:311:HIS:ND1	1.84	0.92
2:R:97:ASN:HD22	2:R:97:ASN:H	1.18	0.92
1:B:548:THR:H	4:B:902:CMP:HN61	1.07	0.92
1:C:308:VAL:HB	1:C:311:HIS:ND1	1.85	0.92
1:B:188:LEU:HD23	1:B:188:LEU:N	1.85	0.92
2:S:97:ASN:H	2:S:97:ASN:HD22	1.17	0.92
1:B:187:SER:C	1:B:188:LEU:O	2.05	0.91
1:C:187:SER:C	1:C:188:LEU:O	2.05	0.91
1:E:308:VAL:HB	1:E:311:HIS:ND1	1.83	0.91
1:B:308:VAL:HB	1:B:311:HIS:ND1	1.84	0.91
1:E:186:LYS:HA	1:E:190:PRO:CD	1.99	0.91
1:D:635:ILE:H	1:D:635:ILE:HD12	1.35	0.91
2:P:65:PHE:HB2	2:P:66:PRO:HD3	1.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:65:PHE:HB2	2:Q:66:PRO:HD3	1.51	0.91
1:B:635:ILE:H	1:B:635:ILE:HD12	1.36	0.91
1:C:635:ILE:H	1:C:635:ILE:HD12	1.35	0.91
2:T:97:ASN:H	2:T:97:ASN:HD22	1.18	0.91
1:C:405:LEU:HD13	1:C:453:VAL:HG21	1.52	0.91
2:O:97:ASN:HD22	2:O:97:ASN:H	1.19	0.91
2:P:97:ASN:HD22	2:P:97:ASN:H	1.19	0.91
1:F:405:LEU:HD13	1:F:453:VAL:HG21	1.53	0.91
2:S:65:PHE:HB2	2:S:66:PRO:HD3	1.50	0.91
1:A:131:ARG:H	1:A:170:TYR:HE2	1.16	0.91
1:D:405:LEU:HD13	1:D:453:VAL:HG21	1.53	0.91
2:T:65:PHE:HB2	2:T:66:PRO:HD3	1.50	0.90
1:B:131:ARG:H	1:B:170:TYR:HE2	1.17	0.90
2:R:65:PHE:HB2	2:R:66:PRO:HD3	1.53	0.90
1:A:635:ILE:H	1:A:635:ILE:HD12	1.34	0.90
1:B:179:LEU:C	1:B:183:SER:HB2	1.96	0.90
1:A:187:SER:C	1:A:188:LEU:O	2.04	0.90
1:E:405:LEU:HD13	1:E:453:VAL:HG21	1.53	0.90
2:P:97:ASN:H	2:P:97:ASN:ND2	1.70	0.90
2:Q:30:LYS:HD3	2:Q:30:LYS:H	1.37	0.90
2:S:5:THR:HG23	2:S:8:GLN:HB2	1.54	0.90
2:S:30:LYS:HD3	2:S:30:LYS:H	1.37	0.90
1:F:131:ARG:H	1:F:170:TYR:HE2	1.16	0.89
1:A:188:LEU:HD23	1:A:188:LEU:N	1.85	0.89
1:C:188:LEU:HD23	1:C:188:LEU:N	1.85	0.89
1:F:188:LEU:HD23	1:F:188:LEU:N	1.85	0.89
1:F:635:ILE:H	1:F:635:ILE:HD12	1.37	0.89
1:D:187:SER:C	1:D:188:LEU:O	2.05	0.89
1:A:179:LEU:C	1:A:183:SER:HB2	1.97	0.89
1:A:405:LEU:HD13	1:A:453:VAL:HG21	1.54	0.89
2:P:5:THR:HG23	2:P:8:GLN:HB2	1.54	0.89
1:D:179:LEU:O	1:D:183:SER:N	2.04	0.89
1:A:275:GLY:HA2	1:A:278:LYS:HG3	1.55	0.89
2:R:5:THR:HG23	2:R:8:GLN:HB2	1.55	0.89
2:R:13:LYS:HZ3	2:R:65:PHE:HB3	1.35	0.89
2:R:30:LYS:H	2:R:30:LYS:HD3	1.37	0.89
2:T:30:LYS:H	2:T:30:LYS:HD3	1.36	0.89
1:D:131:ARG:H	1:D:170:TYR:HE2	1.13	0.89
2:R:100:ILE:HB	2:R:136:VAL:HG23	1.55	0.89
1:D:275:GLY:HA2	1:D:278:LYS:HG3	1.55	0.88
1:F:187:SER:C	1:F:188:LEU:O	2.04	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:5:THR:HG23	2:O:8:GLN:HB2	1.55	0.88
1:B:405:LEU:HD13	1:B:453:VAL:HG21	1.54	0.88
2:P:100:ILE:HB	2:P:136:VAL:HG23	1.55	0.88
2:Q:5:THR:HG23	2:Q:8:GLN:HB2	1.55	0.88
1:D:175:LYS:HB2	1:D:175:LYS:NZ	1.88	0.88
2:O:30:LYS:H	2:O:30:LYS:HD3	1.37	0.88
1:B:128:MET:HE2	1:B:239:HIS:NE2	1.88	0.88
1:C:759:GLN:HE21	1:C:759:GLN:HA	1.38	0.88
1:F:479:LYS:HG2	1:F:488:LEU:HD21	1.56	0.88
2:P:30:LYS:HD3	2:P:30:LYS:H	1.37	0.88
2:T:5:THR:HG23	2:T:8:GLN:HB2	1.55	0.88
1:B:630:ARG:CZ	2:P:83:GLU:HG2	2.04	0.88
1:D:89:ILE:HG22	1:D:93:VAL:HG11	1.55	0.88
2:O:100:ILE:HB	2:O:136:VAL:HG23	1.56	0.88
2:Q:97:ASN:H	2:Q:97:ASN:HD22	1.20	0.88
1:A:89:ILE:HG22	1:A:93:VAL:HG11	1.55	0.88
1:A:175:LYS:HB2	1:A:175:LYS:NZ	1.89	0.88
1:E:635:ILE:HD12	1:E:635:ILE:H	1.36	0.88
1:F:175:LYS:HB2	1:F:175:LYS:NZ	1.89	0.88
1:B:89:ILE:HG22	1:B:93:VAL:HG11	1.56	0.88
1:C:275:GLY:HA2	1:C:278:LYS:HG3	1.54	0.88
1:E:175:LYS:NZ	1:E:175:LYS:HB2	1.88	0.88
1:F:89:ILE:HG22	1:F:93:VAL:HG11	1.56	0.88
1:E:188:LEU:HD23	1:E:188:LEU:N	1.85	0.87
2:Q:100:ILE:HB	2:Q:136:VAL:HG23	1.55	0.87
2:S:97:ASN:H	2:S:97:ASN:ND2	1.69	0.87
1:B:275:GLY:HA2	1:B:278:LYS:HG3	1.56	0.87
1:C:678:VAL:HG22	1:C:745:TYR:CE2	2.09	0.87
2:R:13:LYS:NZ	2:R:65:PHE:HB3	1.88	0.87
1:B:759:GLN:HA	1:B:759:GLN:HE21	1.39	0.87
1:E:759:GLN:HA	1:E:759:GLN:HE21	1.40	0.87
1:C:175:LYS:HB2	1:C:175:LYS:NZ	1.90	0.87
1:D:188:LEU:HD23	1:D:188:LEU:N	1.85	0.87
1:E:479:LYS:HG2	1:E:488:LEU:HD21	1.57	0.87
1:F:759:GLN:HE21	1:F:759:GLN:HA	1.40	0.87
1:C:142:VAL:HG22	1:C:154:ILE:HD12	1.56	0.87
1:E:89:ILE:HG22	1:E:93:VAL:HG11	1.57	0.87
2:O:97:ASN:H	2:O:97:ASN:ND2	1.70	0.87
1:D:722:ILE:HG23	1:D:760:VAL:HG13	1.57	0.87
1:E:131:ARG:H	1:E:170:TYR:HE2	1.18	0.87
1:F:134:LYS:HG2	1:F:136:PRO:CD	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:13:LYS:NZ	2:S:65:PHE:HB3	1.90	0.87
2:T:100:ILE:HB	2:T:136:VAL:HG23	1.55	0.86
2:O:13:LYS:HZ3	2:O:65:PHE:HB3	1.38	0.86
1:D:464:VAL:HG23	1:D:465:LEU:HD12	1.57	0.86
1:C:479:LYS:HG2	1:C:488:LEU:HD21	1.54	0.86
1:E:275:GLY:HA2	1:E:278:LYS:HG3	1.56	0.86
1:C:89:ILE:HG22	1:C:93:VAL:HG11	1.58	0.86
1:C:769:SER:O	1:C:769:SER:OG	1.90	0.86
1:F:678:VAL:HG22	1:F:745:TYR:CE2	2.10	0.86
2:T:13:LYS:NZ	2:T:65:PHE:HB3	1.91	0.86
1:A:678:VAL:HG22	1:A:745:TYR:CE2	2.09	0.86
1:B:175:LYS:HB2	1:B:175:LYS:NZ	1.89	0.86
1:B:186:LYS:HA	1:B:190:PRO:CD	2.04	0.86
1:C:134:LYS:HG2	1:C:136:PRO:HD3	1.54	0.86
2:Q:13:LYS:NZ	2:Q:65:PHE:HB3	1.90	0.86
1:D:678:VAL:HG22	1:D:745:TYR:CE2	2.10	0.86
1:E:179:LEU:C	1:E:183:SER:HB2	2.00	0.86
1:D:759:GLN:HA	1:D:759:GLN:HE21	1.40	0.86
1:A:479:LYS:HG2	1:A:488:LEU:HD21	1.56	0.86
1:B:479:LYS:HG2	1:B:488:LEU:HD21	1.56	0.86
1:D:179:LEU:C	1:D:183:SER:HB2	2.01	0.85
2:S:100:ILE:HB	2:S:136:VAL:HG23	1.56	0.85
1:C:722:ILE:HG23	1:C:760:VAL:HG13	1.58	0.85
1:D:134:LYS:HG2	1:D:136:PRO:CD	2.05	0.85
1:A:464:VAL:HG23	1:A:465:LEU:HD12	1.58	0.85
1:B:142:VAL:HG22	1:B:154:ILE:HD12	1.58	0.85
1:B:678:VAL:HG22	1:B:745:TYR:CE2	2.11	0.85
1:C:464:VAL:HG23	1:C:465:LEU:HD12	1.57	0.85
1:D:142:VAL:HG22	1:D:154:ILE:HD12	1.57	0.85
1:E:678:VAL:HG22	1:E:745:TYR:CE2	2.10	0.85
1:F:464:VAL:HG23	1:F:465:LEU:HD12	1.57	0.85
1:F:722:ILE:HG23	1:F:760:VAL:HG13	1.58	0.85
1:E:630:ARG:CZ	2:S:83:GLU:HG2	2.06	0.85
1:D:479:LYS:HG2	1:D:488:LEU:HD21	1.56	0.85
1:A:165:GLN:CD	1:A:252:ASP:HB3	2.02	0.85
1:F:165:GLN:CD	1:F:252:ASP:HB3	2.01	0.85
1:C:628:PHE:HE2	2:Q:90:ARG:HD3	1.41	0.85
1:E:464:VAL:HG23	1:E:465:LEU:HD12	1.57	0.85
1:D:165:GLN:CD	1:D:252:ASP:HB3	2.02	0.85
2:P:13:LYS:NZ	2:P:65:PHE:HB3	1.91	0.85
1:A:759:GLN:HA	1:A:759:GLN:HE21	1.42	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:SER:OG	1:A:769:SER:O	1.89	0.85
1:B:64:ASN:N	1:B:64:ASN:ND2	2.19	0.85
1:D:131:ARG:HG3	1:D:243:LEU:CD2	2.07	0.85
1:E:131:ARG:HG3	1:E:243:LEU:CD2	2.06	0.85
1:B:74:GLU:HB2	1:B:78:LYS:HB3	1.59	0.84
1:F:630:ARG:CZ	2:T:83:GLU:HG2	2.07	0.84
1:A:142:VAL:HG22	1:A:154:ILE:HD12	1.57	0.84
1:F:275:GLY:HA2	1:F:278:LYS:HG3	1.57	0.84
1:A:186:LYS:HA	1:A:190:PRO:CD	2.07	0.84
2:O:6:GLU:HG3	2:O:7:GLU:N	1.92	0.84
2:S:6:GLU:HG3	2:S:7:GLU:N	1.93	0.84
1:B:722:ILE:HG23	1:B:760:VAL:HG13	1.59	0.84
1:E:722:ILE:HG23	1:E:760:VAL:HG13	1.60	0.84
2:R:97:ASN:H	2:R:97:ASN:ND2	1.69	0.84
1:C:179:LEU:C	1:C:183:SER:HB2	2.03	0.84
2:P:6:GLU:HG3	2:P:7:GLU:N	1.93	0.84
1:B:165:GLN:CD	1:B:252:ASP:HB3	2.03	0.84
1:E:165:GLN:CD	1:E:252:ASP:HB3	2.03	0.84
1:A:722:ILE:HG23	1:A:760:VAL:HG13	1.59	0.84
2:O:13:LYS:NZ	2:O:65:PHE:HB3	1.91	0.84
1:B:464:VAL:HG23	1:B:465:LEU:HD12	1.57	0.84
1:A:630:ARG:CZ	2:O:83:GLU:HG2	2.08	0.83
2:R:6:GLU:HG3	2:R:7:GLU:N	1.92	0.83
1:B:186:LYS:CB	1:B:190:PRO:HD3	2.08	0.83
1:E:74:GLU:HB2	1:E:78:LYS:HB3	1.59	0.83
1:F:142:VAL:HG22	1:F:154:ILE:HD12	1.57	0.83
1:F:186:LYS:CA	1:F:190:PRO:HD3	2.07	0.83
1:F:191:GLU:O	1:F:192:PHE:C	2.20	0.83
1:E:142:VAL:HG22	1:E:154:ILE:HD12	1.58	0.83
2:T:6:GLU:HG3	2:T:7:GLU:N	1.93	0.83
1:C:165:GLN:CD	1:C:252:ASP:HB3	2.03	0.83
1:A:90:PRO:O	1:A:93:VAL:HG12	1.78	0.83
1:E:90:PRO:O	1:E:93:VAL:HG12	1.79	0.83
1:E:628:PHE:HE2	2:S:90:ARG:HD3	1.43	0.83
1:B:288:VAL:HG23	1:B:289:GLU:H	1.44	0.82
1:A:550:SER:HB3	1:A:553:GLN:HG3	1.59	0.82
1:D:186:LYS:HA	1:D:190:PRO:CD	2.05	0.82
1:F:90:PRO:O	1:F:93:VAL:HG12	1.78	0.82
1:F:628:PHE:HE2	2:T:90:ARG:HD3	1.44	0.82
1:B:107:THR:HG21	1:B:115:LYS:HD2	1.61	0.82
1:D:90:PRO:O	1:D:93:VAL:HG12	1.78	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:628:PHE:HE2	2:R:90:ARG:HD3	1.43	0.82
1:D:497:LEU:HD13	1:D:556:MET:HG2	1.62	0.82
1:E:781:ASN:H	1:E:789:ASN:HD21	1.27	0.82
2:Q:97:ASN:H	2:Q:97:ASN:ND2	1.71	0.82
2:R:97:ASN:HD22	2:R:97:ASN:N	1.76	0.82
1:D:630:ARG:CZ	2:R:83:GLU:HG2	2.10	0.81
1:F:769:SER:O	1:F:769:SER:OG	1.89	0.81
1:A:74:GLU:HB2	1:A:78:LYS:HB3	1.62	0.81
1:E:107:THR:HG21	1:E:115:LYS:HD2	1.60	0.81
1:F:140:ARG:HA	1:F:140:ARG:HE	1.44	0.81
1:C:90:PRO:O	1:C:93:VAL:HG12	1.79	0.81
1:C:630:ARG:CZ	2:Q:83:GLU:HG2	2.09	0.81
1:F:64:ASN:HD22	1:F:64:ASN:N	1.76	0.81
2:Q:6:GLU:HG3	2:Q:7:GLU:N	1.92	0.81
1:B:718:ARG:O	1:B:722:ILE:HG13	1.80	0.81
1:F:107:THR:HG21	1:F:115:LYS:HD2	1.62	0.81
1:E:288:VAL:HG23	1:E:289:GLU:H	1.45	0.81
1:A:628:PHE:HE2	2:O:90:ARG:HD3	1.43	0.81
1:E:769:SER:O	1:E:769:SER:OG	1.90	0.81
1:D:288:VAL:HG23	1:D:289:GLU:H	1.46	0.81
1:E:131:ARG:HG3	1:E:243:LEU:HD22	1.62	0.81
1:B:550:SER:HB3	1:B:553:GLN:HG3	1.62	0.81
1:C:324:THR:HB	1:C:499:PRO:HA	1.63	0.81
1:C:718:ARG:O	1:C:722:ILE:HG13	1.81	0.81
1:B:140:ARG:HA	1:B:140:ARG:HE	1.45	0.80
1:D:403:LEU:HD21	1:D:405:LEU:HD11	1.63	0.80
1:F:324:THR:HB	1:F:499:PRO:HA	1.64	0.80
1:F:781:ASN:H	1:F:789:ASN:HD21	1.28	0.80
2:T:97:ASN:H	2:T:97:ASN:ND2	1.70	0.80
1:C:288:VAL:HG23	1:C:289:GLU:H	1.47	0.80
1:A:140:ARG:HA	1:A:140:ARG:HE	1.46	0.80
1:B:628:PHE:HE2	2:P:90:ARG:HD3	1.44	0.80
2:P:12:PHE:HZ	2:P:76:MET:HE3	1.46	0.80
1:F:217:LYS:HB2	1:F:236:GLU:CD	2.07	0.80
2:S:12:PHE:HZ	2:S:76:MET:HE3	1.47	0.80
1:C:457:THR:HG21	1:C:468:LYS:HA	1.64	0.80
2:O:106:ARG:O	2:O:110:THR:HG23	1.81	0.80
1:D:131:ARG:HG3	1:D:243:LEU:HD22	1.64	0.80
1:E:217:LYS:HB2	1:E:236:GLU:CD	2.07	0.80
1:A:288:VAL:HG23	1:A:289:GLU:H	1.46	0.80
1:D:324:THR:HB	1:D:499:PRO:HA	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:VAL:HG23	1:F:289:GLU:H	1.47	0.80
1:F:718:ARG:O	1:F:722:ILE:HG13	1.81	0.80
1:B:781:ASN:H	1:B:789:ASN:HD21	1.28	0.80
1:C:140:ARG:HA	1:C:140:ARG:HE	1.46	0.80
1:C:550:SER:HB3	1:C:553:GLN:HG3	1.63	0.80
1:A:497:LEU:HD13	1:A:556:MET:HG2	1.64	0.79
1:B:90:PRO:O	1:B:93:VAL:HG12	1.80	0.79
1:B:318:ILE:HG23	1:B:322:LEU:HD12	1.64	0.79
1:B:403:LEU:HD21	1:B:405:LEU:HD11	1.64	0.79
1:D:550:SER:HB3	1:D:553:GLN:HG3	1.63	0.79
1:E:140:ARG:NE	1:E:140:ARG:HA	1.98	0.79
2:P:100:ILE:HB	2:P:136:VAL:CG2	2.12	0.79
2:Q:106:ARG:O	2:Q:110:THR:HG23	1.81	0.79
1:E:140:ARG:HA	1:E:140:ARG:HE	1.45	0.79
2:T:106:ARG:O	2:T:110:THR:HG23	1.82	0.79
1:A:718:ARG:O	1:A:722:ILE:HG13	1.82	0.79
1:C:403:LEU:HD21	1:C:405:LEU:HD11	1.64	0.79
1:F:140:ARG:HA	1:F:140:ARG:NE	1.98	0.79
1:F:457:THR:HG21	1:F:468:LYS:HA	1.64	0.79
1:F:550:SER:HB3	1:F:553:GLN:HG3	1.62	0.79
1:A:318:ILE:HG23	1:A:322:LEU:HD12	1.65	0.79
1:F:497:LEU:HD13	1:F:556:MET:HG2	1.64	0.79
2:R:106:ARG:O	2:R:110:THR:HG23	1.82	0.79
1:A:107:THR:HG21	1:A:115:LYS:HD2	1.64	0.79
1:A:296:LEU:CD2	1:A:606:LYS:HE2	2.13	0.79
1:D:781:ASN:H	1:D:789:ASN:HD21	1.28	0.79
1:E:318:ILE:HG23	1:E:322:LEU:HD12	1.64	0.79
1:E:550:SER:HB3	1:E:553:GLN:HG3	1.63	0.79
1:B:324:THR:HB	1:B:499:PRO:HA	1.64	0.79
1:E:457:THR:HG21	1:E:468:LYS:HA	1.64	0.79
1:F:501:LEU:HB2	1:F:623:ASP:O	1.82	0.79
1:A:324:THR:HB	1:A:499:PRO:HA	1.65	0.79
1:C:694:VAL:HG23	2:Q:18:LEU:HD11	1.64	0.79
1:D:140:ARG:HA	1:D:140:ARG:HE	1.46	0.79
1:D:457:THR:HG21	1:D:468:LYS:HA	1.64	0.79
1:D:718:ARG:O	1:D:722:ILE:HG13	1.82	0.79
1:D:769:SER:O	1:D:769:SER:OG	1.89	0.79
1:A:540:ARG:NH2	2:O:87:GLU:OE1	2.16	0.79
1:A:781:ASN:H	1:A:789:ASN:HD21	1.28	0.79
1:B:186:LYS:HB2	1:B:190:PRO:HD3	1.65	0.79
1:C:134:LYS:HG2	1:C:136:PRO:CD	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:THR:HB	1:E:499:PRO:HA	1.65	0.79
1:F:403:LEU:HD21	1:F:405:LEU:HD11	1.64	0.79
2:P:106:ARG:O	2:P:110:THR:HG23	1.83	0.79
1:A:457:THR:HG21	1:A:468:LYS:HA	1.63	0.79
2:S:100:ILE:HB	2:S:136:VAL:CG2	2.13	0.79
1:A:217:LYS:HB2	1:A:236:GLU:CD	2.08	0.78
2:S:97:ASN:HD22	2:S:97:ASN:N	1.75	0.78
1:A:550:SER:HB3	1:A:553:GLN:CG	2.12	0.78
1:B:497:LEU:HD13	1:B:556:MET:HG2	1.65	0.78
1:D:71:PHE:HB3	1:D:108:ASP:HB2	1.65	0.78
1:D:318:ILE:HG23	1:D:322:LEU:HD12	1.65	0.78
1:B:412:GLU:C	1:B:414:LYS:H	1.92	0.78
1:C:781:ASN:H	1:C:789:ASN:HD21	1.28	0.78
1:E:694:VAL:HG23	2:S:18:LEU:HD11	1.65	0.78
2:Q:100:ILE:HB	2:Q:136:VAL:CG2	2.13	0.78
1:C:217:LYS:HB2	1:C:236:GLU:CD	2.07	0.78
1:F:318:ILE:HG23	1:F:322:LEU:HD12	1.64	0.78
2:R:6:GLU:HG3	2:R:7:GLU:H	1.48	0.78
1:B:154:ILE:HG13	1:B:171:TYR:CE1	2.19	0.78
1:B:217:LYS:HB2	1:B:236:GLU:CD	2.08	0.78
1:C:71:PHE:HB3	1:C:108:ASP:HB2	1.65	0.78
1:E:412:GLU:C	1:E:414:LYS:H	1.91	0.78
1:A:403:LEU:HD21	1:A:405:LEU:HD11	1.66	0.78
1:D:153:ILE:O	1:D:154:ILE:HD13	1.84	0.78
2:O:12:PHE:HZ	2:O:76:MET:HE3	1.49	0.78
2:S:106:ARG:O	2:S:110:THR:HG23	1.83	0.78
1:F:550:SER:HB3	1:F:553:GLN:CG	2.14	0.78
2:O:100:ILE:HB	2:O:136:VAL:CG2	2.13	0.78
2:T:49:GLN:HE21	2:T:49:GLN:H	1.32	0.78
1:C:497:LEU:HD13	1:C:556:MET:HG2	1.66	0.78
1:C:175:LYS:HB2	1:C:175:LYS:HZ2	1.48	0.78
1:F:74:GLU:HB2	1:F:78:LYS:HB3	1.64	0.78
2:R:100:ILE:HB	2:R:136:VAL:CG2	2.13	0.78
1:F:540:ARG:NH2	2:T:87:GLU:OE1	2.16	0.77
1:B:540:ARG:NH2	2:P:87:GLU:OE1	2.18	0.77
1:D:140:ARG:HA	1:D:140:ARG:NE	1.98	0.77
1:E:286:GLU:O	1:E:290:LYS:HB2	1.85	0.77
2:S:6:GLU:HG3	2:S:7:GLU:H	1.49	0.77
1:A:71:PHE:HB3	1:A:108:ASP:HB2	1.65	0.77
1:C:318:ILE:HG23	1:C:322:LEU:HD12	1.66	0.77
1:B:140:ARG:HA	1:B:140:ARG:NE	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLU:O	1:B:290:LYS:HB2	1.84	0.77
1:B:457:THR:HG21	1:B:468:LYS:HA	1.64	0.77
2:Q:49:GLN:HE21	2:Q:49:GLN:H	1.32	0.77
2:Q:6:GLU:HG3	2:Q:7:GLU:H	1.49	0.77
2:T:100:ILE:HB	2:T:136:VAL:CG2	2.13	0.77
1:A:286:GLU:O	1:A:290:LYS:HB2	1.84	0.77
1:B:71:PHE:HB3	1:B:108:ASP:HB2	1.65	0.77
1:C:550:SER:HB3	1:C:553:GLN:CG	2.15	0.77
1:D:694:VAL:HG23	2:R:18:LEU:HD11	1.66	0.77
1:E:71:PHE:HB3	1:E:108:ASP:HB2	1.65	0.77
2:T:6:GLU:HG3	2:T:7:GLU:H	1.50	0.77
2:T:12:PHE:HZ	2:T:76:MET:HE3	1.50	0.77
1:B:776:LEU:O	1:B:776:LEU:HD23	1.85	0.77
1:C:140:ARG:HA	1:C:140:ARG:NE	1.99	0.77
1:D:715:GLU:HA	1:D:718:ARG:NH1	1.99	0.77
1:E:718:ARG:O	1:E:722:ILE:HG13	1.84	0.77
1:F:153:ILE:O	1:F:154:ILE:HD13	1.85	0.77
1:F:154:ILE:HG13	1:F:171:TYR:CE1	2.20	0.77
1:A:154:ILE:HG13	1:A:171:TYR:CE1	2.19	0.77
1:A:412:GLU:C	1:A:414:LYS:H	1.91	0.77
1:B:153:ILE:O	1:B:154:ILE:HD13	1.85	0.77
1:D:217:LYS:HB2	1:D:236:GLU:CD	2.09	0.77
2:R:64:ASP:OD1	2:R:66:PRO:HD2	1.84	0.77
1:A:140:ARG:HA	1:A:140:ARG:NE	1.98	0.77
1:F:71:PHE:HB3	1:F:108:ASP:HB2	1.65	0.77
2:P:64:ASP:OD1	2:P:66:PRO:HD2	1.85	0.77
1:C:191:GLU:O	1:C:193:LEU:N	2.17	0.77
1:C:678:VAL:HG22	1:C:745:TYR:HE2	1.49	0.77
1:E:497:LEU:HD13	1:E:556:MET:HG2	1.66	0.77
1:A:657:ILE:HG13	1:A:756:ILE:HD13	1.67	0.76
1:B:715:GLU:HA	1:B:718:ARG:NH1	2.00	0.76
1:D:74:GLU:HB2	1:D:78:LYS:HB3	1.66	0.76
1:D:412:GLU:C	1:D:414:LYS:H	1.91	0.76
1:E:153:ILE:O	1:E:154:ILE:HD13	1.85	0.76
2:Q:64:ASP:OD1	2:Q:66:PRO:HD2	1.85	0.76
1:B:134:LYS:CG	1:B:136:PRO:HD3	2.14	0.76
1:B:550:SER:HB3	1:B:553:GLN:CG	2.14	0.76
1:E:154:ILE:HG13	1:E:171:TYR:CE1	2.20	0.76
1:E:403:LEU:HD21	1:E:405:LEU:HD11	1.66	0.76
1:F:664:ILE:HG21	2:T:15:ALA:HB2	1.68	0.76
1:F:694:VAL:HG23	2:T:18:LEU:HD11	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:6:GLU:HG3	2:O:7:GLU:H	1.49	0.76
2:Q:36:MET:HE1	2:Q:51:MET:HE1	1.67	0.76
1:A:153:ILE:O	1:A:154:ILE:HD13	1.85	0.76
1:C:776:LEU:HD23	1:C:776:LEU:O	1.85	0.76
1:B:657:ILE:HG13	1:B:756:ILE:HD13	1.67	0.76
1:C:664:ILE:HG21	2:Q:15:ALA:HB2	1.68	0.76
2:O:3:GLN:N	2:O:77:LYS:HZ2	1.83	0.76
1:E:540:ARG:NH2	2:S:87:GLU:OE1	2.18	0.76
1:F:657:ILE:HG13	1:F:756:ILE:HD13	1.66	0.76
1:B:462:ILE:HD11	1:B:466:GLY:HA2	1.67	0.76
1:C:657:ILE:HG13	1:C:756:ILE:HD13	1.68	0.76
1:D:210:PHE:HD1	1:D:214:PHE:HB2	1.51	0.76
1:E:73:ASN:ND2	1:E:74:GLU:OE2	2.18	0.76
1:E:715:GLU:HA	1:E:718:ARG:NH1	2.01	0.76
2:R:36:MET:HE1	2:R:51:MET:HE1	1.68	0.76
1:C:107:THR:HG21	1:C:115:LYS:HD2	1.68	0.76
1:D:286:GLU:O	1:D:290:LYS:HB2	1.85	0.76
1:A:73:ASN:ND2	1:A:74:GLU:OE2	2.18	0.76
1:A:120:LEU:HD13	1:A:120:LEU:C	2.11	0.76
1:C:286:GLU:O	1:C:290:LYS:HB2	1.85	0.76
1:F:210:PHE:HD1	1:F:214:PHE:HB2	1.51	0.76
2:Q:97:ASN:HD22	2:Q:97:ASN:N	1.77	0.76
1:A:776:LEU:O	1:A:776:LEU:HD23	1.86	0.76
1:B:120:LEU:O	1:B:120:LEU:CD1	2.34	0.76
1:B:120:LEU:HD13	1:B:120:LEU:C	2.11	0.76
1:A:210:PHE:HD1	1:A:214:PHE:HB2	1.51	0.75
1:B:210:PHE:HD1	1:B:214:PHE:HB2	1.51	0.75
1:C:462:ILE:HD11	1:C:466:GLY:HA2	1.68	0.75
1:D:776:LEU:O	1:D:776:LEU:HD23	1.86	0.75
1:F:715:GLU:HA	1:F:718:ARG:NH1	2.00	0.75
1:F:776:LEU:HD23	1:F:776:LEU:O	1.86	0.75
2:O:64:ASP:OD1	2:O:66:PRO:HD2	1.85	0.75
2:R:12:PHE:HZ	2:R:76:MET:HE3	1.51	0.75
2:S:49:GLN:HE21	2:S:49:GLN:H	1.32	0.75
1:C:128:MET:HE2	1:C:239:HIS:NE2	2.00	0.75
1:D:462:ILE:HD11	1:D:466:GLY:HA2	1.68	0.75
2:S:117:THR:HG23	2:S:120:GLU:HB2	1.68	0.75
1:A:715:GLU:HA	1:A:718:ARG:NH1	2.01	0.75
1:B:199:LEU:C	1:B:201:ASP:H	1.94	0.75
1:C:715:GLU:HA	1:C:718:ARG:NH1	2.00	0.75
1:D:120:LEU:HD13	1:D:120:LEU:C	2.11	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:O	1:E:120:LEU:CD1	2.34	0.75
1:F:120:LEU:CD1	1:F:120:LEU:O	2.34	0.75
1:F:678:VAL:HG22	1:F:745:TYR:HE2	1.50	0.75
1:A:120:LEU:O	1:A:120:LEU:CD1	2.34	0.75
1:A:478:ALA:HB1	1:A:486:LYS:O	1.86	0.75
1:D:120:LEU:O	1:D:120:LEU:CD1	2.34	0.75
1:D:540:ARG:NH2	2:R:87:GLU:OE1	2.19	0.75
2:O:97:ASN:HD22	2:O:97:ASN:N	1.76	0.75
1:A:678:VAL:HG22	1:A:745:TYR:HE2	1.49	0.75
1:C:153:ILE:O	1:C:154:ILE:HD13	1.87	0.75
1:C:412:GLU:C	1:C:414:LYS:H	1.92	0.75
1:E:550:SER:HB3	1:E:553:GLN:CG	2.15	0.75
2:P:3:GLN:N	2:P:77:LYS:HZ2	1.83	0.75
2:Q:12:PHE:HZ	2:Q:76:MET:HE3	1.52	0.75
2:S:64:ASP:OD1	2:S:66:PRO:HD2	1.86	0.75
1:B:478:ALA:HB1	1:B:486:LYS:O	1.86	0.75
1:D:296:LEU:CD2	1:D:606:LYS:HE2	2.17	0.75
1:E:210:PHE:HD1	1:E:214:PHE:HB2	1.51	0.75
1:F:218:LEU:HD11	1:F:225:ILE:HD11	1.68	0.75
2:O:117:THR:HG23	2:O:120:GLU:HB2	1.69	0.75
1:C:540:ARG:NH2	2:Q:87:GLU:OE1	2.20	0.75
1:E:236:GLU:HA	1:E:239:HIS:CD2	2.22	0.75
1:E:462:ILE:HD11	1:E:466:GLY:HA2	1.69	0.75
1:F:462:ILE:HD11	1:F:466:GLY:HA2	1.67	0.75
2:P:6:GLU:HG3	2:P:7:GLU:H	1.50	0.75
1:E:188:LEU:CD2	1:E:188:LEU:N	2.46	0.75
2:R:49:GLN:HE21	2:R:49:GLN:H	1.32	0.75
1:C:120:LEU:C	1:C:120:LEU:HD13	2.11	0.75
1:D:550:SER:HB3	1:D:553:GLN:CG	2.15	0.75
1:F:120:LEU:C	1:F:120:LEU:HD13	2.11	0.75
2:Q:117:THR:HG23	2:Q:120:GLU:HB2	1.69	0.75
1:C:120:LEU:CD1	1:C:120:LEU:O	2.34	0.74
1:C:478:ALA:HB1	1:C:486:LYS:O	1.86	0.74
1:D:186:LYS:CB	1:D:190:PRO:HD3	2.17	0.74
1:E:180:ASP:CG	1:E:181:ILE:H	1.93	0.74
2:T:117:THR:HG23	2:T:120:GLU:HB2	1.69	0.74
1:A:236:GLU:HA	1:A:239:HIS:CD2	2.22	0.74
1:A:694:VAL:HG23	2:O:18:LEU:HD11	1.68	0.74
1:E:120:LEU:C	1:E:120:LEU:HD13	2.11	0.74
2:O:36:MET:CE	2:O:43:PRO:HG3	2.17	0.74
1:A:165:GLN:NE2	1:A:252:ASP:HB3	2.02	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HB2	1:B:175:LYS:HZ2	1.51	0.74
1:B:236:GLU:HA	1:B:239:HIS:CD2	2.23	0.74
1:C:210:PHE:HD1	1:C:214:PHE:HB2	1.50	0.74
2:R:3:GLN:N	2:R:77:LYS:HZ2	1.84	0.74
2:T:64:ASP:OD1	2:T:66:PRO:HD2	1.87	0.74
2:O:36:MET:HE1	2:O:51:MET:HE1	1.68	0.74
2:P:117:THR:HG23	2:P:120:GLU:HB2	1.69	0.74
2:R:117:THR:HG23	2:R:120:GLU:HB2	1.69	0.74
1:D:154:ILE:HG13	1:D:171:TYR:CE1	2.21	0.74
1:D:175:LYS:HB2	1:D:175:LYS:HZ2	1.48	0.74
1:D:657:ILE:HG13	1:D:756:ILE:HD13	1.69	0.74
1:F:478:ALA:HB1	1:F:486:LYS:O	1.87	0.74
2:O:49:GLN:HE21	2:O:49:GLN:H	1.32	0.74
1:A:186:LYS:CB	1:A:190:PRO:HD3	2.17	0.74
1:A:218:LEU:HD11	1:A:225:ILE:HD11	1.69	0.74
1:C:74:GLU:HB2	1:C:78:LYS:HB3	1.67	0.74
1:E:671:ARG:NH1	1:E:677:GLY:HA3	2.03	0.74
1:E:678:VAL:HG22	1:E:745:TYR:HE2	1.51	0.74
1:F:412:GLU:C	1:F:414:LYS:H	1.92	0.74
2:S:3:GLN:N	2:S:77:LYS:HZ2	1.83	0.74
1:B:678:VAL:HG22	1:B:745:TYR:HE2	1.51	0.74
1:C:123:GLU:HG2	1:C:124:GLU:N	2.02	0.74
1:F:64:ASN:N	1:F:64:ASN:ND2	2.32	0.74
1:F:165:GLN:NE2	1:F:252:ASP:HB3	2.02	0.74
1:F:286:GLU:O	1:F:290:LYS:HB2	1.87	0.74
1:A:671:ARG:NH1	1:A:677:GLY:HA3	2.02	0.74
1:C:671:ARG:NH1	1:C:677:GLY:HA3	2.03	0.74
1:D:218:LEU:HD11	1:D:225:ILE:HD11	1.68	0.74
1:E:185:ASP:O	1:E:190:PRO:HA	1.87	0.74
1:E:478:ALA:HB1	1:E:486:LYS:O	1.87	0.74
1:E:657:ILE:HG13	1:E:756:ILE:HD13	1.68	0.74
1:F:180:ASP:C	1:F:182:ILE:H	1.96	0.74
2:P:49:GLN:HE21	2:P:49:GLN:H	1.32	0.74
2:S:36:MET:HE1	2:S:51:MET:HE1	1.68	0.74
2:T:3:GLN:N	2:T:77:LYS:HZ2	1.85	0.74
1:B:694:VAL:HG23	2:P:18:LEU:HD11	1.68	0.74
1:C:148:GLU:HG3	1:C:149:THR:N	2.03	0.74
1:C:154:ILE:HG13	1:C:171:TYR:CE1	2.23	0.74
1:E:186:LYS:CB	1:E:190:PRO:HD3	2.17	0.74
1:D:165:GLN:NE2	1:D:252:ASP:HB3	2.02	0.74
1:E:199:LEU:C	1:E:201:ASP:H	1.92	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:664:ILE:HG21	2:S:15:ALA:HB2	1.70	0.74
1:B:165:GLN:NE2	1:B:252:ASP:HB3	2.03	0.73
1:B:769:SER:O	1:B:769:SER:OG	1.89	0.73
1:D:678:VAL:HG22	1:D:745:TYR:HE2	1.51	0.73
1:E:165:GLN:NE2	1:E:252:ASP:HB3	2.03	0.73
1:F:236:GLU:HA	1:F:239:HIS:CD2	2.23	0.73
2:R:31:GLU:O	2:R:35:VAL:HG23	1.89	0.73
1:C:236:GLU:HA	1:C:239:HIS:CD2	2.23	0.73
1:D:73:ASN:ND2	1:D:74:GLU:OE2	2.18	0.73
1:D:478:ALA:HB1	1:D:486:LYS:O	1.87	0.73
1:E:189:ASP:O	1:E:191:GLU:N	2.21	0.73
2:T:36:MET:CE	2:T:43:PRO:HG3	2.18	0.73
1:A:299:GLU:HG2	1:A:299:GLU:O	1.88	0.73
1:C:131:ARG:HG3	1:C:243:LEU:CD2	2.18	0.73
1:C:218:LEU:HD11	1:C:225:ILE:HD11	1.68	0.73
2:Q:3:GLN:N	2:Q:77:LYS:HZ2	1.84	0.73
1:A:462:ILE:HD11	1:A:466:GLY:HA2	1.69	0.73
1:B:185:ASP:O	1:B:190:PRO:HA	1.89	0.73
1:B:671:ARG:NH1	1:B:677:GLY:HA3	2.04	0.73
1:E:776:LEU:HD23	1:E:776:LEU:O	1.87	0.73
2:P:36:MET:HE1	2:P:51:MET:HE1	1.69	0.73
1:E:218:LEU:HD11	1:E:225:ILE:HD11	1.69	0.73
1:F:73:ASN:ND2	1:F:74:GLU:OE2	2.18	0.73
1:C:197:LYS:HD3	1:C:263:ASP:HB3	1.70	0.73
1:D:236:GLU:HA	1:D:239:HIS:CD2	2.23	0.73
1:E:197:LYS:HD3	1:E:263:ASP:HB3	1.70	0.73
1:F:671:ARG:NH1	1:F:677:GLY:HA3	2.04	0.73
1:A:664:ILE:HG21	2:O:15:ALA:HB2	1.69	0.73
1:B:189:ASP:O	1:B:191:GLU:N	2.21	0.73
1:C:462:ILE:HG12	1:C:463:THR:H	1.54	0.73
2:T:36:MET:HE1	2:T:51:MET:HE1	1.69	0.73
1:B:197:LYS:HD3	1:B:263:ASP:HB3	1.71	0.73
1:D:107:THR:HG21	1:D:115:LYS:HD2	1.70	0.73
1:D:462:ILE:HG12	1:D:463:THR:N	2.03	0.73
1:D:548:THR:N	4:D:904:CMP:HN61	1.86	0.73
1:E:299:GLU:O	1:E:299:GLU:HG2	1.89	0.73
1:B:217:LYS:HZ2	1:B:217:LYS:HB3	1.52	0.73
1:B:288:VAL:HG23	1:B:289:GLU:N	2.03	0.73
1:C:178:SER:OG	1:C:179:LEU:HD23	1.88	0.73
1:C:186:LYS:HA	1:C:190:PRO:CD	2.15	0.73
1:E:191:GLU:O	1:E:193:LEU:N	2.20	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:VAL:HG23	1:E:289:GLU:N	2.04	0.73
2:Q:36:MET:CE	2:Q:43:PRO:HG3	2.18	0.73
1:B:180:ASP:CG	1:B:181:ILE:H	1.95	0.72
1:C:299:GLU:HG2	1:C:299:GLU:O	1.89	0.72
1:C:446:ILE:HD11	1:C:451:ASN:HB3	1.71	0.72
1:E:781:ASN:H	1:E:789:ASN:ND2	1.87	0.72
1:F:462:ILE:HG12	1:F:463:THR:N	2.03	0.72
1:A:462:ILE:HG12	1:A:463:THR:H	1.54	0.72
1:B:218:LEU:HD11	1:B:225:ILE:HD11	1.69	0.72
1:C:462:ILE:HG12	1:C:463:THR:N	2.03	0.72
1:C:781:ASN:H	1:C:789:ASN:ND2	1.88	0.72
1:D:197:LYS:HD3	1:D:263:ASP:HB3	1.72	0.72
1:A:781:ASN:H	1:A:789:ASN:ND2	1.88	0.72
2:P:31:GLU:O	2:P:35:VAL:HG23	1.89	0.72
1:B:697:ILE:HD13	1:B:732:ILE:CD1	2.20	0.72
1:B:715:GLU:HA	1:B:718:ARG:HH12	1.55	0.72
1:C:191:GLU:O	1:C:192:PHE:C	2.32	0.72
1:D:462:ILE:HG12	1:D:463:THR:H	1.53	0.72
1:A:175:LYS:HB2	1:A:175:LYS:HZ2	1.54	0.72
1:A:199:LEU:C	1:A:201:ASP:H	1.97	0.72
1:B:134:LYS:HG2	1:B:136:PRO:CG	2.20	0.72
1:B:462:ILE:HG12	1:B:463:THR:N	2.03	0.72
1:C:105:TYR:HB2	1:C:153:ILE:HG12	1.69	0.72
1:F:105:TYR:HB2	1:F:153:ILE:HG12	1.71	0.72
2:T:31:GLU:O	2:T:35:VAL:HG23	1.89	0.72
1:A:105:TYR:HB2	1:A:153:ILE:HG12	1.71	0.72
1:B:105:TYR:HB2	1:B:153:ILE:HG12	1.71	0.72
1:C:776:LEU:O	1:C:780:LEU:HD22	1.90	0.72
1:E:105:TYR:HB2	1:E:153:ILE:HG12	1.72	0.72
1:F:131:ARG:HG3	1:F:243:LEU:CD2	2.19	0.72
1:A:462:ILE:HG12	1:A:463:THR:N	2.04	0.72
1:B:296:LEU:CD2	1:B:606:LYS:HE2	2.16	0.72
1:F:462:ILE:HG12	1:F:463:THR:H	1.54	0.72
1:A:123:GLU:HG2	1:A:124:GLU:N	2.05	0.72
1:A:197:LYS:HD3	1:A:263:ASP:HB3	1.71	0.72
1:D:664:ILE:HG21	2:R:15:ALA:HB2	1.71	0.72
2:O:31:GLU:O	2:O:35:VAL:HG23	1.90	0.72
1:D:148:GLU:HG3	1:D:149:THR:N	2.05	0.72
1:E:134:LYS:HG2	1:E:136:PRO:CG	2.20	0.72
1:D:299:GLU:O	1:D:299:GLU:HG2	1.89	0.71
1:E:697:ILE:HD13	1:E:732:ILE:CD1	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:31:GLU:O	2:S:35:VAL:HG23	1.89	0.71
1:E:462:ILE:HG12	1:E:463:THR:H	1.54	0.71
1:A:697:ILE:HD13	1:A:732:ILE:CD1	2.20	0.71
1:E:462:ILE:HG12	1:E:463:THR:N	2.04	0.71
1:E:715:GLU:HA	1:E:718:ARG:HH12	1.55	0.71
1:F:548:THR:N	4:F:906:CMP:HN61	1.87	0.71
2:T:97:ASN:HD22	2:T:97:ASN:N	1.76	0.71
1:B:299:GLU:O	1:B:299:GLU:HG2	1.89	0.71
1:C:165:GLN:NE2	1:C:252:ASP:HB3	2.04	0.71
1:D:671:ARG:NH1	1:D:677:GLY:HA3	2.04	0.71
1:E:134:LYS:CG	1:E:136:PRO:HD3	2.17	0.71
1:F:781:ASN:H	1:F:789:ASN:ND2	1.88	0.71
1:A:131:ARG:HG3	1:A:243:LEU:HD22	1.73	0.71
1:B:73:ASN:ND2	1:B:74:GLU:OE2	2.18	0.71
1:F:776:LEU:O	1:F:780:LEU:HD22	1.91	0.71
1:A:131:ARG:HG3	1:A:243:LEU:CD2	2.20	0.71
1:B:70:GLU:HB2	1:B:107:THR:HG22	1.73	0.71
1:C:73:ASN:ND2	1:C:74:GLU:OE2	2.18	0.71
1:B:597:ASN:HB2	1:B:598:PRO:HD2	1.73	0.71
1:E:180:ASP:C	1:E:182:ILE:H	1.97	0.71
1:A:715:GLU:HA	1:A:718:ARG:HH12	1.56	0.71
1:B:128:MET:HE2	1:B:239:HIS:CE1	2.25	0.71
1:D:776:LEU:O	1:D:780:LEU:HD22	1.91	0.71
1:A:191:GLU:O	1:A:192:PHE:C	2.32	0.71
1:B:462:ILE:HG12	1:B:463:THR:H	1.53	0.71
2:P:12:PHE:CE1	2:P:72:MET:HG3	2.26	0.71
2:P:36:MET:CE	2:P:43:PRO:HG3	2.20	0.71
1:B:776:LEU:O	1:B:780:LEU:HD22	1.90	0.71
1:D:781:ASN:H	1:D:789:ASN:ND2	1.88	0.71
1:F:197:LYS:HD3	1:F:263:ASP:HB3	1.72	0.71
1:F:199:LEU:C	1:F:201:ASP:H	1.98	0.71
1:F:299:GLU:HG2	1:F:299:GLU:O	1.90	0.71
1:D:288:VAL:HG23	1:D:289:GLU:N	2.05	0.70
1:E:184:LYS:HZ1	1:E:191:GLU:HB2	1.55	0.70
1:E:776:LEU:O	1:E:780:LEU:HD22	1.91	0.70
2:S:12:PHE:CE1	2:S:72:MET:HG3	2.25	0.70
1:A:70:GLU:HB2	1:A:107:THR:HG22	1.73	0.70
1:B:781:ASN:H	1:B:789:ASN:ND2	1.88	0.70
1:D:178:SER:OG	1:D:179:LEU:HD23	1.90	0.70
1:E:128:MET:HE2	1:E:239:HIS:NE2	2.06	0.70
1:F:89:ILE:HG22	1:F:93:VAL:CG1	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:LYS:CG	1:A:136:PRO:HD3	2.20	0.70
1:B:373:LYS:HD3	1:B:376:GLN:NE2	2.06	0.70
1:D:446:ILE:HD11	1:D:451:ASN:HB3	1.71	0.70
1:E:597:ASN:HB2	1:E:598:PRO:HD2	1.73	0.70
1:F:597:ASN:HB2	1:F:598:PRO:HD2	1.72	0.70
1:A:776:LEU:O	1:A:780:LEU:HD22	1.91	0.70
1:C:137:PHE:HD2	1:C:137:PHE:C	2.00	0.70
1:C:257:LEU:HD12	1:C:261:ALA:HB3	1.73	0.70
1:C:288:VAL:HG23	1:C:289:GLU:N	2.05	0.70
1:E:191:GLU:O	1:E:192:PHE:C	2.35	0.70
1:F:288:VAL:HG23	1:F:289:GLU:N	2.05	0.70
2:Q:31:GLU:O	2:Q:35:VAL:HG23	1.91	0.70
1:A:89:ILE:HG22	1:A:93:VAL:CG1	2.20	0.70
1:D:123:GLU:HG2	1:D:124:GLU:N	2.05	0.70
1:E:89:ILE:HG22	1:E:93:VAL:CG1	2.22	0.70
1:F:175:LYS:HB2	1:F:175:LYS:HZ2	1.54	0.70
2:P:97:ASN:HD22	2:P:97:ASN:N	1.76	0.70
1:A:137:PHE:HD2	1:A:137:PHE:C	1.99	0.70
1:A:597:ASN:HB2	1:A:598:PRO:HD2	1.73	0.70
1:F:123:GLU:HG2	1:F:124:GLU:N	2.05	0.70
2:T:12:PHE:CE1	2:T:72:MET:HG3	2.26	0.70
1:C:333:LYS:H	1:C:333:LYS:HD2	1.57	0.70
1:A:288:VAL:HG23	1:A:289:GLU:N	2.04	0.70
1:B:89:ILE:HG22	1:B:93:VAL:CG1	2.21	0.70
1:B:664:ILE:HG21	2:P:15:ALA:HB2	1.72	0.70
1:E:137:PHE:HD2	1:E:137:PHE:C	1.99	0.70
2:O:12:PHE:CE1	2:O:72:MET:HG3	2.26	0.70
1:B:333:LYS:H	1:B:333:LYS:HD2	1.57	0.70
1:C:715:GLU:HA	1:C:718:ARG:HH12	1.54	0.70
1:D:105:TYR:HB2	1:D:153:ILE:HG12	1.72	0.70
1:D:442:TYR:HD1	1:D:455:TYR:HD1	1.40	0.70
1:F:137:PHE:HD2	1:F:137:PHE:C	2.00	0.70
2:R:12:PHE:CE1	2:R:72:MET:HG3	2.26	0.70
1:B:137:PHE:HD2	1:B:137:PHE:C	1.99	0.70
1:B:792:VAL:O	1:B:796:ILE:HG12	1.92	0.70
1:C:442:TYR:HD1	1:C:455:TYR:HD1	1.39	0.70
1:D:659:THR:OG1	1:D:662:GLU:HB2	1.92	0.70
1:F:333:LYS:H	1:F:333:LYS:HD2	1.56	0.70
1:F:792:VAL:O	1:F:796:ILE:HG12	1.92	0.70
2:S:58:ASP:C	2:S:60:ASN:H	2.00	0.70
1:C:186:LYS:CB	1:C:190:PRO:HD3	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ASN:HB2	1:D:598:PRO:HD2	1.73	0.69
1:E:373:LYS:HD3	1:E:376:GLN:NE2	2.07	0.69
1:A:442:TYR:HD1	1:A:455:TYR:HD1	1.40	0.69
1:A:446:ILE:HD11	1:A:451:ASN:HB3	1.73	0.69
1:A:548:THR:N	4:A:901:CMP:HN61	1.86	0.69
1:C:792:VAL:O	1:C:796:ILE:HG12	1.91	0.69
1:D:137:PHE:HD2	1:D:137:PHE:C	2.00	0.69
1:D:217:LYS:HZ2	1:D:217:LYS:HB3	1.56	0.69
1:E:333:LYS:H	1:E:333:LYS:HD2	1.57	0.69
1:F:178:SER:OG	1:F:179:LEU:HD23	1.90	0.69
1:F:715:GLU:HA	1:F:718:ARG:HH12	1.56	0.69
2:Q:12:PHE:CE1	2:Q:72:MET:HG3	2.26	0.69
1:A:792:VAL:O	1:A:796:ILE:HG12	1.93	0.69
1:D:715:GLU:HA	1:D:718:ARG:HH12	1.55	0.69
1:B:446:ILE:HD11	1:B:451:ASN:HB3	1.75	0.69
1:E:446:ILE:HD11	1:E:451:ASN:HB3	1.75	0.69
1:E:501:LEU:HB2	1:E:623:ASP:O	1.92	0.69
1:F:115:LYS:HZ3	1:F:115:LYS:HB3	1.57	0.69
1:F:697:ILE:HD13	1:F:732:ILE:CD1	2.22	0.69
1:A:134:LYS:HG2	1:A:136:PRO:CG	2.21	0.69
1:A:333:LYS:H	1:A:333:LYS:HD2	1.58	0.69
1:D:792:VAL:O	1:D:796:ILE:HG12	1.92	0.69
1:E:659:THR:OG1	1:E:662:GLU:HB2	1.91	0.69
1:B:426:ILE:HD13	1:B:431:LYS:HA	1.74	0.69
1:C:128:MET:O	1:C:128:MET:HG2	1.91	0.69
1:E:792:VAL:O	1:E:796:ILE:HG12	1.92	0.69
1:F:426:ILE:HD13	1:F:431:LYS:HA	1.75	0.69
1:F:659:THR:OG1	1:F:662:GLU:HB2	1.92	0.69
1:A:186:LYS:HB2	1:A:190:PRO:HD3	1.74	0.69
1:D:89:ILE:HG22	1:D:93:VAL:CG1	2.21	0.69
1:D:373:LYS:HD3	1:D:376:GLN:NE2	2.07	0.69
1:F:446:ILE:HD11	1:F:451:ASN:HB3	1.73	0.69
2:R:36:MET:CE	2:R:43:PRO:HG3	2.20	0.69
1:B:123:GLU:HG2	1:B:124:GLU:N	2.07	0.69
1:C:278:LYS:HE3	1:C:279:ILE:HD11	1.75	0.69
1:C:597:ASN:HB2	1:C:598:PRO:HD2	1.73	0.69
1:D:389:LYS:HA	1:D:392:THR:HB	1.73	0.69
1:D:697:ILE:HD13	1:D:732:ILE:CD1	2.22	0.69
1:E:426:ILE:HD13	1:E:431:LYS:HA	1.75	0.69
2:T:49:GLN:HE21	2:T:49:GLN:N	1.90	0.69
1:A:128:MET:O	1:A:128:MET:CG	2.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:HA	1:A:392:THR:HB	1.74	0.69
1:A:426:ILE:HD13	1:A:431:LYS:HA	1.75	0.69
1:C:373:LYS:HD3	1:C:376:GLN:NE2	2.08	0.69
1:C:426:ILE:HD13	1:C:431:LYS:HA	1.75	0.69
2:P:58:ASP:C	2:P:60:ASN:H	2.01	0.69
2:T:58:ASP:C	2:T:60:ASN:H	2.00	0.69
1:A:373:LYS:HD3	1:A:376:GLN:NE2	2.07	0.68
1:A:501:LEU:HB2	1:A:623:ASP:O	1.93	0.68
1:B:389:LYS:HA	1:B:392:THR:HB	1.74	0.68
1:C:389:LYS:HA	1:C:392:THR:HB	1.74	0.68
1:C:501:LEU:HB2	1:C:623:ASP:O	1.92	0.68
1:D:333:LYS:HD2	1:D:333:LYS:H	1.58	0.68
1:E:70:GLU:HB2	1:E:107:THR:HG22	1.75	0.68
1:F:389:LYS:HA	1:F:392:THR:HB	1.74	0.68
2:O:58:ASP:C	2:O:60:ASN:H	2.01	0.68
2:P:49:GLN:HE21	2:P:49:GLN:N	1.90	0.68
1:B:442:TYR:HD1	1:B:455:TYR:HD1	1.39	0.68
1:C:180:ASP:C	1:C:182:ILE:H	2.01	0.68
1:F:373:LYS:HD3	1:F:376:GLN:NE2	2.08	0.68
1:F:442:TYR:HD1	1:F:455:TYR:HD1	1.40	0.68
1:F:737:LYS:HE2	1:F:737:LYS:HA	1.75	0.68
2:Q:49:GLN:HE21	2:Q:49:GLN:N	1.91	0.68
1:B:115:LYS:HB3	1:B:115:LYS:NZ	2.09	0.68
1:C:697:ILE:HD13	1:C:732:ILE:CD1	2.23	0.68
1:E:389:LYS:HA	1:E:392:THR:HB	1.74	0.68
1:A:278:LYS:HE3	1:A:279:ILE:HD11	1.76	0.68
1:B:180:ASP:C	1:B:182:ILE:H	2.00	0.68
1:D:426:ILE:HD13	1:D:431:LYS:HA	1.76	0.68
1:A:99:GLU:C	1:A:101:GLY:H	2.02	0.68
1:A:548:THR:N	4:A:901:CMP:N6	2.37	0.68
1:B:278:LYS:HE3	1:B:279:ILE:HD11	1.76	0.68
1:E:123:GLU:HG2	1:E:124:GLU:N	2.08	0.68
1:E:175:LYS:HB2	1:E:175:LYS:HZ2	1.55	0.68
1:E:186:LYS:O	1:E:188:LEU:O	2.11	0.68
2:R:58:ASP:C	2:R:60:ASN:H	2.00	0.68
2:R:58:ASP:HB3	2:R:62:THR:HG23	1.75	0.68
2:S:49:GLN:HE21	2:S:49:GLN:N	1.91	0.68
1:A:657:ILE:HG13	1:A:756:ILE:CD1	2.24	0.68
1:C:89:ILE:HG22	1:C:93:VAL:CG1	2.23	0.68
1:C:137:PHE:C	1:C:137:PHE:CD2	2.72	0.68
1:F:148:GLU:HG3	1:F:149:THR:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:58:ASP:C	2:Q:60:ASN:H	2.01	0.68
2:S:36:MET:CE	2:S:43:PRO:HG3	2.20	0.68
1:A:223:LYS:HD3	1:A:224:SER:N	2.09	0.68
1:D:188:LEU:CD2	1:D:188:LEU:N	2.46	0.68
1:D:278:LYS:HE3	1:D:279:ILE:HD11	1.76	0.68
1:F:257:LEU:HD12	1:F:261:ALA:HB3	1.76	0.68
2:O:58:ASP:HB3	2:O:62:THR:HG23	1.75	0.68
2:T:58:ASP:HB3	2:T:62:THR:HG23	1.75	0.68
1:A:115:LYS:NZ	1:A:115:LYS:HB3	2.09	0.68
1:A:137:PHE:C	1:A:137:PHE:CD2	2.72	0.68
1:B:659:THR:OG1	1:B:662:GLU:HB2	1.93	0.68
1:E:296:LEU:CD2	1:E:606:LYS:HE2	2.19	0.68
1:F:142:VAL:HG13	1:F:154:ILE:CD1	2.24	0.68
1:F:278:LYS:HE3	1:F:279:ILE:HD11	1.76	0.68
1:A:186:LYS:O	1:A:188:LEU:O	2.11	0.68
1:B:99:GLU:C	1:B:101:GLY:H	2.01	0.68
1:B:368:GLN:HB2	1:B:384:ASN:OD1	1.94	0.68
1:C:412:GLU:C	1:C:414:LYS:N	2.51	0.68
1:D:724:ARG:HG3	1:D:724:ARG:HH11	1.59	0.68
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.09	0.68
1:E:278:LYS:HE3	1:E:279:ILE:HD11	1.76	0.68
1:E:548:THR:N	4:E:905:CMP:HN61	1.86	0.68
1:C:188:LEU:CD2	1:C:188:LEU:N	2.46	0.67
1:C:505:LYS:C	1:C:507:GLN:H	2.02	0.67
1:B:144:GLU:HG2	1:B:177:ILE:HD11	1.75	0.67
1:D:322:LEU:HD13	1:D:556:MET:HE1	1.77	0.67
1:E:223:LYS:HD3	1:E:224:SER:N	2.09	0.67
1:E:442:TYR:HD1	1:E:455:TYR:HD1	1.39	0.67
2:Q:58:ASP:HB3	2:Q:62:THR:HG23	1.74	0.67
1:A:142:VAL:HG13	1:A:154:ILE:HD11	1.76	0.67
1:B:223:LYS:HD3	1:B:224:SER:N	2.09	0.67
1:D:180:ASP:C	1:D:182:ILE:H	2.01	0.67
1:E:254:ARG:H	1:E:254:ARG:HD2	1.60	0.67
1:F:254:ARG:H	1:F:254:ARG:HD2	1.59	0.67
1:B:254:ARG:H	1:B:254:ARG:HD2	1.59	0.67
1:C:657:ILE:HG13	1:C:756:ILE:CD1	2.24	0.67
1:E:99:GLU:C	1:E:101:GLY:H	2.02	0.67
1:E:426:ILE:CD1	1:E:431:LYS:HA	2.25	0.67
1:F:525:LYS:HE2	2:T:114:GLU:HG2	1.77	0.67
2:R:121:VAL:C	2:R:123:GLN:H	2.02	0.67
1:B:737:LYS:HA	1:B:737:LYS:HE2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:THR:OG1	1:C:662:GLU:HB2	1.94	0.67
1:E:137:PHE:C	1:E:137:PHE:CD2	2.72	0.67
1:F:179:LEU:HB2	1:F:183:SER:HB2	1.76	0.67
1:F:450:ASN:ND2	1:F:452:GLU:HG3	2.10	0.67
1:A:178:SER:OG	1:A:179:LEU:HD23	1.94	0.67
1:B:426:ILE:CD1	1:B:431:LYS:HA	2.25	0.67
1:C:446:ILE:HG13	1:C:452:GLU:O	1.94	0.67
1:D:186:LYS:HB2	1:D:190:PRO:HD3	1.74	0.67
1:D:412:GLU:C	1:D:414:LYS:N	2.51	0.67
1:E:505:LYS:C	1:E:507:GLN:H	2.02	0.67
2:O:49:GLN:HE21	2:O:49:GLN:N	1.91	0.67
1:C:737:LYS:HE2	1:C:737:LYS:HA	1.76	0.67
1:D:191:GLU:O	1:D:192:PHE:C	2.37	0.67
1:D:548:THR:N	4:D:904:CMP:N6	2.38	0.67
1:E:737:LYS:HA	1:E:737:LYS:HE2	1.77	0.67
1:F:186:LYS:O	1:F:188:LEU:O	2.11	0.67
1:F:426:ILE:CD1	1:F:431:LYS:HA	2.25	0.67
1:F:505:LYS:C	1:F:507:GLN:H	2.03	0.67
2:Q:16:PHE:HA	2:Q:35:VAL:HG11	1.77	0.67
2:R:16:PHE:HA	2:R:35:VAL:HG11	1.77	0.67
2:S:16:PHE:HA	2:S:35:VAL:HG11	1.77	0.67
2:T:49:GLN:N	2:T:49:GLN:NE2	2.43	0.67
1:B:137:PHE:C	1:B:137:PHE:CD2	2.72	0.67
1:F:223:LYS:HD3	1:F:224:SER:N	2.10	0.67
1:A:142:VAL:HG13	1:A:154:ILE:CD1	2.25	0.67
1:B:657:ILE:HG13	1:B:756:ILE:CD1	2.24	0.67
1:C:368:GLN:HB2	1:C:384:ASN:OD1	1.94	0.67
1:D:595:ILE:HG22	1:D:596:ILE:N	2.10	0.67
2:Q:49:GLN:N	2:Q:49:GLN:NE2	2.43	0.67
2:S:58:ASP:HB3	2:S:62:THR:HG23	1.75	0.67
1:A:134:LYS:HG2	1:A:136:PRO:HG3	1.77	0.67
1:A:737:LYS:HE2	1:A:737:LYS:HA	1.77	0.67
1:B:724:ARG:HH11	1:B:724:ARG:HG3	1.59	0.67
1:C:322:LEU:HD13	1:C:556:MET:HE1	1.77	0.67
1:C:724:ARG:HH11	1:C:724:ARG:HG3	1.58	0.67
1:D:99:GLU:C	1:D:101:GLY:H	2.02	0.67
1:D:199:LEU:C	1:D:201:ASP:H	2.03	0.67
1:D:368:GLN:HB2	1:D:384:ASN:OD1	1.95	0.67
1:D:657:ILE:HG13	1:D:756:ILE:CD1	2.25	0.67
1:F:137:PHE:C	1:F:137:PHE:CD2	2.72	0.67
1:F:142:VAL:HG13	1:F:154:ILE:HD11	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LYS:HB2	1:F:190:PRO:HD3	1.77	0.67
2:R:49:GLN:HE21	2:R:49:GLN:N	1.91	0.67
1:B:178:SER:OG	1:B:179:LEU:HD23	1.95	0.66
1:B:630:ARG:NE	2:P:83:GLU:HG2	2.10	0.66
1:C:186:LYS:HB2	1:C:190:PRO:HD3	1.77	0.66
1:F:115:LYS:HB3	1:F:115:LYS:NZ	2.10	0.66
1:F:131:ARG:HG3	1:F:243:LEU:HD22	1.77	0.66
2:Q:121:VAL:C	2:Q:123:GLN:H	2.02	0.66
1:A:180:ASP:CG	1:A:181:ILE:H	2.02	0.66
1:A:257:LEU:O	1:A:257:LEU:HG	1.95	0.66
1:A:659:THR:OG1	1:A:662:GLU:HB2	1.94	0.66
1:C:426:ILE:CD1	1:C:431:LYS:HA	2.25	0.66
1:D:446:ILE:HG13	1:D:452:GLU:O	1.95	0.66
1:F:368:GLN:HB2	1:F:384:ASN:OD1	1.95	0.66
1:F:657:ILE:HG13	1:F:756:ILE:CD1	2.23	0.66
2:P:16:PHE:HA	2:P:35:VAL:HG11	1.77	0.66
1:A:130:SER:HB2	1:A:170:TYR:CE2	2.30	0.66
1:A:540:ARG:HD3	1:A:627:TYR:OH	1.95	0.66
1:C:186:LYS:O	1:C:188:LEU:O	2.13	0.66
1:E:178:SER:OG	1:E:179:LEU:HD23	1.96	0.66
1:A:191:GLU:O	1:A:193:LEU:N	2.27	0.66
1:A:426:ILE:CD1	1:A:431:LYS:HA	2.25	0.66
1:B:142:VAL:HG13	1:B:154:ILE:HD11	1.78	0.66
1:B:505:LYS:C	1:B:507:GLN:H	2.02	0.66
1:D:450:ASN:ND2	1:D:452:GLU:HG3	2.10	0.66
1:F:296:LEU:CD2	1:F:606:LYS:HE2	2.20	0.66
1:F:529:VAL:HG21	2:T:109:MET:HE1	1.75	0.66
2:P:49:GLN:N	2:P:49:GLN:NE2	2.43	0.66
1:A:180:ASP:C	1:A:182:ILE:H	2.01	0.66
1:B:548:THR:N	4:B:902:CMP:HN61	1.87	0.66
1:C:254:ARG:H	1:C:254:ARG:HD2	1.60	0.66
1:C:345:THR:HG22	1:C:490:ALA:O	1.95	0.66
1:C:607:ASN:HB3	1:C:609:GLU:OE2	1.95	0.66
1:D:223:LYS:HD3	1:D:224:SER:N	2.10	0.66
1:E:368:GLN:HB2	1:E:384:ASN:OD1	1.95	0.66
1:E:525:LYS:HE2	2:S:114:GLU:HG2	1.77	0.66
1:F:581:GLN:NE2	1:F:629:ASN:H	1.94	0.66
2:O:121:VAL:C	2:O:123:GLN:H	2.01	0.66
2:P:58:ASP:HB3	2:P:62:THR:HG23	1.76	0.66
1:B:186:LYS:O	1:B:188:LEU:O	2.13	0.66
1:D:115:LYS:NZ	1:D:115:LYS:HB3	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:49:GLN:N	2:O:49:GLN:NE2	2.43	0.66
1:C:99:GLU:C	1:C:101:GLY:H	2.02	0.66
1:C:548:THR:N	4:C:903:CMP:HN61	1.87	0.66
1:F:607:ASN:HB3	1:F:609:GLU:OE2	1.96	0.66
1:B:345:THR:HG22	1:B:490:ALA:O	1.96	0.66
1:D:426:ILE:CD1	1:D:431:LYS:HA	2.25	0.66
1:D:529:VAL:HG21	2:R:109:MET:HE1	1.77	0.66
1:E:412:GLU:C	1:E:414:LYS:N	2.51	0.66
1:A:148:GLU:HG3	1:A:149:THR:N	2.10	0.66
1:D:607:ASN:HB3	1:D:609:GLU:OE2	1.96	0.66
1:D:658:PRO:HG3	1:D:752:LEU:HD22	1.78	0.66
1:E:131:ARG:HG3	1:E:243:LEU:HD21	1.77	0.66
1:E:142:VAL:HG13	1:E:154:ILE:HD11	1.78	0.66
1:F:99:GLU:C	1:F:101:GLY:H	2.03	0.66
2:T:121:VAL:C	2:T:123:GLN:H	2.02	0.66
1:A:658:PRO:HG3	1:A:752:LEU:HD22	1.78	0.66
1:B:112:VAL:O	1:B:114:HIS:N	2.29	0.66
1:D:254:ARG:H	1:D:254:ARG:HD2	1.60	0.66
1:E:112:VAL:O	1:E:114:HIS:N	2.29	0.66
1:E:134:LYS:C	1:E:136:PRO:HD3	2.21	0.66
1:F:658:PRO:HG3	1:F:752:LEU:HD22	1.79	0.66
1:A:173:ILE:HD12	1:A:243:LEU:CD2	2.26	0.65
1:A:185:ASP:O	1:A:190:PRO:HA	1.96	0.65
1:A:345:THR:HG22	1:A:490:ALA:O	1.96	0.65
1:A:412:GLU:C	1:A:414:LYS:N	2.51	0.65
1:B:412:GLU:C	1:B:414:LYS:N	2.52	0.65
1:E:142:VAL:HG13	1:E:154:ILE:CD1	2.26	0.65
1:F:332:ASN:OD1	1:F:334:LEU:HD13	1.97	0.65
1:F:655:ASN:HD22	1:F:655:ASN:N	1.93	0.65
2:S:49:GLN:N	2:S:49:GLN:NE2	2.43	0.65
2:S:65:PHE:HB2	2:S:66:PRO:CD	2.25	0.65
1:A:607:ASN:HB3	1:A:609:GLU:OE2	1.96	0.65
1:B:142:VAL:HG13	1:B:154:ILE:CD1	2.26	0.65
1:F:173:ILE:HD12	1:F:243:LEU:CD2	2.26	0.65
2:P:65:PHE:HB2	2:P:66:PRO:CD	2.26	0.65
1:A:581:GLN:NE2	1:A:629:ASN:H	1.93	0.65
1:C:142:VAL:HG13	1:C:154:ILE:CD1	2.26	0.65
1:C:216:GLU:HG3	1:C:217:LYS:HG2	1.78	0.65
1:C:257:LEU:HG	1:C:257:LEU:O	1.95	0.65
1:D:134:LYS:HG2	1:D:136:PRO:CG	2.26	0.65
1:D:257:LEU:HD12	1:D:261:ALA:HB3	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ILE:HD12	1:E:243:LEU:CD2	2.27	0.65
1:E:630:ARG:NE	2:S:83:GLU:HG2	2.12	0.65
1:F:338:LEU:HD21	1:F:409:ARG:CZ	2.26	0.65
1:F:595:ILE:HG22	1:F:596:ILE:N	2.12	0.65
2:O:16:PHE:HA	2:O:35:VAL:HG11	1.77	0.65
1:A:338:LEU:HD21	1:A:409:ARG:CZ	2.25	0.65
1:B:581:GLN:NE2	1:B:629:ASN:H	1.94	0.65
1:C:173:ILE:HD12	1:C:243:LEU:CD2	2.26	0.65
1:C:217:LYS:HB3	1:C:217:LYS:HZ2	1.60	0.65
1:C:223:LYS:HD3	1:C:224:SER:N	2.10	0.65
1:E:186:LYS:HB2	1:E:190:PRO:HD3	1.78	0.65
1:F:172:GLU:HB3	1:F:246:SER:HA	1.79	0.65
1:A:172:GLU:HB3	1:A:246:SER:HA	1.78	0.65
1:B:338:LEU:HD21	1:B:409:ARG:CZ	2.26	0.65
1:B:450:ASN:ND2	1:B:452:GLU:HG3	2.11	0.65
1:C:172:GLU:HB3	1:C:246:SER:HA	1.79	0.65
1:C:450:ASN:ND2	1:C:452:GLU:HG3	2.12	0.65
1:C:759:GLN:HE21	1:C:759:GLN:CA	2.09	0.65
1:D:134:LYS:C	1:D:136:PRO:HD3	2.22	0.65
1:D:142:VAL:HG13	1:D:154:ILE:HD11	1.78	0.65
1:D:172:GLU:HB3	1:D:246:SER:HA	1.78	0.65
1:D:175:LYS:NZ	1:D:175:LYS:CB	2.60	0.65
1:D:737:LYS:HE2	1:D:737:LYS:HA	1.77	0.65
1:E:657:ILE:HG13	1:E:756:ILE:CD1	2.25	0.65
2:R:49:GLN:N	2:R:49:GLN:NE2	2.44	0.65
1:A:450:ASN:ND2	1:A:452:GLU:HG3	2.10	0.65
1:A:724:ARG:HG3	1:A:724:ARG:HH11	1.61	0.65
1:B:191:GLU:O	1:B:192:PHE:C	2.40	0.65
1:C:635:ILE:HD12	1:C:635:ILE:N	2.11	0.65
1:D:655:ASN:HD22	1:D:655:ASN:N	1.94	0.65
1:F:120:LEU:CD1	1:F:120:LEU:C	2.70	0.65
1:F:134:LYS:HG2	1:F:136:PRO:CG	2.26	0.65
1:F:216:GLU:HG3	1:F:217:LYS:HG2	1.79	0.65
2:T:12:PHE:CD1	2:T:72:MET:HG3	2.32	0.65
1:A:141:PHE:HB2	1:A:155:ASN:OD1	1.97	0.65
1:A:505:LYS:C	1:A:507:GLN:H	2.03	0.65
1:D:134:LYS:HG2	1:D:136:PRO:HG3	1.79	0.65
1:D:354:SER:O	1:D:371:SER:HB2	1.96	0.65
1:D:747:ASN:O	1:D:750:GLN:HB2	1.97	0.65
1:E:508:ILE:HG23	1:E:536:TYR:CE2	2.32	0.65
2:T:16:PHE:HA	2:T:35:VAL:HG11	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:VAL:HG21	2:O:109:MET:HE1	1.79	0.65
1:B:189:ASP:O	1:B:190:PRO:C	2.36	0.65
1:C:142:VAL:HG13	1:C:154:ILE:HD11	1.77	0.65
1:D:191:GLU:O	1:D:193:LEU:N	2.30	0.65
1:D:218:LEU:C	1:D:220:LEU:H	2.05	0.65
1:E:120:LEU:CD1	1:E:120:LEU:C	2.70	0.65
2:P:12:PHE:CD1	2:P:72:MET:HG3	2.32	0.65
1:B:141:PHE:HB2	1:B:155:ASN:OD1	1.97	0.65
1:B:173:ILE:HD12	1:B:243:LEU:CD2	2.27	0.65
1:C:115:LYS:NZ	1:C:115:LYS:HB3	2.11	0.65
1:C:540:ARG:HD3	1:C:627:TYR:OH	1.97	0.65
1:C:595:ILE:HG22	1:C:596:ILE:N	2.12	0.65
1:C:658:PRO:HG3	1:C:752:LEU:HD22	1.79	0.65
1:D:257:LEU:O	1:D:257:LEU:HG	1.97	0.65
1:D:338:LEU:HD21	1:D:409:ARG:CZ	2.27	0.65
1:E:450:ASN:ND2	1:E:452:GLU:HG3	2.12	0.65
1:E:635:ILE:HD12	1:E:635:ILE:N	2.12	0.65
1:F:180:ASP:O	1:F:182:ILE:N	2.30	0.65
2:S:5:THR:CG2	2:S:8:GLN:HB2	2.27	0.65
2:S:121:VAL:C	2:S:123:GLN:H	2.02	0.65
1:A:134:LYS:C	1:A:136:PRO:HD3	2.21	0.65
1:A:257:LEU:O	1:A:265:PHE:HB2	1.97	0.65
1:B:172:GLU:HB3	1:B:246:SER:HA	1.79	0.65
1:B:525:LYS:HE2	2:P:114:GLU:HG2	1.77	0.65
1:C:120:LEU:C	1:C:120:LEU:CD1	2.70	0.65
1:C:257:LEU:O	1:C:265:PHE:HB2	1.97	0.65
1:C:504:ILE:O	1:C:507:GLN:HB3	1.97	0.65
1:C:529:VAL:HG21	2:Q:109:MET:HE1	1.78	0.65
1:C:655:ASN:HD22	1:C:655:ASN:N	1.93	0.65
1:D:141:PHE:HB2	1:D:155:ASN:OD1	1.97	0.65
1:D:142:VAL:HG13	1:D:154:ILE:CD1	2.26	0.65
1:D:173:ILE:HD12	1:D:243:LEU:CD2	2.26	0.65
1:E:134:LYS:HG2	1:E:136:PRO:HG3	1.78	0.65
1:E:172:GLU:HB3	1:E:246:SER:HA	1.79	0.65
1:E:540:ARG:HD3	1:E:627:TYR:OH	1.96	0.65
1:E:595:ILE:HG22	1:E:596:ILE:N	2.12	0.65
1:F:134:LYS:C	1:F:136:PRO:HD3	2.22	0.65
2:Q:5:THR:CG2	2:Q:8:GLN:HB2	2.27	0.65
1:A:595:ILE:HG22	1:A:596:ILE:N	2.12	0.64
1:B:120:LEU:CD1	1:B:120:LEU:C	2.70	0.64
1:B:658:PRO:HG3	1:B:752:LEU:HD22	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:LYS:HE2	2:Q:114:GLU:HG2	1.79	0.64
1:D:70:GLU:HB2	1:D:107:THR:HG22	1.79	0.64
1:D:505:LYS:C	1:D:507:GLN:H	2.03	0.64
1:F:186:LYS:CB	1:F:190:PRO:HD3	2.27	0.64
2:R:12:PHE:HE1	2:R:72:MET:HE2	1.62	0.64
1:A:112:VAL:O	1:A:114:HIS:N	2.28	0.64
1:B:134:LYS:HG2	1:B:136:PRO:HG3	1.79	0.64
1:C:354:SER:O	1:C:371:SER:HB2	1.96	0.64
1:D:120:LEU:C	1:D:120:LEU:CD1	2.70	0.64
1:E:581:GLN:NE2	1:E:629:ASN:H	1.95	0.64
1:E:607:ASN:HB3	1:E:609:GLU:OE2	1.96	0.64
1:E:658:PRO:HG3	1:E:752:LEU:HD22	1.79	0.64
1:E:724:ARG:HH11	1:E:724:ARG:HG3	1.61	0.64
2:R:65:PHE:HB2	2:R:66:PRO:CD	2.27	0.64
2:T:65:PHE:HB2	2:T:66:PRO:CD	2.25	0.64
1:A:120:LEU:C	1:A:120:LEU:CD1	2.70	0.64
1:A:127:SER:HB3	1:A:133:GLU:OE2	1.97	0.64
1:A:525:LYS:HE2	2:O:114:GLU:HG2	1.78	0.64
1:B:332:ASN:OD1	1:B:334:LEU:HD13	1.96	0.64
1:C:134:LYS:C	1:C:136:PRO:HD3	2.22	0.64
1:D:332:ASN:OD1	1:D:334:LEU:HD13	1.98	0.64
1:E:175:LYS:NZ	1:E:175:LYS:CB	2.61	0.64
1:E:216:GLU:HG3	1:E:217:LYS:HG2	1.78	0.64
1:E:332:ASN:OD1	1:E:334:LEU:HD13	1.97	0.64
1:E:338:LEU:HD21	1:E:409:ARG:CZ	2.26	0.64
1:E:548:THR:N	4:E:905:CMP:N6	2.38	0.64
1:F:184:LYS:HZ1	1:F:191:GLU:HB2	1.63	0.64
2:T:69:LEU:HD12	2:T:69:LEU:O	1.97	0.64
1:B:322:LEU:HD13	1:B:556:MET:HE1	1.79	0.64
1:B:529:VAL:HG21	2:P:109:MET:HE1	1.79	0.64
1:B:728:ALA:O	1:B:732:ILE:HG12	1.97	0.64
1:B:747:ASN:O	1:B:750:GLN:HB2	1.98	0.64
1:C:120:LEU:O	1:C:120:LEU:HD12	1.97	0.64
1:D:186:LYS:O	1:D:188:LEU:O	2.14	0.64
1:D:345:THR:HG22	1:D:490:ALA:O	1.97	0.64
1:D:504:ILE:O	1:D:507:GLN:HB3	1.97	0.64
1:E:187:SER:N	1:E:188:LEU:O	2.31	0.64
1:E:345:THR:HG22	1:E:490:ALA:O	1.98	0.64
2:P:121:VAL:C	2:P:123:GLN:H	2.02	0.64
2:R:12:PHE:CD1	2:R:72:MET:HG3	2.32	0.64
2:T:5:THR:CG2	2:T:8:GLN:HB2	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASN:OD1	1:A:334:LEU:HD13	1.97	0.64
1:A:504:ILE:O	1:A:507:GLN:HB3	1.98	0.64
1:C:131:ARG:HG3	1:C:243:LEU:HD22	1.78	0.64
1:C:338:LEU:HD21	1:C:409:ARG:CZ	2.27	0.64
1:C:692:GLU:O	1:C:696:LYS:HG3	1.98	0.64
1:D:120:LEU:O	1:D:120:LEU:HD12	1.97	0.64
1:D:525:LYS:HE2	2:R:114:GLU:HG2	1.78	0.64
1:E:257:LEU:O	1:E:265:PHE:HB2	1.97	0.64
1:E:322:LEU:HD13	1:E:556:MET:HE1	1.78	0.64
1:E:692:GLU:O	1:E:696:LYS:HG3	1.98	0.64
1:F:120:LEU:O	1:F:120:LEU:HD12	1.97	0.64
1:F:134:LYS:HG2	1:F:136:PRO:HG3	1.79	0.64
1:F:724:ARG:HH11	1:F:724:ARG:HG3	1.61	0.64
2:Q:12:PHE:CD1	2:Q:72:MET:HG3	2.32	0.64
2:Q:12:PHE:HE1	2:Q:72:MET:HE2	1.63	0.64
2:R:92:PHE:O	2:R:94:LYS:N	2.30	0.64
1:A:216:GLU:HG3	1:A:217:LYS:HG2	1.79	0.64
1:A:254:ARG:H	1:A:254:ARG:HD2	1.61	0.64
1:B:447:SER:HB3	1:B:450:ASN:O	1.98	0.64
1:B:540:ARG:HD3	1:B:627:TYR:OH	1.97	0.64
1:B:595:ILE:HG22	1:B:596:ILE:N	2.12	0.64
1:B:607:ASN:HB3	1:B:609:GLU:OE2	1.98	0.64
1:E:504:ILE:O	1:E:507:GLN:HB3	1.97	0.64
1:F:345:THR:HG22	1:F:490:ALA:O	1.98	0.64
2:P:55:VAL:HG21	2:P:67:GLU:OE1	1.98	0.64
2:S:12:PHE:CD1	2:S:72:MET:HG3	2.32	0.64
1:A:83:GLN:C	1:A:85:LEU:H	2.06	0.64
1:A:368:GLN:HB2	1:A:384:ASN:OD1	1.97	0.64
1:A:635:ILE:HD12	1:A:635:ILE:N	2.10	0.64
1:B:134:LYS:C	1:B:136:PRO:HD3	2.23	0.64
1:B:257:LEU:HG	1:B:257:LEU:O	1.96	0.64
1:B:655:ASN:HD22	1:B:655:ASN:N	1.94	0.64
1:C:508:ILE:HG23	1:C:536:TYR:CE2	2.33	0.64
1:F:257:LEU:O	1:F:265:PHE:HB2	1.97	0.64
1:F:322:LEU:HD13	1:F:556:MET:HE1	1.79	0.64
1:F:508:ILE:HG23	1:F:536:TYR:CE2	2.33	0.64
1:A:508:ILE:HG23	1:A:536:TYR:CE2	2.33	0.64
1:B:218:LEU:C	1:B:220:LEU:H	2.05	0.64
1:C:199:LEU:C	1:C:201:ASP:H	2.06	0.64
1:D:759:GLN:HE21	1:D:759:GLN:CA	2.10	0.64
1:E:180:ASP:O	1:E:182:ILE:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:120:LEU:HD12	1.97	0.64
1:B:257:LEU:O	1:B:265:PHE:HB2	1.97	0.64
1:C:141:PHE:HB2	1:C:155:ASN:OD1	1.98	0.64
1:C:405:LEU:HD13	1:C:453:VAL:CG2	2.28	0.64
1:D:692:GLU:O	1:D:696:LYS:HG3	1.98	0.64
1:E:747:ASN:O	1:E:750:GLN:HB2	1.98	0.64
1:F:540:ARG:HD3	1:F:627:TYR:OH	1.97	0.64
1:C:332:ASN:OD1	1:C:334:LEU:HD13	1.97	0.64
1:C:457:THR:OG1	1:C:468:LYS:HG3	1.97	0.64
1:D:540:ARG:HD3	1:D:627:TYR:OH	1.98	0.64
1:F:217:LYS:HG3	1:F:236:GLU:HG3	1.80	0.64
2:P:121:VAL:C	2:P:123:GLN:N	2.55	0.64
1:A:310:GLU:OE2	1:A:340:LYS:HD2	1.98	0.63
1:A:457:THR:OG1	1:A:468:LYS:HG3	1.98	0.63
1:B:66:LEU:HD12	1:B:103:GLU:HA	1.81	0.63
1:B:504:ILE:O	1:B:507:GLN:HB3	1.97	0.63
2:S:55:VAL:HG21	2:S:67:GLU:OE1	1.98	0.63
2:S:69:LEU:HD12	2:S:69:LEU:O	1.98	0.63
2:T:121:VAL:C	2:T:123:GLN:N	2.56	0.63
1:B:216:GLU:HG3	1:B:217:LYS:HG2	1.79	0.63
1:B:426:ILE:HD11	1:B:431:LYS:HG2	1.81	0.63
1:C:296:LEU:CD2	1:C:606:LYS:HE2	2.21	0.63
1:D:131:ARG:HG3	1:D:243:LEU:HD21	1.78	0.63
1:D:216:GLU:HG3	1:D:217:LYS:HG2	1.79	0.63
1:E:310:GLU:OE2	1:E:340:LYS:HD2	1.98	0.63
1:F:66:LEU:HD12	1:F:103:GLU:HA	1.80	0.63
1:F:187:SER:N	1:F:188:LEU:O	2.31	0.63
1:A:187:SER:N	1:A:188:LEU:O	2.31	0.63
1:C:747:ASN:O	1:C:750:GLN:HB2	1.97	0.63
1:E:257:LEU:HD12	1:E:261:ALA:HB3	1.81	0.63
1:F:188:LEU:CD2	1:F:188:LEU:N	2.46	0.63
2:R:55:VAL:HG21	2:R:67:GLU:OE1	1.98	0.63
1:A:322:LEU:HD13	1:A:556:MET:HE1	1.80	0.63
1:B:508:ILE:HG23	1:B:536:TYR:CE2	2.33	0.63
1:C:112:VAL:O	1:C:114:HIS:N	2.29	0.63
1:C:581:GLN:NE2	1:C:629:ASN:H	1.96	0.63
1:D:581:GLN:NE2	1:D:629:ASN:H	1.95	0.63
1:E:529:VAL:HG21	2:S:109:MET:HE1	1.79	0.63
1:F:310:GLU:OE2	1:F:340:LYS:HD2	1.99	0.63
2:O:65:PHE:HB2	2:O:66:PRO:CD	2.25	0.63
1:A:144:GLU:HG2	1:A:177:ILE:HD11	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ILE:HG12	1:A:447:SER:N	2.13	0.63
1:C:501:LEU:HD11	2:Q:108:VAL:HG13	1.80	0.63
1:E:120:LEU:O	1:E:120:LEU:HD12	1.97	0.63
1:E:457:THR:OG1	1:E:468:LYS:HG3	1.99	0.63
1:F:182:ILE:O	1:F:187:SER:HB2	1.99	0.63
2:Q:33:GLY:O	2:Q:37:ARG:HG3	1.99	0.63
1:B:191:GLU:O	1:B:193:LEU:N	2.31	0.63
1:C:83:GLN:C	1:C:85:LEU:H	2.07	0.63
1:D:457:THR:OG1	1:D:468:LYS:HG3	1.99	0.63
1:D:508:ILE:HG23	1:D:536:TYR:CE2	2.34	0.63
1:D:520:PRO:HG2	1:D:521:ASN:H	1.64	0.63
1:E:257:LEU:O	1:E:257:LEU:HG	1.96	0.63
1:E:426:ILE:HD11	1:E:431:LYS:HG2	1.81	0.63
1:F:112:VAL:O	1:F:114:HIS:N	2.30	0.63
1:F:180:ASP:CG	1:F:181:ILE:H	2.05	0.63
1:F:257:LEU:O	1:F:257:LEU:HG	1.96	0.63
1:F:504:ILE:O	1:F:507:GLN:HB3	1.98	0.63
2:O:12:PHE:CD1	2:O:72:MET:HG3	2.33	0.63
2:O:12:PHE:HE1	2:O:72:MET:HE2	1.64	0.63
2:P:5:THR:CG2	2:P:8:GLN:HB2	2.28	0.63
2:Q:92:PHE:O	2:Q:94:LYS:N	2.31	0.63
2:T:55:VAL:HG21	2:T:67:GLU:OE1	1.98	0.63
1:A:244:ALA:HB2	1:A:264:MET:HE3	1.81	0.63
1:B:83:GLN:C	1:B:85:LEU:H	2.06	0.63
1:E:144:GLU:HG2	1:E:177:ILE:HD11	1.81	0.63
1:A:128:MET:HE2	1:A:239:HIS:CE1	2.33	0.63
1:A:426:ILE:HD11	1:A:431:LYS:HG2	1.81	0.63
1:C:217:LYS:HG3	1:C:236:GLU:HG3	1.81	0.63
1:C:310:GLU:OE2	1:C:340:LYS:HD2	1.99	0.63
1:D:447:SER:HB3	1:D:450:ASN:O	1.99	0.63
1:E:161:ILE:CG2	1:E:168:GLU:HB2	2.28	0.63
1:B:403:LEU:HG	1:B:405:LEU:HD12	1.81	0.63
1:B:548:THR:N	4:B:902:CMP:N6	2.38	0.63
1:C:728:ALA:O	1:C:732:ILE:HG12	1.99	0.63
1:D:137:PHE:C	1:D:137:PHE:CD2	2.72	0.63
1:D:635:ILE:HD12	1:D:635:ILE:N	2.11	0.63
1:E:66:LEU:HD12	1:E:103:GLU:HA	1.81	0.63
1:E:141:PHE:HB2	1:E:155:ASN:OD1	1.99	0.63
1:E:360:VAL:HG21	1:E:365:PRO:HB3	1.80	0.63
1:E:447:SER:HB3	1:E:450:ASN:O	1.99	0.63
1:F:70:GLU:HB2	1:F:107:THR:HG22	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:ILE:HD11	1:F:431:LYS:HG2	1.81	0.63
1:F:728:ALA:O	1:F:732:ILE:HG12	1.99	0.63
2:O:55:VAL:HG21	2:O:67:GLU:OE1	1.99	0.63
1:A:184:LYS:HZ1	1:A:191:GLU:HB2	1.64	0.62
1:A:594:PHE:HE2	1:A:596:ILE:HD11	1.64	0.62
1:A:692:GLU:O	1:A:696:LYS:HG3	1.99	0.62
1:A:747:ASN:O	1:A:750:GLN:HB2	1.98	0.62
1:B:244:ALA:HB2	1:B:264:MET:HE3	1.81	0.62
1:B:447:SER:OG	1:B:448:ASP:N	2.32	0.62
1:C:446:ILE:HG12	1:C:447:SER:N	2.13	0.62
1:E:728:ALA:O	1:E:732:ILE:HG12	1.99	0.62
1:F:412:GLU:C	1:F:414:LYS:N	2.52	0.62
2:R:121:VAL:C	2:R:123:GLN:N	2.56	0.62
1:B:217:LYS:HG3	1:B:236:GLU:HG3	1.81	0.62
1:B:310:GLU:OE2	1:B:340:LYS:HD2	1.98	0.62
1:D:115:LYS:HB3	1:D:115:LYS:HZ3	1.63	0.62
1:E:218:LEU:C	1:E:220:LEU:H	2.07	0.62
1:E:377:GLN:O	1:E:378:LEU:HD12	1.99	0.62
1:F:141:PHE:HB2	1:F:155:ASN:OD1	1.99	0.62
1:F:193:LEU:O	1:F:197:LYS:HB2	1.99	0.62
2:P:69:LEU:HD12	2:P:69:LEU:O	1.99	0.62
1:A:257:LEU:HD12	1:A:261:ALA:HB3	1.80	0.62
1:B:186:LYS:HB2	1:B:190:PRO:CD	2.29	0.62
1:C:426:ILE:HD11	1:C:431:LYS:HG2	1.81	0.62
1:E:152:LEU:HD21	1:E:154:ILE:HD11	1.80	0.62
1:E:193:LEU:O	1:E:197:LYS:HB2	2.00	0.62
1:E:446:ILE:HG12	1:E:447:SER:N	2.13	0.62
1:F:175:LYS:NZ	1:F:175:LYS:CB	2.62	0.62
1:F:747:ASN:O	1:F:750:GLN:HB2	1.99	0.62
2:T:12:PHE:HE1	2:T:72:MET:HE2	1.63	0.62
1:A:120:LEU:O	1:A:120:LEU:HD12	1.97	0.62
1:A:193:LEU:O	1:A:197:LYS:HB2	1.99	0.62
1:C:700:TYR:CE1	1:C:727:GLN:HB3	2.34	0.62
1:E:752:LEU:O	1:E:756:ILE:HG12	1.99	0.62
1:F:446:ILE:HG12	1:F:447:SER:N	2.13	0.62
2:O:121:VAL:C	2:O:123:GLN:N	2.55	0.62
1:A:217:LYS:HG3	1:A:236:GLU:HG3	1.81	0.62
1:A:759:GLN:HE21	1:A:759:GLN:CA	2.11	0.62
1:B:592:GLU:HB3	1:B:604:LEU:HD11	1.81	0.62
1:B:635:ILE:HD12	1:B:635:ILE:N	2.12	0.62
1:C:83:GLN:C	1:C:85:LEU:N	2.57	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LYS:HG2	1:C:136:PRO:HG3	1.82	0.62
1:D:217:LYS:HG3	1:D:236:GLU:HG3	1.81	0.62
1:D:257:LEU:O	1:D:265:PHE:HB2	1.99	0.62
1:E:217:LYS:HG3	1:E:236:GLU:HG3	1.81	0.62
1:F:403:LEU:HG	1:F:405:LEU:HD12	1.81	0.62
2:R:69:LEU:HD12	2:R:69:LEU:O	1.99	0.62
1:B:161:ILE:CG2	1:B:168:GLU:HB2	2.29	0.62
1:B:360:VAL:HG21	1:B:365:PRO:HB3	1.81	0.62
1:D:83:GLN:C	1:D:85:LEU:N	2.57	0.62
1:D:112:VAL:O	1:D:114:HIS:N	2.29	0.62
1:D:403:LEU:HG	1:D:405:LEU:HD12	1.81	0.62
1:D:743:PRO:HA	1:D:746:LYS:HB3	1.82	0.62
1:E:107:THR:CG2	1:E:115:LYS:HD2	2.29	0.62
1:A:83:GLN:C	1:A:85:LEU:N	2.57	0.62
1:A:354:SER:O	1:A:371:SER:HB2	1.99	0.62
1:A:403:LEU:HG	1:A:405:LEU:HD12	1.82	0.62
1:B:457:THR:OG1	1:B:468:LYS:HG3	1.99	0.62
1:C:189:ASP:O	1:C:191:GLU:N	2.32	0.62
1:D:185:ASP:O	1:D:190:PRO:HA	1.99	0.62
1:D:426:ILE:HD11	1:D:431:LYS:HG2	1.81	0.62
1:E:592:GLU:HB3	1:E:604:LEU:HD11	1.82	0.62
2:O:33:GLY:O	2:O:37:ARG:HG3	2.00	0.62
1:B:152:LEU:HD21	1:B:154:ILE:HD11	1.81	0.62
1:C:447:SER:HB3	1:C:450:ASN:O	2.00	0.62
1:C:743:PRO:HA	1:C:746:LYS:HB3	1.82	0.62
1:C:752:LEU:O	1:C:756:ILE:HG12	1.99	0.62
1:D:83:GLN:C	1:D:85:LEU:H	2.07	0.62
1:D:193:LEU:O	1:D:197:LYS:HB2	1.99	0.62
1:D:310:GLU:OE2	1:D:340:LYS:HD2	1.99	0.62
1:D:360:VAL:HG21	1:D:365:PRO:HB3	1.80	0.62
1:D:728:ALA:O	1:D:732:ILE:HG12	2.00	0.62
1:E:403:LEU:HG	1:E:405:LEU:HD12	1.82	0.62
1:F:405:LEU:HD13	1:F:453:VAL:CG2	2.29	0.62
2:P:12:PHE:HE1	2:P:72:MET:HE2	1.64	0.62
1:A:447:SER:HB3	1:A:450:ASN:O	1.98	0.62
1:E:447:SER:OG	1:E:448:ASP:N	2.33	0.62
1:F:186:LYS:HA	1:F:190:PRO:CD	2.25	0.62
1:A:630:ARG:NE	2:O:83:GLU:HG2	2.15	0.62
1:A:728:ALA:O	1:A:732:ILE:HG12	1.99	0.62
1:B:184:LYS:HZ1	1:B:191:GLU:HB2	1.64	0.62
1:B:446:ILE:HG12	1:B:447:SER:N	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ARG:HB3	1:C:254:ARG:HH11	1.65	0.62
1:D:501:LEU:HD11	2:R:108:VAL:HG13	1.81	0.62
1:E:127:SER:HB3	1:E:133:GLU:OE2	2.00	0.62
1:F:83:GLN:C	1:F:85:LEU:H	2.08	0.62
2:O:69:LEU:HD12	2:O:69:LEU:O	2.00	0.62
2:P:12:PHE:CZ	2:P:76:MET:HE3	2.32	0.62
2:Q:65:PHE:HB2	2:Q:66:PRO:CD	2.26	0.62
2:S:12:PHE:HE1	2:S:72:MET:HE2	1.63	0.62
2:S:121:VAL:C	2:S:123:GLN:N	2.56	0.62
1:B:520:PRO:HG2	1:B:521:ASN:H	1.65	0.61
1:B:639:ASN:C	1:B:639:ASN:HD22	2.08	0.61
1:D:187:SER:N	1:D:188:LEU:O	2.33	0.61
1:E:301:ALA:O	1:E:303:LYS:N	2.33	0.61
1:E:520:PRO:HG2	1:E:521:ASN:H	1.65	0.61
1:F:107:THR:CG2	1:F:115:LYS:HD2	2.30	0.61
2:Q:55:VAL:HG21	2:Q:67:GLU:OE1	1.98	0.61
2:R:33:GLY:O	2:R:37:ARG:HG3	2.00	0.61
1:A:527:LYS:HD2	2:O:145:MET:O	2.00	0.61
1:A:655:ASN:HD22	1:A:655:ASN:N	1.95	0.61
1:B:115:LYS:HB3	1:B:115:LYS:HZ3	1.66	0.61
1:C:66:LEU:HD12	1:C:103:GLU:HA	1.81	0.61
1:C:70:GLU:HB2	1:C:107:THR:HG22	1.82	0.61
1:C:244:ALA:HB2	1:C:264:MET:HE3	1.80	0.61
1:C:409:ARG:NE	1:C:413:LEU:HD21	2.15	0.61
1:E:83:GLN:C	1:E:85:LEU:H	2.07	0.61
1:E:185:ASP:O	1:E:190:PRO:CA	2.48	0.61
1:E:668:SER:CA	2:S:14:GLU:HG3	2.26	0.61
1:E:743:PRO:HA	1:E:746:LYS:HB3	1.82	0.61
1:F:127:SER:HB3	1:F:133:GLU:OE2	1.99	0.61
1:F:520:PRO:HG2	1:F:521:ASN:H	1.65	0.61
1:F:548:THR:N	4:F:906:CMP:N6	2.38	0.61
2:P:33:GLY:O	2:P:37:ARG:HG3	2.00	0.61
1:A:218:LEU:C	1:A:220:LEU:H	2.05	0.61
1:A:520:PRO:HG2	1:A:521:ASN:H	1.64	0.61
1:E:197:LYS:HZ2	1:E:197:LYS:HB3	1.66	0.61
1:E:639:ASN:C	1:E:639:ASN:HD22	2.07	0.61
1:F:191:GLU:C	1:F:193:LEU:N	2.59	0.61
1:F:409:ARG:NE	1:F:413:LEU:HD21	2.15	0.61
1:A:377:GLN:O	1:A:378:LEU:HD12	2.01	0.61
1:B:252:ASP:CG	1:B:253:HIS:H	2.09	0.61
1:C:128:MET:O	1:C:128:MET:CG	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ILE:HG12	1:D:447:SER:N	2.13	0.61
1:E:501:LEU:HD11	2:S:108:VAL:HG13	1.82	0.61
1:F:244:ALA:HB2	1:F:264:MET:HE3	1.81	0.61
1:F:360:VAL:HG21	1:F:365:PRO:HB3	1.81	0.61
1:F:501:LEU:HD11	2:T:108:VAL:HG13	1.82	0.61
2:T:92:PHE:O	2:T:94:LYS:N	2.32	0.61
1:A:343:VAL:HG13	1:A:487:PRO:HG2	1.82	0.61
1:B:83:GLN:C	1:B:85:LEU:N	2.56	0.61
1:F:79:ILE:C	1:F:81:GLN:H	2.09	0.61
1:F:368:GLN:HG3	1:F:383:GLY:C	2.25	0.61
2:O:92:PHE:O	2:O:94:LYS:N	2.32	0.61
2:Q:36:MET:HE3	2:Q:43:PRO:CG	2.27	0.61
1:A:409:ARG:NE	1:A:413:LEU:HD21	2.15	0.61
1:B:743:PRO:HA	1:B:746:LYS:HB3	1.82	0.61
1:C:180:ASP:O	1:C:182:ILE:N	2.33	0.61
1:C:193:LEU:O	1:C:197:LYS:HB2	2.01	0.61
1:C:218:LEU:C	1:C:220:LEU:H	2.06	0.61
1:E:376:GLN:C	1:E:378:LEU:H	2.08	0.61
1:F:301:ALA:O	1:F:303:LYS:N	2.34	0.61
1:A:372:LYS:HG3	1:A:373:LYS:HG2	1.82	0.61
1:B:180:ASP:C	1:B:182:ILE:N	2.58	0.61
1:B:193:LEU:O	1:B:197:LYS:HB2	2.00	0.61
1:B:372:LYS:HG3	1:B:373:LYS:HG2	1.81	0.61
1:D:244:ALA:HB2	1:D:264:MET:HE3	1.82	0.61
1:E:355:SER:HB3	1:E:361:ALA:HA	1.83	0.61
1:F:446:ILE:HG13	1:F:452:GLU:O	2.00	0.61
2:Q:69:LEU:HD12	2:Q:69:LEU:O	2.00	0.61
1:B:185:ASP:O	1:B:190:PRO:CA	2.49	0.61
1:B:752:LEU:O	1:B:756:ILE:HG12	2.00	0.61
1:B:759:GLN:HE21	1:B:759:GLN:CA	2.09	0.61
1:C:403:LEU:HG	1:C:405:LEU:HD12	1.81	0.61
1:D:409:ARG:NE	1:D:413:LEU:HD21	2.16	0.61
1:D:752:LEU:O	1:D:756:ILE:HG12	1.99	0.61
1:F:83:GLN:C	1:F:85:LEU:N	2.57	0.61
1:F:457:THR:OG1	1:F:468:LYS:HG3	1.99	0.61
1:A:66:LEU:HD12	1:A:103:GLU:HA	1.83	0.61
1:A:446:ILE:HG13	1:A:452:GLU:O	2.01	0.61
1:B:83:GLN:O	1:B:85:LEU:N	2.34	0.61
1:B:128:MET:CG	1:B:128:MET:O	2.49	0.61
1:C:639:ASN:HD22	1:C:639:ASN:C	2.07	0.61
1:D:180:ASP:CG	1:D:181:ILE:H	2.09	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LYS:HG3	1:D:373:LYS:HG2	1.82	0.61
1:D:639:ASN:C	1:D:639:ASN:HD22	2.09	0.61
1:F:403:LEU:CD2	1:F:405:LEU:HD11	2.30	0.61
1:F:700:TYR:CE1	1:F:727:GLN:HB3	2.35	0.61
2:O:5:THR:CG2	2:O:8:GLN:HB2	2.28	0.61
1:A:515:LYS:HG2	1:A:515:LYS:O	2.01	0.61
1:B:257:LEU:HD12	1:B:261:ALA:HB3	1.83	0.61
1:C:360:VAL:HG21	1:C:365:PRO:HB3	1.80	0.61
1:C:376:GLN:C	1:C:378:LEU:H	2.08	0.61
1:D:189:ASP:O	1:D:191:GLU:N	2.33	0.61
1:D:368:GLN:HG3	1:D:383:GLY:C	2.25	0.61
1:D:403:LEU:CD2	1:D:405:LEU:HD11	2.30	0.61
1:F:630:ARG:NE	2:T:83:GLU:HG2	2.16	0.61
1:A:115:LYS:HB3	1:A:115:LYS:HZ3	1.66	0.60
1:B:368:GLN:HB3	1:B:380:VAL:HG13	1.83	0.60
1:B:376:GLN:C	1:B:378:LEU:H	2.09	0.60
1:C:187:SER:N	1:C:188:LEU:O	2.34	0.60
1:C:372:LYS:HG3	1:C:373:LYS:HG2	1.82	0.60
1:D:66:LEU:HD12	1:D:103:GLU:HA	1.81	0.60
1:E:79:ILE:C	1:E:81:GLN:H	2.09	0.60
2:S:12:PHE:CZ	2:S:76:MET:HE3	2.33	0.60
1:B:131:ARG:HG3	1:B:243:LEU:CD2	2.31	0.60
1:B:187:SER:N	1:B:188:LEU:O	2.34	0.60
1:C:128:MET:HE2	1:C:239:HIS:CE1	2.36	0.60
1:C:131:ARG:HG3	1:C:243:LEU:HD21	1.83	0.60
1:D:182:ILE:O	1:D:187:SER:HB2	2.00	0.60
1:D:377:GLN:O	1:D:378:LEU:HD12	2.00	0.60
1:D:700:TYR:CE1	1:D:727:GLN:HB3	2.36	0.60
1:E:244:ALA:HB2	1:E:264:MET:HE3	1.82	0.60
1:E:252:ASP:CG	1:E:253:HIS:H	2.09	0.60
1:E:405:LEU:HD13	1:E:453:VAL:CG2	2.29	0.60
1:E:735:VAL:HG12	1:E:741:ILE:HD13	1.82	0.60
1:F:254:ARG:HB3	1:F:254:ARG:HH11	1.67	0.60
1:A:189:ASP:O	1:A:191:GLU:N	2.34	0.60
1:B:107:THR:CG2	1:B:115:LYS:HD2	2.31	0.60
1:B:692:GLU:O	1:B:696:LYS:HG3	2.00	0.60
1:C:127:SER:HB3	1:C:133:GLU:OE2	2.01	0.60
1:C:182:ILE:O	1:C:187:SER:HB2	2.02	0.60
1:C:197:LYS:HZ2	1:C:197:LYS:HB3	1.65	0.60
1:C:403:LEU:CD2	1:C:405:LEU:HD11	2.30	0.60
1:E:372:LYS:HG3	1:E:373:LYS:HG2	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:LEU:HD21	1:F:154:ILE:HD11	1.82	0.60
1:F:515:LYS:NZ	1:F:515:LYS:HB3	2.15	0.60
1:A:301:ALA:O	1:A:303:LYS:N	2.34	0.60
1:A:368:GLN:HG3	1:A:383:GLY:C	2.26	0.60
1:A:700:TYR:CE1	1:A:727:GLN:HB3	2.35	0.60
1:B:136:PRO:O	1:B:137:PHE:C	2.45	0.60
1:B:355:SER:HB3	1:B:361:ALA:HA	1.83	0.60
1:B:515:LYS:NZ	1:B:515:LYS:HB3	2.16	0.60
1:B:527:LYS:HD2	2:P:145:MET:O	2.02	0.60
1:C:180:ASP:CG	1:C:181:ILE:H	2.08	0.60
1:C:343:VAL:HG13	1:C:487:PRO:HG2	1.82	0.60
1:E:165:GLN:C	1:E:167:LYS:H	2.09	0.60
1:E:655:ASN:HD22	1:E:655:ASN:N	1.98	0.60
1:F:499:PRO:HG2	1:F:504:ILE:HD11	1.83	0.60
1:A:752:LEU:O	1:A:756:ILE:HG12	2.00	0.60
1:B:180:ASP:O	1:B:182:ILE:N	2.34	0.60
1:B:354:SER:O	1:B:371:SER:HB2	2.01	0.60
1:B:409:ARG:NE	1:B:413:LEU:HD21	2.15	0.60
1:C:337:ASN:ND2	1:C:412:GLU:OE2	2.35	0.60
1:D:527:LYS:HD2	2:R:145:MET:O	2.01	0.60
1:E:368:GLN:HB3	1:E:380:VAL:HG13	1.83	0.60
1:E:409:ARG:NE	1:E:413:LEU:HD21	2.15	0.60
1:F:635:ILE:HD12	1:F:635:ILE:N	2.12	0.60
1:F:743:PRO:HA	1:F:746:LYS:HB3	1.82	0.60
2:T:33:GLY:O	2:T:37:ARG:HG3	2.01	0.60
1:A:368:GLN:HB3	1:A:380:VAL:HG13	1.83	0.60
1:A:376:GLN:C	1:A:378:LEU:H	2.09	0.60
1:B:337:ASN:ND2	1:B:412:GLU:OE2	2.34	0.60
1:C:122:GLU:O	1:C:122:GLU:HG2	2.02	0.60
1:C:134:LYS:HG2	1:C:136:PRO:CG	2.31	0.60
1:C:499:PRO:HG2	1:C:504:ILE:HD11	1.84	0.60
1:C:735:VAL:HG12	1:C:741:ILE:HD13	1.83	0.60
1:D:76:LEU:O	1:D:80:GLN:N	2.35	0.60
1:D:152:LEU:HD21	1:D:154:ILE:HD11	1.82	0.60
1:D:343:VAL:HG13	1:D:487:PRO:HG2	1.82	0.60
1:F:136:PRO:O	1:F:137:PHE:C	2.45	0.60
1:F:550:SER:H	1:F:553:GLN:HE21	1.49	0.60
1:F:692:GLU:O	1:F:696:LYS:HG3	2.01	0.60
1:F:752:LEU:O	1:F:756:ILE:HG12	2.00	0.60
1:C:248:TYR:C	1:C:248:TYR:CD2	2.80	0.60
1:C:301:ALA:O	1:C:303:LYS:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:GLN:HG3	1:C:383:GLY:C	2.26	0.60
1:D:180:ASP:O	1:D:182:ILE:N	2.34	0.60
1:E:148:GLU:HG3	1:E:149:THR:N	2.16	0.60
1:E:368:GLN:HG3	1:E:383:GLY:C	2.26	0.60
1:F:122:GLU:O	1:F:122:GLU:HG2	2.02	0.60
1:F:248:TYR:C	1:F:248:TYR:CD2	2.80	0.60
1:F:377:GLN:O	1:F:378:LEU:HD12	2.01	0.60
1:F:447:SER:HB3	1:F:450:ASN:O	2.00	0.60
1:F:594:PHE:HE2	1:F:596:ILE:HD11	1.67	0.60
1:B:79:ILE:C	1:B:81:GLN:H	2.09	0.60
1:B:175:LYS:NZ	1:B:175:LYS:CB	2.61	0.60
1:B:301:ALA:O	1:B:303:LYS:N	2.35	0.60
1:B:405:LEU:HD13	1:B:453:VAL:CG2	2.29	0.60
1:C:520:PRO:HG2	1:C:521:ASN:H	1.65	0.60
1:D:301:ALA:O	1:D:303:LYS:N	2.34	0.60
1:D:499:PRO:HG2	1:D:504:ILE:HD11	1.84	0.60
1:E:122:GLU:O	1:E:122:GLU:HG2	2.02	0.60
1:E:175:LYS:HB2	1:E:175:LYS:HZ3	1.66	0.60
1:E:700:TYR:CE1	1:E:727:GLN:HB3	2.36	0.60
1:F:268:MET:O	1:F:271:LEU:HB2	2.02	0.60
1:F:654:ILE:C	1:F:655:ASN:HD22	2.09	0.60
1:A:743:PRO:HA	1:A:746:LYS:HB3	1.83	0.60
1:B:188:LEU:CD2	1:B:188:LEU:N	2.46	0.60
1:B:499:PRO:HG2	1:B:504:ILE:HD11	1.83	0.60
1:B:515:LYS:O	1:B:515:LYS:HG2	2.02	0.60
1:C:252:ASP:CG	1:C:253:HIS:H	2.09	0.60
1:C:377:GLN:O	1:C:378:LEU:HD12	2.02	0.60
1:C:594:PHE:HE2	1:C:596:ILE:HD11	1.67	0.60
1:C:654:ILE:C	1:C:655:ASN:HD22	2.10	0.60
1:D:136:PRO:O	1:D:137:PHE:C	2.45	0.60
1:F:354:SER:O	1:F:371:SER:HB2	2.01	0.60
1:A:210:PHE:CD1	1:A:214:PHE:HB2	2.36	0.60
1:A:355:SER:HB3	1:A:361:ALA:HA	1.84	0.60
1:A:499:PRO:HG2	1:A:504:ILE:HD11	1.84	0.60
1:B:76:LEU:O	1:B:80:GLN:N	2.35	0.60
1:B:122:GLU:O	1:B:122:GLU:HG2	2.02	0.60
1:B:165:GLN:C	1:B:167:LYS:H	2.09	0.60
1:B:594:PHE:HE2	1:B:596:ILE:HD11	1.66	0.60
1:C:515:LYS:NZ	1:C:515:LYS:HB3	2.16	0.60
1:E:83:GLN:O	1:E:85:LEU:N	2.35	0.60
1:E:116:GLU:O	1:E:117:LEU:HD22	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:PHE:CD1	1:E:214:PHE:HB2	2.36	0.60
1:E:403:LEU:CD2	1:E:405:LEU:HD11	2.32	0.60
1:F:372:LYS:HG3	1:F:373:LYS:HG2	1.82	0.60
2:S:33:GLY:O	2:S:37:ARG:HG3	2.02	0.60
1:A:136:PRO:O	1:A:137:PHE:C	2.45	0.59
1:A:180:ASP:O	1:A:182:ILE:N	2.35	0.59
1:A:248:TYR:C	1:A:248:TYR:CD2	2.80	0.59
1:A:254:ARG:HB3	1:A:254:ARG:HH11	1.66	0.59
1:A:360:VAL:HG21	1:A:365:PRO:HB3	1.82	0.59
1:A:501:LEU:HD11	2:O:108:VAL:HG13	1.82	0.59
1:A:735:VAL:HG12	1:A:741:ILE:HD13	1.83	0.59
1:B:156:ILE:HD12	1:B:156:ILE:N	2.17	0.59
1:B:735:VAL:HG12	1:B:741:ILE:HD13	1.82	0.59
1:D:735:VAL:HG12	1:D:741:ILE:HD13	1.83	0.59
1:E:248:TYR:C	1:E:248:TYR:CD2	2.80	0.59
1:B:700:TYR:CE1	1:B:727:GLN:HB3	2.37	0.59
1:C:116:GLU:O	1:C:117:LEU:HD22	2.02	0.59
1:C:185:ASP:O	1:C:190:PRO:HA	2.01	0.59
1:C:504:ILE:O	1:C:507:GLN:CB	2.50	0.59
1:D:83:GLN:O	1:D:85:LEU:N	2.35	0.59
1:D:144:GLU:HG2	1:D:177:ILE:HD11	1.83	0.59
1:D:173:ILE:HG13	1:D:242:SER:CB	2.27	0.59
1:D:252:ASP:CG	1:D:253:HIS:H	2.10	0.59
1:D:346:LYS:HG3	1:D:350:VAL:HB	1.84	0.59
1:D:594:PHE:HE2	1:D:596:ILE:HD11	1.67	0.59
1:F:185:ASP:O	1:F:190:PRO:HA	2.02	0.59
1:F:337:ASN:ND2	1:F:412:GLU:OE2	2.34	0.59
1:F:376:GLN:C	1:F:378:LEU:H	2.09	0.59
1:A:152:LEU:HD21	1:A:154:ILE:HD11	1.83	0.59
1:B:248:TYR:C	1:B:248:TYR:CD2	2.80	0.59
1:B:671:ARG:O	1:B:674:SER:O	2.21	0.59
1:C:79:ILE:C	1:C:81:GLN:H	2.10	0.59
1:C:136:PRO:O	1:C:137:PHE:C	2.45	0.59
1:C:152:LEU:HD21	1:C:154:ILE:HD11	1.84	0.59
1:C:165:GLN:C	1:C:167:LYS:H	2.10	0.59
1:D:592:GLU:HB3	1:D:604:LEU:HD11	1.82	0.59
1:E:343:VAL:HG13	1:E:487:PRO:HG2	1.82	0.59
1:E:354:SER:O	1:E:371:SER:HB2	2.02	0.59
1:E:527:LYS:HD2	2:S:145:MET:O	2.02	0.59
1:F:735:VAL:HG12	1:F:741:ILE:HD13	1.83	0.59
1:A:189:ASP:O	1:A:190:PRO:C	2.39	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:CG	1:A:253:HIS:H	2.10	0.59
1:B:368:GLN:HG3	1:B:383:GLY:C	2.26	0.59
1:B:504:ILE:O	1:B:507:GLN:CB	2.51	0.59
1:C:515:LYS:O	1:C:515:LYS:HG2	2.02	0.59
1:D:128:MET:HG2	1:D:128:MET:O	2.01	0.59
1:D:376:GLN:C	1:D:378:LEU:H	2.09	0.59
1:E:83:GLN:C	1:E:85:LEU:N	2.57	0.59
1:E:136:PRO:O	1:E:137:PHE:C	2.46	0.59
1:F:71:PHE:CB	1:F:108:ASP:HB2	2.33	0.59
1:F:301:ALA:C	1:F:303:LYS:N	2.59	0.59
1:F:355:SER:HB3	1:F:361:ALA:HA	1.85	0.59
1:F:368:GLN:HB3	1:F:380:VAL:HG13	1.83	0.59
1:B:343:VAL:HG13	1:B:487:PRO:HG2	1.84	0.59
1:C:355:SER:HB3	1:C:361:ALA:HA	1.84	0.59
1:D:116:GLU:O	1:D:117:LEU:HD22	2.03	0.59
1:D:254:ARG:HB3	1:D:254:ARG:HH11	1.66	0.59
1:D:323:ASN:C	1:D:323:ASN:HD22	2.10	0.59
1:E:199:LEU:C	1:E:201:ASP:N	2.61	0.59
2:T:36:MET:HE3	2:T:43:PRO:CG	2.27	0.59
1:A:165:GLN:C	1:A:167:LYS:H	2.10	0.59
1:A:180:ASP:C	1:A:182:ILE:N	2.61	0.59
1:A:594:PHE:CE1	1:A:602:PHE:HB3	2.38	0.59
1:B:116:GLU:O	1:B:117:LEU:HD22	2.03	0.59
1:C:76:LEU:O	1:C:80:GLN:N	2.34	0.59
1:C:197:LYS:HB3	1:C:197:LYS:NZ	2.18	0.59
1:D:654:ILE:C	1:D:655:ASN:HD22	2.11	0.59
2:P:92:PHE:O	2:P:94:LYS:N	2.33	0.59
1:A:671:ARG:O	1:A:674:SER:O	2.21	0.59
1:C:71:PHE:CB	1:C:108:ASP:HB2	2.33	0.59
1:C:123:GLU:HG2	1:C:124:GLU:H	1.66	0.59
1:C:368:GLN:HB3	1:C:380:VAL:HG13	1.82	0.59
1:C:557:LEU:HD11	1:C:575:VAL:HG12	1.85	0.59
1:D:337:ASN:ND2	1:D:412:GLU:OE2	2.35	0.59
1:F:165:GLN:C	1:F:167:LYS:H	2.10	0.59
1:F:346:LYS:HG3	1:F:350:VAL:HB	1.85	0.59
1:F:515:LYS:HG2	1:F:515:LYS:O	2.02	0.59
1:F:550:SER:H	1:F:553:GLN:NE2	2.00	0.59
1:A:76:LEU:O	1:A:80:GLN:N	2.36	0.59
1:A:175:LYS:NZ	1:A:175:LYS:CB	2.62	0.59
1:A:515:LYS:NZ	1:A:515:LYS:HB3	2.17	0.59
1:B:134:LYS:O	1:B:135:VAL:HG12	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PHE:CD1	1:B:214:PHE:HB2	2.36	0.59
1:C:592:GLU:HB3	1:C:604:LEU:HD11	1.84	0.59
1:D:403:LEU:HG	1:D:405:LEU:CD1	2.33	0.59
1:E:76:LEU:O	1:E:80:GLN:N	2.35	0.59
1:E:180:ASP:O	1:E:183:SER:N	2.35	0.59
1:F:115:LYS:C	1:F:117:LEU:H	2.11	0.59
1:F:210:PHE:CD1	1:F:214:PHE:HB2	2.36	0.59
1:A:78:LYS:HD2	1:A:156:ILE:HD13	1.84	0.59
1:A:83:GLN:O	1:A:85:LEU:N	2.36	0.59
1:A:122:GLU:HG2	1:A:122:GLU:O	2.02	0.59
1:A:550:SER:H	1:A:553:GLN:HE21	1.48	0.59
1:B:364:ILE:O	1:B:477:MET:HG2	2.03	0.59
1:C:83:GLN:O	1:C:85:LEU:N	2.36	0.59
1:C:175:LYS:NZ	1:C:175:LYS:CB	2.62	0.59
1:C:184:LYS:NZ	1:C:191:GLU:HB2	2.17	0.59
1:D:180:ASP:O	1:D:183:SER:N	2.35	0.59
1:D:264:MET:O	1:D:267:TYR:HB3	2.03	0.59
1:E:337:ASN:ND2	1:E:412:GLU:OE2	2.35	0.59
1:E:515:LYS:NZ	1:E:515:LYS:HB3	2.17	0.59
2:T:12:PHE:CZ	2:T:76:MET:HE3	2.36	0.59
1:A:248:TYR:CD2	1:A:248:TYR:O	2.56	0.59
1:A:346:LYS:HG3	1:A:350:VAL:HB	1.85	0.59
1:A:550:SER:H	1:A:553:GLN:NE2	2.01	0.59
1:B:74:GLU:HB2	1:B:78:LYS:CB	2.33	0.59
1:B:501:LEU:HD11	2:P:108:VAL:HG13	1.84	0.59
1:C:115:LYS:HD3	1:C:153:ILE:HD13	1.84	0.59
1:C:346:LYS:HG3	1:C:350:VAL:HB	1.85	0.59
1:D:368:GLN:HB3	1:D:380:VAL:HG13	1.83	0.59
1:D:504:ILE:O	1:D:507:GLN:CB	2.51	0.59
1:E:264:MET:O	1:E:267:TYR:HB3	2.03	0.59
1:E:515:LYS:O	1:E:515:LYS:HG2	2.02	0.59
1:F:161:ILE:CG2	1:F:168:GLU:HB2	2.33	0.59
1:F:403:LEU:HG	1:F:405:LEU:CD1	2.33	0.59
1:A:337:ASN:ND2	1:A:412:GLU:OE2	2.34	0.58
1:B:197:LYS:HZ2	1:B:197:LYS:HB3	1.68	0.58
1:B:377:GLN:O	1:B:378:LEU:HD12	2.02	0.58
1:C:186:LYS:HE3	1:C:234:LEU:HB2	1.84	0.58
1:D:122:GLU:HG2	1:D:122:GLU:O	2.02	0.58
1:D:127:SER:HB3	1:D:133:GLU:OE2	2.03	0.58
1:D:165:GLN:C	1:D:167:LYS:H	2.10	0.58
1:E:759:GLN:HE21	1:E:759:GLN:CA	2.10	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:LYS:HB2	1:F:175:LYS:HZ3	1.68	0.58
1:F:639:ASN:HD22	1:F:639:ASN:C	2.08	0.58
1:A:412:GLU:O	1:A:414:LYS:N	2.37	0.58
1:A:598:PRO:HG3	1:A:624:TYR:OH	2.02	0.58
1:A:639:ASN:C	1:A:639:ASN:HD22	2.09	0.58
1:B:131:ARG:HG3	1:B:243:LEU:HD22	1.83	0.58
1:B:173:ILE:C	1:B:175:LYS:N	2.60	0.58
1:B:197:LYS:HB3	1:B:197:LYS:NZ	2.18	0.58
1:B:602:PHE:N	1:B:602:PHE:CD2	2.72	0.58
1:D:210:PHE:CD1	1:D:214:PHE:HB2	2.36	0.58
1:D:355:SER:HB3	1:D:361:ALA:HA	1.84	0.58
1:E:248:TYR:CD2	1:E:248:TYR:O	2.56	0.58
1:E:412:GLU:O	1:E:414:LYS:N	2.36	0.58
1:E:598:PRO:HG3	1:E:624:TYR:OH	2.03	0.58
1:F:130:SER:HB2	1:F:170:TYR:CE2	2.38	0.58
1:F:364:ILE:O	1:F:477:MET:HG2	2.03	0.58
1:A:323:ASN:C	1:A:323:ASN:HD22	2.12	0.58
1:B:412:GLU:O	1:B:414:LYS:N	2.36	0.58
1:B:788:ASP:O	1:B:792:VAL:HG23	2.03	0.58
1:C:550:SER:H	1:C:553:GLN:HE21	1.51	0.58
1:D:199:LEU:HD11	1:D:226:ASP:OD2	2.03	0.58
1:D:550:SER:H	1:D:553:GLN:HE21	1.50	0.58
1:E:184:LYS:NZ	1:E:191:GLU:HB2	2.19	0.58
1:E:185:ASP:O	1:E:190:PRO:CD	2.51	0.58
1:E:197:LYS:HB3	1:E:197:LYS:NZ	2.17	0.58
1:E:594:PHE:HE2	1:E:596:ILE:HD11	1.67	0.58
2:Q:121:VAL:C	2:Q:123:GLN:N	2.56	0.58
2:R:5:THR:CG2	2:R:8:GLN:HB2	2.28	0.58
1:A:173:ILE:HG13	1:A:242:SER:CB	2.29	0.58
1:B:192:PHE:O	1:B:196:ILE:HG13	2.03	0.58
1:D:71:PHE:CB	1:D:108:ASP:HB2	2.33	0.58
1:D:184:LYS:HZ1	1:D:191:GLU:HB2	1.66	0.58
1:D:318:ILE:CG2	1:D:322:LEU:HD12	2.32	0.58
1:D:515:LYS:HG2	1:D:515:LYS:O	2.02	0.58
1:F:217:LYS:NZ	1:F:217:LYS:HB3	2.19	0.58
1:F:318:ILE:CG2	1:F:322:LEU:HD12	2.32	0.58
1:B:346:LYS:HG3	1:B:350:VAL:HB	1.85	0.58
1:D:301:ALA:C	1:D:303:LYS:N	2.60	0.58
1:D:515:LYS:HB3	1:D:515:LYS:NZ	2.17	0.58
1:D:630:ARG:NE	2:R:83:GLU:HG2	2.18	0.58
1:D:788:ASP:O	1:D:792:VAL:HG23	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:670:ILE:HG21	1:E:744:GLU:HB2	1.85	0.58
1:F:252:ASP:CG	1:F:253:HIS:H	2.11	0.58
2:O:12:PHE:CZ	2:O:76:MET:HE3	2.35	0.58
2:Q:12:PHE:CZ	2:Q:76:MET:HE3	2.38	0.58
2:S:92:PHE:O	2:S:94:LYS:N	2.33	0.58
1:A:79:ILE:C	1:A:81:GLN:H	2.11	0.58
1:A:164:GLU:O	1:A:167:LYS:HE3	2.03	0.58
1:A:186:LYS:HE3	1:A:234:LEU:HB2	1.86	0.58
1:A:264:MET:O	1:A:267:TYR:HB3	2.03	0.58
1:A:301:ALA:C	1:A:303:LYS:N	2.60	0.58
1:A:654:ILE:C	1:A:655:ASN:HD22	2.11	0.58
1:A:670:ILE:HG21	1:A:744:GLU:HB2	1.86	0.58
1:B:264:MET:O	1:B:267:TYR:HB3	2.04	0.58
1:B:403:LEU:HG	1:B:405:LEU:CD1	2.34	0.58
1:C:670:ILE:HG21	1:C:744:GLU:HB2	1.85	0.58
1:D:405:LEU:HD13	1:D:453:VAL:CG2	2.29	0.58
1:D:670:ILE:HG21	1:D:744:GLU:HB2	1.86	0.58
1:E:301:ALA:C	1:E:303:LYS:N	2.59	0.58
1:E:364:ILE:O	1:E:477:MET:HG2	2.04	0.58
1:F:76:LEU:O	1:F:80:GLN:N	2.35	0.58
1:F:83:GLN:O	1:F:85:LEU:N	2.37	0.58
1:B:71:PHE:CB	1:B:108:ASP:HB2	2.33	0.58
1:C:164:GLU:O	1:C:167:LYS:HE3	2.04	0.58
1:C:199:LEU:HD11	1:C:226:ASP:OD2	2.04	0.58
1:C:210:PHE:CD1	1:C:214:PHE:HB2	2.35	0.58
1:D:248:TYR:C	1:D:248:TYR:CD2	2.80	0.58
1:D:412:GLU:O	1:D:414:LYS:N	2.36	0.58
1:E:254:ARG:HB3	1:E:254:ARG:HH11	1.69	0.58
1:E:499:PRO:HG2	1:E:504:ILE:HD11	1.85	0.58
1:F:197:LYS:NZ	1:F:197:LYS:HB3	2.19	0.58
1:A:116:GLU:O	1:A:117:LEU:HD22	2.04	0.58
1:A:403:LEU:CD2	1:A:405:LEU:HD11	2.31	0.58
1:A:504:ILE:O	1:A:507:GLN:CB	2.52	0.58
1:B:403:LEU:CD2	1:B:405:LEU:HD11	2.30	0.58
1:B:594:PHE:CE1	1:B:602:PHE:HB3	2.39	0.58
1:B:670:ILE:HG21	1:B:744:GLU:HB2	1.86	0.58
1:D:268:MET:O	1:D:271:LEU:HB2	2.04	0.58
1:E:199:LEU:HD11	1:E:226:ASP:OD2	2.04	0.58
1:F:788:ASP:O	1:F:792:VAL:HG23	2.03	0.58
1:A:71:PHE:CB	1:A:108:ASP:HB2	2.33	0.58
1:A:173:ILE:C	1:A:175:LYS:N	2.61	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:O	1:A:477:MET:HG2	2.04	0.58
1:A:592:GLU:HB3	1:A:604:LEU:HD11	1.84	0.58
1:B:127:SER:HB3	1:B:133:GLU:OE2	2.04	0.58
1:B:186:LYS:HE3	1:B:234:LEU:HB2	1.86	0.58
1:D:602:PHE:N	1:D:602:PHE:CD2	2.72	0.58
1:E:403:LEU:HG	1:E:405:LEU:CD1	2.34	0.58
1:F:116:GLU:O	1:F:117:LEU:HD22	2.03	0.58
1:F:655:ASN:N	1:F:655:ASN:ND2	2.51	0.58
1:F:670:ILE:HG21	1:F:744:GLU:HB2	1.86	0.58
1:A:275:GLY:O	1:A:278:LYS:HB2	2.04	0.58
1:A:403:LEU:HG	1:A:405:LEU:CD1	2.34	0.58
1:B:225:ILE:HG12	1:B:229:PHE:HE2	1.69	0.58
1:C:318:ILE:CG2	1:C:322:LEU:HD12	2.34	0.58
1:C:693:SER:O	1:C:696:LYS:HB2	2.04	0.58
1:C:788:ASP:O	1:C:792:VAL:HG23	2.04	0.58
1:D:79:ILE:C	1:D:81:GLN:H	2.11	0.58
1:D:248:TYR:HD2	1:D:248:TYR:O	1.87	0.58
1:D:594:PHE:CE1	1:D:602:PHE:HB3	2.38	0.58
1:E:346:LYS:HG3	1:E:350:VAL:HB	1.85	0.58
1:E:504:ILE:O	1:E:507:GLN:CB	2.51	0.58
2:R:36:MET:HE3	2:R:43:PRO:CG	2.28	0.58
1:A:405:LEU:HD13	1:A:453:VAL:CG2	2.29	0.57
1:B:323:ASN:HD22	1:B:323:ASN:C	2.12	0.57
1:C:403:LEU:HG	1:C:405:LEU:CD1	2.34	0.57
1:D:134:LYS:CG	1:D:136:PRO:HD3	2.27	0.57
1:D:196:ILE:HA	1:D:199:LEU:HD12	1.86	0.57
1:D:197:LYS:NZ	1:D:197:LYS:HB3	2.18	0.57
1:D:248:TYR:CD2	1:D:248:TYR:O	2.57	0.57
1:D:671:ARG:O	1:D:674:SER:O	2.22	0.57
1:F:218:LEU:C	1:F:220:LEU:H	2.06	0.57
1:F:592:GLU:HB3	1:F:604:LEU:HD11	1.85	0.57
1:A:156:ILE:N	1:A:156:ILE:HD12	2.19	0.57
1:A:199:LEU:HD11	1:A:226:ASP:OD2	2.04	0.57
1:A:318:ILE:CG2	1:A:322:LEU:HD12	2.33	0.57
1:B:301:ALA:C	1:B:303:LYS:N	2.60	0.57
1:C:464:VAL:CG2	1:C:465:LEU:HD12	2.33	0.57
1:C:557:LEU:HD11	1:C:575:VAL:CG1	2.34	0.57
1:D:186:LYS:HE3	1:D:234:LEU:HB2	1.85	0.57
1:E:550:SER:H	1:E:553:GLN:HE21	1.50	0.57
1:E:594:PHE:CE1	1:E:602:PHE:HB3	2.39	0.57
1:F:164:GLU:O	1:F:167:LYS:HE3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:O	1:A:248:TYR:HD2	1.87	0.57
1:A:788:ASP:O	1:A:792:VAL:HG23	2.04	0.57
1:B:164:GLU:O	1:B:167:LYS:HE3	2.05	0.57
1:C:301:ALA:C	1:C:303:LYS:N	2.60	0.57
1:C:364:ILE:O	1:C:477:MET:HG2	2.04	0.57
1:C:412:GLU:O	1:C:414:LYS:N	2.37	0.57
1:C:548:THR:N	4:C:903:CMP:N6	2.38	0.57
1:D:156:ILE:HD12	1:D:156:ILE:N	2.19	0.57
1:E:156:ILE:HD12	1:E:156:ILE:N	2.19	0.57
1:F:164:GLU:C	1:F:166:SER:H	2.13	0.57
1:F:192:PHE:HA	1:F:195:LEU:HB3	1.86	0.57
1:F:661:ALA:O	1:F:665:LYS:HD3	2.05	0.57
2:O:36:MET:HE3	2:O:43:PRO:CG	2.27	0.57
1:A:192:PHE:O	1:A:196:ILE:HG13	2.04	0.57
1:A:339:ILE:O	1:A:340:LYS:C	2.47	0.57
1:B:268:MET:O	1:B:271:LEU:HB2	2.04	0.57
1:C:655:ASN:N	1:C:655:ASN:ND2	2.52	0.57
1:D:115:LYS:C	1:D:117:LEU:H	2.11	0.57
1:D:164:GLU:C	1:D:166:SER:H	2.12	0.57
1:D:443:GLU:HG3	1:D:458:LYS:HG2	1.86	0.57
1:E:115:LYS:C	1:E:117:LEU:H	2.11	0.57
1:E:186:LYS:HB2	1:E:190:PRO:CD	2.34	0.57
1:E:602:PHE:N	1:E:602:PHE:CD2	2.71	0.57
1:F:196:ILE:HA	1:F:199:LEU:HD12	1.87	0.57
1:F:343:VAL:HG13	1:F:487:PRO:HG2	1.86	0.57
1:A:268:MET:O	1:A:271:LEU:HB2	2.04	0.57
1:B:254:ARG:HB3	1:B:254:ARG:HH11	1.68	0.57
1:C:338:LEU:O	1:C:343:VAL:HG23	2.05	0.57
1:C:630:ARG:NE	2:Q:83:GLU:HG2	2.18	0.57
1:D:598:PRO:HG3	1:D:624:TYR:OH	2.03	0.57
1:E:268:MET:O	1:E:271:LEU:HB2	2.04	0.57
1:E:275:GLY:O	1:E:278:LYS:HB2	2.03	0.57
1:E:550:SER:H	1:E:553:GLN:NE2	2.03	0.57
1:F:248:TYR:CD2	1:F:248:TYR:O	2.57	0.57
1:F:504:ILE:O	1:F:507:GLN:CB	2.52	0.57
1:F:508:ILE:HG12	1:F:536:TYR:CD2	2.40	0.57
1:A:180:ASP:O	1:A:183:SER:N	2.36	0.57
1:B:78:LYS:HD2	1:B:156:ILE:HD13	1.85	0.57
1:B:192:PHE:HA	1:B:195:LEU:HB3	1.86	0.57
1:B:764:LEU:C	1:B:766:HIS:H	2.12	0.57
1:C:173:ILE:HG13	1:C:242:SER:CB	2.27	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:MET:O	1:C:267:TYR:HB3	2.05	0.57
1:C:527:LYS:HD2	2:Q:145:MET:O	2.04	0.57
1:D:115:LYS:HD3	1:D:153:ILE:HD13	1.86	0.57
1:D:275:GLY:O	1:D:278:LYS:HB2	2.04	0.57
1:D:339:ILE:O	1:D:340:LYS:C	2.47	0.57
1:F:180:ASP:O	1:F:183:SER:N	2.38	0.57
1:F:598:PRO:HG3	1:F:624:TYR:OH	2.04	0.57
1:A:196:ILE:HA	1:A:199:LEU:HD12	1.87	0.57
1:A:275:GLY:HA2	1:A:278:LYS:CG	2.32	0.57
1:B:180:ASP:O	1:B:183:SER:N	2.36	0.57
1:B:598:PRO:HG3	1:B:624:TYR:OH	2.04	0.57
1:B:632:TYR:O	1:B:633:ASN:HB2	2.05	0.57
1:C:115:LYS:C	1:C:117:LEU:H	2.11	0.57
1:C:156:ILE:N	1:C:156:ILE:HD12	2.19	0.57
1:C:323:ASN:C	1:C:323:ASN:HD22	2.10	0.57
1:D:128:MET:O	1:D:128:MET:CG	2.49	0.57
1:D:338:LEU:O	1:D:343:VAL:HG23	2.05	0.57
1:E:164:GLU:O	1:E:167:LYS:HE3	2.05	0.57
1:E:550:SER:HB3	1:E:553:GLN:HB2	1.87	0.57
1:F:115:LYS:HD3	1:F:153:ILE:HD13	1.86	0.57
1:F:527:LYS:HD2	2:T:145:MET:O	2.03	0.57
1:F:594:PHE:CE1	1:F:602:PHE:HB3	2.40	0.57
2:P:84:GLU:N	2:P:84:GLU:OE2	2.38	0.57
1:A:175:LYS:HB2	1:A:175:LYS:HZ3	1.68	0.57
1:A:225:ILE:HG12	1:A:229:PHE:HE2	1.69	0.57
1:A:338:LEU:O	1:A:343:VAL:HG23	2.05	0.57
1:B:148:GLU:HG3	1:B:149:THR:N	2.18	0.57
1:B:244:ALA:HB3	1:B:268:MET:HE3	1.87	0.57
1:B:368:GLN:CB	1:B:380:VAL:HG13	2.35	0.57
1:B:550:SER:H	1:B:553:GLN:NE2	2.03	0.57
1:C:217:LYS:HB3	1:C:217:LYS:NZ	2.19	0.57
1:C:248:TYR:CD2	1:C:248:TYR:O	2.57	0.57
1:C:268:MET:O	1:C:271:LEU:HB2	2.04	0.57
1:E:368:GLN:CB	1:E:380:VAL:HG13	2.35	0.57
1:E:788:ASP:O	1:E:792:VAL:HG23	2.04	0.57
1:F:264:MET:O	1:F:267:TYR:HB3	2.04	0.57
1:A:161:ILE:CG2	1:A:168:GLU:HB2	2.34	0.57
1:A:184:LYS:NZ	1:A:191:GLU:HB2	2.20	0.57
1:B:122:GLU:HG3	1:B:147:ARG:HB2	1.87	0.57
1:B:173:ILE:HG13	1:B:242:SER:CB	2.28	0.57
1:B:248:TYR:CD2	1:B:248:TYR:O	2.58	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLY:O	1:B:278:LYS:HB2	2.05	0.57
1:B:654:ILE:C	1:B:655:ASN:HD22	2.12	0.57
1:C:107:THR:CG2	1:C:115:LYS:HD2	2.35	0.57
1:C:597:ASN:C	1:C:599:GLU:H	2.13	0.57
1:D:123:GLU:HG2	1:D:124:GLU:H	1.70	0.57
1:D:776:LEU:O	1:D:780:LEU:CD2	2.53	0.57
1:F:144:GLU:HG2	1:F:177:ILE:HD11	1.87	0.57
1:A:122:GLU:HG3	1:A:147:ARG:HB2	1.87	0.57
1:A:443:GLU:HG3	1:A:458:LYS:HG2	1.87	0.57
1:C:196:ILE:HA	1:C:199:LEU:HD12	1.87	0.57
1:C:594:PHE:CE1	1:C:602:PHE:HB3	2.39	0.57
1:D:122:GLU:HG3	1:D:147:ARG:HB2	1.87	0.57
1:D:217:LYS:HB3	1:D:217:LYS:NZ	2.20	0.57
1:D:655:ASN:N	1:D:655:ASN:ND2	2.52	0.57
1:E:71:PHE:CB	1:E:108:ASP:HB2	2.33	0.57
1:E:196:ILE:HA	1:E:199:LEU:HD12	1.87	0.57
1:E:284:LYS:HA	1:E:284:LYS:HE3	1.87	0.57
1:F:275:GLY:O	1:F:278:LYS:HB2	2.04	0.57
1:F:412:GLU:O	1:F:414:LYS:N	2.37	0.57
2:R:84:GLU:N	2:R:84:GLU:OE2	2.38	0.57
1:A:301:ALA:C	1:A:303:LYS:H	2.13	0.56
1:B:184:LYS:HZ2	1:B:191:GLU:HG3	1.71	0.56
1:C:78:LYS:HD2	1:C:156:ILE:HD13	1.86	0.56
1:C:275:GLY:O	1:C:278:LYS:HB2	2.05	0.56
1:C:368:GLN:CB	1:C:380:VAL:HG13	2.34	0.56
1:C:776:LEU:O	1:C:780:LEU:CD2	2.53	0.56
1:D:124:GLU:OE2	1:D:129:ASN:ND2	2.38	0.56
1:E:78:LYS:HD2	1:E:156:ILE:HD13	1.86	0.56
1:F:199:LEU:HD11	1:F:226:ASP:OD2	2.04	0.56
1:F:284:LYS:HA	1:F:284:LYS:HE3	1.87	0.56
1:F:339:ILE:O	1:F:340:LYS:C	2.46	0.56
2:S:36:MET:HE3	2:S:43:PRO:CG	2.28	0.56
1:A:197:LYS:NZ	1:A:197:LYS:HB3	2.19	0.56
1:B:217:LYS:HB3	1:B:217:LYS:NZ	2.19	0.56
1:C:180:ASP:O	1:C:183:SER:N	2.36	0.56
1:C:284:LYS:HA	1:C:284:LYS:HE3	1.87	0.56
1:C:598:PRO:HG3	1:C:624:TYR:OH	2.05	0.56
1:D:364:ILE:O	1:D:477:MET:HG2	2.05	0.56
1:E:161:ILE:HG23	1:E:168:GLU:HB2	1.86	0.56
1:F:78:LYS:HD2	1:F:156:ILE:HD13	1.86	0.56
1:F:192:PHE:O	1:F:196:ILE:HG13	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:557:LEU:HD11	1:F:575:VAL:HG12	1.87	0.56
1:F:597:ASN:C	1:F:599:GLU:H	2.14	0.56
1:A:115:LYS:C	1:A:117:LEU:H	2.12	0.56
1:A:326:ILE:HG22	1:A:328:PHE:CE1	2.40	0.56
1:A:776:LEU:O	1:A:780:LEU:CD2	2.53	0.56
1:B:154:ILE:HG13	1:B:171:TYR:CD1	2.41	0.56
1:B:301:ALA:C	1:B:303:LYS:H	2.14	0.56
1:B:318:ILE:CG2	1:B:322:LEU:HD12	2.33	0.56
1:C:550:SER:H	1:C:553:GLN:NE2	2.02	0.56
1:D:76:LEU:H	1:D:76:LEU:CD2	2.19	0.56
1:E:164:GLU:C	1:E:166:SER:H	2.12	0.56
1:E:192:PHE:HA	1:E:195:LEU:HB3	1.87	0.56
1:E:217:LYS:HB3	1:E:217:LYS:NZ	2.20	0.56
1:E:301:ALA:C	1:E:303:LYS:H	2.13	0.56
1:E:338:LEU:O	1:E:343:VAL:HG23	2.05	0.56
1:E:508:ILE:HG12	1:E:536:TYR:CD2	2.40	0.56
1:E:597:ASN:C	1:E:599:GLU:H	2.13	0.56
1:E:661:ALA:O	1:E:665:LYS:HD3	2.05	0.56
1:F:131:ARG:HG3	1:F:243:LEU:HD21	1.87	0.56
1:F:301:ALA:C	1:F:303:LYS:H	2.13	0.56
1:F:668:SER:CA	2:T:14:GLU:HG3	2.29	0.56
2:P:21:LYS:C	2:P:21:LYS:HD3	2.30	0.56
2:Q:25:GLY:HA3	2:Q:65:PHE:CE1	2.41	0.56
2:S:21:LYS:C	2:S:21:LYS:HD3	2.30	0.56
2:T:11:GLU:O	2:T:13:LYS:N	2.38	0.56
1:B:164:GLU:C	1:B:166:SER:H	2.13	0.56
1:B:738:SER:OG	1:B:739:LYS:N	2.38	0.56
1:D:550:SER:H	1:D:553:GLN:NE2	2.02	0.56
1:D:661:ALA:O	1:D:665:LYS:HD3	2.04	0.56
1:E:122:GLU:HG3	1:E:147:ARG:HB2	1.87	0.56
1:F:134:LYS:CG	1:F:136:PRO:HD3	2.27	0.56
1:A:217:LYS:NZ	1:A:217:LYS:HB3	2.19	0.56
1:A:334:LEU:H	1:A:334:LEU:HD12	1.70	0.56
1:B:196:ILE:HA	1:B:199:LEU:HD12	1.87	0.56
1:B:338:LEU:O	1:B:343:VAL:HG23	2.06	0.56
1:C:122:GLU:HG3	1:C:147:ARG:HB2	1.87	0.56
1:C:144:GLU:HG2	1:C:177:ILE:HD11	1.88	0.56
1:D:284:LYS:HA	1:D:284:LYS:HE3	1.87	0.56
1:D:738:SER:OG	1:D:739:LYS:N	2.38	0.56
1:E:252:ASP:O	1:E:254:ARG:HD2	2.05	0.56
1:F:175:LYS:O	1:F:177:ILE:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:LYS:O	1:F:178:SER:N	2.38	0.56
1:F:602:PHE:CD2	1:F:602:PHE:N	2.71	0.56
1:F:759:GLN:HE21	1:F:759:GLN:CA	2.10	0.56
2:R:25:GLY:HA3	2:R:65:PHE:CE1	2.41	0.56
1:A:333:LYS:HA	1:A:336:THR:OG1	2.06	0.56
1:A:764:LEU:C	1:A:766:HIS:H	2.13	0.56
1:B:199:LEU:HD11	1:B:226:ASP:OD2	2.04	0.56
1:B:284:LYS:HA	1:B:284:LYS:HE3	1.87	0.56
1:B:550:SER:H	1:B:553:GLN:HE21	1.51	0.56
1:D:275:GLY:HA2	1:D:278:LYS:CG	2.31	0.56
1:D:320:ARG:O	1:D:321:GLU:C	2.49	0.56
1:D:470:ASN:O	1:D:472:ARG:HG3	2.06	0.56
1:E:186:LYS:HE3	1:E:234:LEU:HB2	1.87	0.56
1:E:217:LYS:HB3	1:E:217:LYS:HZ2	1.70	0.56
1:E:225:ILE:HG12	1:E:229:PHE:HE2	1.71	0.56
1:F:172:GLU:O	1:F:175:LYS:HB3	2.06	0.56
1:F:368:GLN:CB	1:F:380:VAL:HG13	2.35	0.56
1:F:557:LEU:HD11	1:F:575:VAL:CG1	2.36	0.56
2:Q:21:LYS:C	2:Q:21:LYS:HD3	2.30	0.56
2:T:21:LYS:C	2:T:21:LYS:HD3	2.31	0.56
2:T:76:MET:HG3	2:T:76:MET:O	2.06	0.56
1:A:192:PHE:HA	1:A:195:LEU:HB3	1.87	0.56
1:A:368:GLN:CB	1:A:380:VAL:HG13	2.34	0.56
1:A:597:ASN:C	1:A:599:GLU:H	2.14	0.56
1:B:115:LYS:C	1:B:117:LEU:H	2.13	0.56
1:B:161:ILE:HG23	1:B:168:GLU:HB2	1.87	0.56
1:C:164:GLU:C	1:C:166:SER:H	2.13	0.56
1:C:184:LYS:HD2	1:C:188:LEU:HG	1.88	0.56
1:C:279:ILE:O	1:C:283:LEU:HD13	2.06	0.56
1:D:192:PHE:O	1:D:196:ILE:HG13	2.05	0.56
2:R:21:LYS:HD3	2:R:21:LYS:C	2.30	0.56
2:S:25:GLY:HA3	2:S:65:PHE:CE1	2.41	0.56
2:S:76:MET:HG3	2:S:76:MET:O	2.06	0.56
1:A:128:MET:O	1:A:128:MET:HG3	2.05	0.56
1:A:164:GLU:C	1:A:166:SER:H	2.13	0.56
1:B:115:LYS:HD3	1:B:153:ILE:HD13	1.87	0.56
1:B:275:GLY:HA2	1:B:278:LYS:CG	2.33	0.56
1:B:550:SER:HB3	1:B:553:GLN:HB2	1.88	0.56
1:C:130:SER:HB2	1:C:170:TYR:CE2	2.40	0.56
1:C:709:ASN:HB2	2:Q:130:ILE:HG23	1.87	0.56
1:D:301:ALA:C	1:D:303:LYS:H	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:GLU:HG3	1:F:147:ARG:HB2	1.87	0.56
1:F:156:ILE:N	1:F:156:ILE:HD12	2.20	0.56
1:F:628:PHE:CD1	1:F:645:TRP:CD1	2.93	0.56
1:A:447:SER:OG	1:A:448:ASP:N	2.37	0.56
1:B:443:GLU:HG3	1:B:458:LYS:HG2	1.87	0.56
1:B:709:ASN:HB2	2:P:130:ILE:HG23	1.87	0.56
1:C:405:LEU:CD1	1:C:453:VAL:HG21	2.32	0.56
1:D:78:LYS:HD2	1:D:156:ILE:HD13	1.87	0.56
1:D:409:ARG:O	1:D:413:LEU:HG	2.06	0.56
1:D:557:LEU:HD11	1:D:575:VAL:CG1	2.36	0.56
1:E:115:LYS:HD3	1:E:153:ILE:HD13	1.87	0.56
1:F:323:ASN:C	1:F:323:ASN:HD22	2.11	0.56
1:F:447:SER:OG	1:F:448:ASP:N	2.39	0.56
2:O:84:GLU:N	2:O:84:GLU:OE2	2.39	0.56
1:B:508:ILE:HG12	1:B:536:TYR:CD2	2.41	0.56
1:C:339:ILE:O	1:C:340:LYS:C	2.47	0.56
1:C:443:GLU:HG3	1:C:458:LYS:HG2	1.87	0.56
1:D:333:LYS:C	1:D:335:ALA:H	2.14	0.56
1:D:333:LYS:HA	1:D:336:THR:OG1	2.06	0.56
1:D:597:ASN:C	1:D:599:GLU:H	2.14	0.56
1:F:128:MET:CG	1:F:128:MET:O	2.50	0.56
1:F:184:LYS:HD2	1:F:188:LEU:HG	1.88	0.56
1:C:96:ILE:O	1:C:100:LEU:HG	2.06	0.55
1:C:173:ILE:C	1:C:175:LYS:N	2.60	0.55
1:C:333:LYS:HA	1:C:336:THR:OG1	2.06	0.55
1:C:550:SER:HB3	1:C:553:GLN:HB2	1.89	0.55
1:D:164:GLU:O	1:D:167:LYS:HE3	2.05	0.55
1:D:368:GLN:CB	1:D:380:VAL:HG13	2.35	0.55
1:E:628:PHE:CD1	1:E:645:TRP:CD1	2.94	0.55
1:E:671:ARG:O	1:E:674:SER:O	2.24	0.55
1:F:334:LEU:HD12	1:F:334:LEU:H	1.70	0.55
1:F:550:SER:HB3	1:F:553:GLN:HB2	1.88	0.55
2:P:16:PHE:HA	2:P:35:VAL:CG1	2.37	0.55
2:S:16:PHE:HA	2:S:35:VAL:CG1	2.37	0.55
1:A:217:LYS:HB3	1:A:217:LYS:HZ2	1.70	0.55
1:A:550:SER:HB3	1:A:553:GLN:CB	2.37	0.55
1:A:722:ILE:HD13	1:A:764:LEU:CD2	2.37	0.55
1:B:628:PHE:CD1	1:B:645:TRP:CD1	2.94	0.55
1:C:184:LYS:HZ1	1:C:191:GLU:HB2	1.71	0.55
1:C:234:LEU:O	1:C:238:GLN:HG3	2.06	0.55
1:D:130:SER:HB2	1:D:170:TYR:CE2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:PHE:O	1:E:196:ILE:HG13	2.06	0.55
1:E:339:ILE:O	1:E:340:LYS:C	2.48	0.55
1:E:654:ILE:C	1:E:655:ASN:HD22	2.14	0.55
1:F:137:PHE:O	1:F:138:ALA:C	2.50	0.55
1:F:165:GLN:OE1	1:F:252:ASP:HB3	2.06	0.55
1:F:699:GLY:O	1:F:702:SER:N	2.40	0.55
2:O:21:LYS:HD3	2:O:21:LYS:C	2.31	0.55
2:Q:65:PHE:CB	2:Q:66:PRO:HD3	2.33	0.55
1:B:248:TYR:O	1:B:248:TYR:HD2	1.89	0.55
1:C:172:GLU:O	1:C:175:LYS:HB3	2.06	0.55
1:C:175:LYS:O	1:C:177:ILE:N	2.40	0.55
1:D:172:GLU:O	1:D:175:LYS:HB3	2.07	0.55
1:D:497:LEU:CD1	1:D:556:MET:HG2	2.36	0.55
1:E:115:LYS:HB3	1:E:115:LYS:HZ3	1.71	0.55
1:E:464:VAL:CG2	1:E:465:LEU:HD12	2.33	0.55
1:E:550:SER:HB3	1:E:553:GLN:CB	2.36	0.55
1:F:409:ARG:O	1:F:413:LEU:HG	2.06	0.55
1:A:137:PHE:O	1:A:138:ALA:C	2.49	0.55
1:A:188:LEU:CD2	1:A:188:LEU:N	2.46	0.55
1:A:197:LYS:HB3	1:A:197:LYS:HZ2	1.71	0.55
1:A:632:TYR:O	1:A:633:ASN:HB2	2.07	0.55
1:E:248:TYR:O	1:E:248:TYR:HD2	1.88	0.55
1:E:323:ASN:HD22	1:E:323:ASN:C	2.13	0.55
1:E:671:ARG:HH12	1:E:677:GLY:HA3	1.72	0.55
1:F:334:LEU:HD12	1:F:334:LEU:N	2.21	0.55
1:F:432:TYR:HE1	1:F:445:ARG:CZ	2.19	0.55
2:O:16:PHE:HA	2:O:35:VAL:CG1	2.37	0.55
2:R:63:ILE:HG13	2:R:67:GLU:HB3	1.89	0.55
1:A:107:THR:CG2	1:A:115:LYS:HD2	2.33	0.55
1:A:470:ASN:O	1:A:472:ARG:HG3	2.06	0.55
1:A:709:ASN:HB2	2:O:130:ILE:HG23	1.88	0.55
1:B:776:LEU:O	1:B:780:LEU:CD2	2.54	0.55
1:D:192:PHE:HA	1:D:195:LEU:HB3	1.87	0.55
1:D:557:LEU:HD11	1:D:575:VAL:HG12	1.88	0.55
1:E:318:ILE:CG2	1:E:322:LEU:HD12	2.32	0.55
1:E:443:GLU:HG3	1:E:458:LYS:HG2	1.87	0.55
1:F:71:PHE:CD1	1:F:73:ASN:HB2	2.42	0.55
1:F:173:ILE:HG13	1:F:242:SER:CB	2.27	0.55
1:F:252:ASP:O	1:F:254:ARG:HD2	2.06	0.55
1:F:338:LEU:O	1:F:343:VAL:HG23	2.06	0.55
1:A:279:ILE:O	1:A:283:LEU:HD13	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:PHE:CD2	1:A:602:PHE:N	2.72	0.55
1:C:301:ALA:C	1:C:303:LYS:H	2.14	0.55
1:C:508:ILE:HG12	1:C:536:TYR:CD2	2.41	0.55
1:C:602:PHE:CD2	1:C:602:PHE:N	2.71	0.55
1:D:96:ILE:O	1:D:100:LEU:HG	2.07	0.55
1:D:464:VAL:CG2	1:D:465:LEU:HD12	2.33	0.55
1:E:179:LEU:HA	1:E:182:ILE:HG22	1.87	0.55
1:E:333:LYS:C	1:E:335:ALA:H	2.15	0.55
1:E:481:VAL:O	1:E:484:VAL:HG23	2.06	0.55
1:F:443:GLU:HG3	1:F:458:LYS:HG2	1.88	0.55
2:P:63:ILE:HG13	2:P:67:GLU:HB3	1.89	0.55
1:A:333:LYS:C	1:A:335:ALA:H	2.15	0.55
1:A:432:TYR:HE1	1:A:445:ARG:CZ	2.20	0.55
1:B:755:ARG:O	1:B:756:ILE:C	2.50	0.55
1:C:115:LYS:HB3	1:C:115:LYS:HZ3	1.69	0.55
1:F:755:ARG:O	1:F:756:ILE:C	2.49	0.55
1:F:776:LEU:O	1:F:780:LEU:CD2	2.53	0.55
1:A:284:LYS:HE3	1:A:284:LYS:HA	1.87	0.55
1:A:628:PHE:CD1	1:A:645:TRP:CD1	2.94	0.55
1:A:671:ARG:HH12	1:A:677:GLY:HA3	1.71	0.55
1:B:172:GLU:O	1:B:175:LYS:HB3	2.06	0.55
1:B:252:ASP:CG	1:B:253:HIS:N	2.65	0.55
1:B:333:LYS:C	1:B:335:ALA:H	2.15	0.55
1:B:339:ILE:O	1:B:340:LYS:C	2.47	0.55
1:C:628:PHE:CE2	2:Q:90:ARG:HD3	2.33	0.55
1:D:173:ILE:C	1:D:175:LYS:N	2.61	0.55
1:F:186:LYS:HE3	1:F:234:LEU:HB2	1.88	0.55
1:F:333:LYS:HA	1:F:336:THR:OG1	2.06	0.55
1:F:432:TYR:CE1	1:F:445:ARG:CZ	2.90	0.55
2:P:25:GLY:HA3	2:P:65:PHE:CE1	2.42	0.55
2:P:36:MET:HE3	2:P:43:PRO:CG	2.28	0.55
2:T:25:GLY:HA3	2:T:65:PHE:CE1	2.42	0.55
1:A:334:LEU:HD12	1:A:334:LEU:N	2.22	0.55
1:A:508:ILE:HG12	1:A:536:TYR:CD2	2.41	0.55
1:A:557:LEU:HD11	1:A:575:VAL:HG12	1.88	0.55
1:A:609:GLU:OE2	1:A:609:GLU:N	2.34	0.55
1:B:97:TYR:CD2	1:B:102:GLY:HA3	2.42	0.55
1:B:334:LEU:H	1:B:334:LEU:HD12	1.70	0.55
1:B:334:LEU:HD12	1:B:334:LEU:N	2.22	0.55
1:B:550:SER:HB3	1:B:553:GLN:CB	2.37	0.55
1:B:697:ILE:HG21	1:B:732:ILE:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:TYR:O	1:C:248:TYR:HD2	1.89	0.55
1:C:470:ASN:O	1:C:472:ARG:HG3	2.07	0.55
1:D:632:TYR:O	1:D:633:ASN:HB2	2.06	0.55
1:D:648:PRO:HA	1:D:651:LYS:HB2	1.89	0.55
1:D:709:ASN:HB2	2:R:130:ILE:HG23	1.87	0.55
1:E:189:ASP:O	1:E:191:GLU:HG2	2.07	0.55
1:E:432:TYR:CE1	1:E:445:ARG:CZ	2.90	0.55
2:O:25:GLY:HA3	2:O:65:PHE:CE1	2.42	0.55
1:B:137:PHE:O	1:B:138:ALA:C	2.50	0.55
1:B:175:LYS:O	1:B:178:SER:N	2.39	0.55
1:B:199:LEU:C	1:B:201:ASP:N	2.62	0.55
1:B:252:ASP:O	1:B:254:ARG:HD2	2.06	0.55
1:C:71:PHE:CD1	1:C:73:ASN:HB2	2.42	0.55
1:C:137:PHE:O	1:C:138:ALA:C	2.50	0.55
1:C:192:PHE:O	1:C:196:ILE:HG13	2.07	0.55
1:C:376:GLN:O	1:C:378:LEU:N	2.40	0.55
1:D:107:THR:CG2	1:D:115:LYS:HD2	2.37	0.55
1:D:189:ASP:O	1:D:190:PRO:C	2.42	0.55
1:D:550:SER:HB3	1:D:553:GLN:HB2	1.89	0.55
1:E:71:PHE:CD1	1:E:73:ASN:HB2	2.42	0.55
1:E:184:LYS:HD2	1:E:188:LEU:HG	1.88	0.55
1:E:244:ALA:HB3	1:E:268:MET:HE3	1.89	0.55
1:E:326:ILE:HG22	1:E:328:PHE:CE1	2.42	0.55
1:E:334:LEU:HD12	1:E:334:LEU:N	2.22	0.55
2:O:63:ILE:HG13	2:O:67:GLU:HB3	1.89	0.55
1:A:74:GLU:HB2	1:A:78:LYS:CB	2.36	0.54
1:A:96:ILE:O	1:A:100:LEU:HG	2.07	0.54
1:A:327:LEU:O	1:A:495:PHE:N	2.40	0.54
1:A:405:LEU:HD12	1:A:405:LEU:N	2.22	0.54
1:B:96:ILE:O	1:B:100:LEU:HG	2.07	0.54
1:B:333:LYS:HA	1:B:336:THR:OG1	2.07	0.54
1:B:597:ASN:C	1:B:599:GLU:H	2.14	0.54
1:D:175:LYS:O	1:D:178:SER:N	2.38	0.54
1:D:184:LYS:HD2	1:D:188:LEU:HG	1.88	0.54
1:D:186:LYS:HB2	1:D:190:PRO:CD	2.36	0.54
1:D:334:LEU:H	1:D:334:LEU:HD12	1.72	0.54
1:D:700:TYR:CD1	1:D:727:GLN:HB3	2.42	0.54
1:E:130:SER:HB2	1:E:170:TYR:CE2	2.43	0.54
1:E:248:TYR:C	1:E:248:TYR:HD2	2.16	0.54
1:E:327:LEU:O	1:E:495:PHE:N	2.40	0.54
1:F:199:LEU:C	1:F:201:ASP:N	2.65	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ILE:HG22	1:F:328:PHE:CE1	2.41	0.54
1:F:333:LYS:C	1:F:335:ALA:H	2.15	0.54
2:P:105:LEU:HD21	2:P:124:MET:SD	2.47	0.54
1:A:184:LYS:HD2	1:A:188:LEU:HG	1.88	0.54
1:A:244:ALA:HB3	1:A:268:MET:HE3	1.89	0.54
1:A:755:ARG:O	1:A:756:ILE:C	2.50	0.54
1:B:410:ILE:HG22	1:B:411:GLU:N	2.22	0.54
1:B:432:TYR:HE1	1:B:445:ARG:CZ	2.20	0.54
1:C:192:PHE:HA	1:C:195:LEU:HB3	1.88	0.54
1:C:244:ALA:HB3	1:C:268:MET:HE3	1.89	0.54
1:C:334:LEU:HD12	1:C:334:LEU:H	1.72	0.54
1:C:432:TYR:HE1	1:C:445:ARG:CZ	2.20	0.54
1:C:632:TYR:O	1:C:633:ASN:HB2	2.08	0.54
1:C:661:ALA:O	1:C:665:LYS:HD3	2.07	0.54
1:C:688:PHE:O	1:C:689:ALA:C	2.51	0.54
1:D:135:VAL:O	1:D:135:VAL:HG22	2.08	0.54
1:D:432:TYR:CE1	1:D:445:ARG:CZ	2.90	0.54
1:F:173:ILE:C	1:F:175:LYS:N	2.61	0.54
2:Q:6:GLU:O	2:Q:9:ILE:N	2.38	0.54
2:R:64:ASP:OD1	2:R:66:PRO:CD	2.55	0.54
2:T:84:GLU:N	2:T:84:GLU:OE2	2.37	0.54
1:A:115:LYS:HD3	1:A:153:ILE:HD13	1.88	0.54
1:A:246:SER:O	1:A:250:ALA:HB2	2.07	0.54
1:A:550:SER:HB3	1:A:553:GLN:HB2	1.89	0.54
1:A:550:SER:HG	1:A:552:TRP:CD1	2.26	0.54
1:A:680:LYS:H	1:A:687:GLU:HG3	1.72	0.54
1:B:80:GLN:O	1:B:80:GLN:HG3	2.08	0.54
1:B:446:ILE:HG13	1:B:452:GLU:O	2.07	0.54
1:C:171:TYR:O	1:C:175:LYS:NZ	2.40	0.54
1:C:252:ASP:O	1:C:254:ARG:HD2	2.06	0.54
1:C:409:ARG:O	1:C:413:LEU:HG	2.06	0.54
1:C:628:PHE:CD1	1:C:645:TRP:CD1	2.95	0.54
1:E:173:ILE:HG13	1:E:242:SER:CB	2.29	0.54
1:E:776:LEU:O	1:E:780:LEU:CD2	2.54	0.54
1:F:248:TYR:C	1:F:248:TYR:HD2	2.16	0.54
1:F:405:LEU:HD12	1:F:405:LEU:N	2.23	0.54
1:F:410:ILE:HG22	1:F:411:GLU:N	2.23	0.54
1:F:550:SER:HB3	1:F:553:GLN:CB	2.37	0.54
1:F:700:TYR:CD1	1:F:727:GLN:HB3	2.42	0.54
2:P:76:MET:HG3	2:P:76:MET:O	2.06	0.54
1:A:234:LEU:O	1:A:238:GLN:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:HD11	1:A:575:VAL:CG1	2.37	0.54
1:A:655:ASN:N	1:A:655:ASN:ND2	2.54	0.54
1:B:171:TYR:O	1:B:175:LYS:NZ	2.41	0.54
1:B:186:LYS:O	1:B:189:ASP:HA	2.08	0.54
1:B:320:ARG:O	1:B:321:GLU:C	2.49	0.54
1:B:655:ASN:N	1:B:655:ASN:ND2	2.53	0.54
1:D:71:PHE:CD1	1:D:73:ASN:HB2	2.42	0.54
1:D:197:LYS:HB3	1:D:197:LYS:HZ2	1.72	0.54
1:F:217:LYS:HB3	1:F:217:LYS:HZ2	1.71	0.54
1:F:680:LYS:H	1:F:687:GLU:HG3	1.72	0.54
2:O:76:MET:HG3	2:O:76:MET:O	2.06	0.54
2:P:26:THR:HA	2:P:64:ASP:HA	1.90	0.54
1:A:97:TYR:CD2	1:A:102:GLY:HA3	2.42	0.54
1:A:154:ILE:HG13	1:A:171:TYR:CD1	2.43	0.54
1:A:172:GLU:O	1:A:175:LYS:HB3	2.07	0.54
1:A:182:ILE:O	1:A:187:SER:HB2	2.06	0.54
1:A:195:LEU:HD21	1:A:227:ILE:HG12	1.90	0.54
1:A:405:LEU:CD1	1:A:453:VAL:HG21	2.34	0.54
1:B:175:LYS:O	1:B:177:ILE:N	2.41	0.54
1:B:184:LYS:HD2	1:B:188:LEU:HG	1.88	0.54
1:B:248:TYR:C	1:B:248:TYR:HD2	2.16	0.54
1:B:409:ARG:O	1:B:413:LEU:HG	2.06	0.54
1:B:661:ALA:O	1:B:665:LYS:HD3	2.07	0.54
1:C:320:ARG:O	1:C:321:GLU:C	2.49	0.54
1:D:171:TYR:O	1:D:175:LYS:NZ	2.41	0.54
1:D:186:LYS:O	1:D:189:ASP:HA	2.08	0.54
1:D:410:ILE:HD13	1:D:419:ILE:CD1	2.37	0.54
1:D:755:ARG:O	1:D:756:ILE:C	2.51	0.54
1:E:74:GLU:HB2	1:E:78:LYS:CB	2.32	0.54
1:E:88:LYS:NZ	1:E:172:GLU:OE2	2.41	0.54
1:E:96:ILE:O	1:E:100:LEU:HG	2.07	0.54
1:E:320:ARG:O	1:E:321:GLU:C	2.50	0.54
1:E:432:TYR:HE1	1:E:445:ARG:CZ	2.20	0.54
1:E:446:ILE:HG13	1:E:452:GLU:O	2.07	0.54
1:F:464:VAL:CG2	1:F:465:LEU:HD12	2.33	0.54
2:O:136:VAL:HG23	2:O:136:VAL:O	2.08	0.54
2:Q:63:ILE:HG13	2:Q:67:GLU:HB3	1.89	0.54
2:S:26:THR:HA	2:S:64:ASP:HA	1.90	0.54
2:T:16:PHE:HA	2:T:35:VAL:CG1	2.37	0.54
2:T:105:LEU:HD21	2:T:124:MET:SD	2.47	0.54
1:A:71:PHE:CD1	1:A:73:ASN:HB2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ARG:O	1:A:413:LEU:HG	2.07	0.54
1:B:71:PHE:CD1	1:B:73:ASN:HB2	2.42	0.54
1:B:405:LEU:HD12	1:B:405:LEU:N	2.23	0.54
1:B:671:ARG:HH12	1:B:677:GLY:HA3	1.73	0.54
1:B:693:SER:O	1:B:696:LYS:HB2	2.07	0.54
1:C:186:LYS:O	1:C:189:ASP:HA	2.08	0.54
1:C:246:SER:O	1:C:250:ALA:HB2	2.08	0.54
1:C:405:LEU:HD12	1:C:405:LEU:N	2.23	0.54
1:C:755:ARG:O	1:C:756:ILE:C	2.50	0.54
1:D:481:VAL:O	1:D:484:VAL:HG23	2.07	0.54
1:D:688:PHE:O	1:D:689:ALA:C	2.51	0.54
1:E:175:LYS:O	1:E:177:ILE:N	2.41	0.54
1:E:186:LYS:O	1:E:189:ASP:HA	2.08	0.54
1:E:275:GLY:HA2	1:E:278:LYS:CG	2.33	0.54
1:E:333:LYS:HA	1:E:336:THR:OG1	2.06	0.54
1:E:409:ARG:O	1:E:413:LEU:HG	2.07	0.54
1:E:688:PHE:O	1:E:689:ALA:C	2.51	0.54
1:F:96:ILE:O	1:F:100:LEU:HG	2.07	0.54
1:F:184:LYS:NZ	1:F:191:GLU:HB2	2.21	0.54
1:F:248:TYR:O	1:F:248:TYR:HD2	1.89	0.54
1:F:320:ARG:O	1:F:321:GLU:C	2.49	0.54
1:A:173:ILE:O	1:A:174:GLY:C	2.51	0.54
1:A:184:LYS:O	1:A:185:ASP:C	2.51	0.54
1:A:252:ASP:CG	1:A:253:HIS:N	2.66	0.54
1:A:481:VAL:O	1:A:484:VAL:HG23	2.07	0.54
1:A:668:SER:CA	2:O:14:GLU:HG3	2.33	0.54
1:A:697:ILE:HG21	1:A:732:ILE:HD11	1.89	0.54
1:C:178:SER:OG	1:C:179:LEU:CD2	2.55	0.54
1:C:275:GLY:HA2	1:C:278:LYS:CG	2.31	0.54
1:D:252:ASP:CG	1:D:253:HIS:N	2.65	0.54
1:D:552:TRP:O	1:D:555:GLN:HG2	2.08	0.54
1:E:172:GLU:O	1:E:175:LYS:HB3	2.07	0.54
1:E:305:SER:OG	1:E:307:LEU:HD13	2.07	0.54
1:E:334:LEU:HD12	1:E:334:LEU:H	1.71	0.54
1:E:697:ILE:HG21	1:E:732:ILE:HD11	1.90	0.54
1:F:410:ILE:HD13	1:F:419:ILE:CD1	2.38	0.54
1:F:632:TYR:O	1:F:633:ASN:HB2	2.08	0.54
2:R:76:MET:HG3	2:R:76:MET:O	2.06	0.54
1:A:135:VAL:O	1:A:135:VAL:HG22	2.08	0.54
1:A:199:LEU:C	1:A:201:ASP:N	2.65	0.54
1:B:184:LYS:O	1:B:185:ASP:C	2.51	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:SER:OG	1:B:307:LEU:HD13	2.08	0.54
1:B:680:LYS:H	1:B:687:GLU:HG3	1.73	0.54
1:C:97:TYR:CD2	1:C:102:GLY:HA3	2.43	0.54
1:C:333:LYS:C	1:C:335:ALA:H	2.15	0.54
1:C:432:TYR:CE1	1:C:445:ARG:CZ	2.90	0.54
1:C:481:VAL:O	1:C:484:VAL:HG23	2.07	0.54
1:E:197:LYS:HE2	1:E:264:MET:HG2	1.90	0.54
1:F:693:SER:O	1:F:696:LYS:HB2	2.08	0.54
2:Q:11:GLU:O	2:Q:13:LYS:N	2.40	0.54
2:R:26:THR:HA	2:R:64:ASP:HA	1.90	0.54
2:R:93:ASP:OD1	2:R:97:ASN:ND2	2.41	0.54
2:R:136:VAL:HG23	2:R:136:VAL:O	2.08	0.54
2:T:65:PHE:CB	2:T:66:PRO:HD3	2.33	0.54
1:A:320:ARG:O	1:A:321:GLU:C	2.49	0.54
1:B:464:VAL:CG2	1:B:465:LEU:HD12	2.33	0.54
1:D:234:LEU:O	1:D:238:GLN:HG3	2.08	0.54
1:D:271:LEU:HD23	1:D:275:GLY:HA3	1.90	0.54
1:D:432:TYR:HE1	1:D:445:ARG:CZ	2.20	0.54
1:E:134:LYS:O	1:E:135:VAL:HG12	2.07	0.54
1:E:180:ASP:C	1:E:182:ILE:N	2.55	0.54
1:E:185:ASP:O	1:E:190:PRO:CG	2.56	0.54
1:F:186:LYS:O	1:F:189:ASP:HA	2.08	0.54
1:F:356:ASP:OD2	1:F:356:ASP:N	2.40	0.54
1:F:481:VAL:O	1:F:484:VAL:HG23	2.08	0.54
1:A:175:LYS:O	1:A:177:ILE:N	2.41	0.54
1:A:410:ILE:HG22	1:A:411:GLU:N	2.23	0.54
1:A:648:PRO:HA	1:A:651:LYS:HB2	1.90	0.54
1:B:279:ILE:O	1:B:283:LEU:HD13	2.08	0.54
1:B:410:ILE:HD13	1:B:419:ILE:CD1	2.37	0.54
1:B:432:TYR:CE1	1:B:445:ARG:CZ	2.90	0.54
1:C:278:LYS:HE3	1:C:279:ILE:CD1	2.38	0.54
1:C:700:TYR:CD1	1:C:727:GLN:HB3	2.42	0.54
1:D:137:PHE:O	1:D:138:ALA:C	2.50	0.54
1:D:184:LYS:O	1:D:185:ASP:C	2.51	0.54
1:D:225:ILE:HG12	1:D:229:PHE:HE2	1.73	0.54
1:D:246:SER:O	1:D:250:ALA:HB2	2.08	0.54
1:D:278:LYS:HE3	1:D:279:ILE:CD1	2.38	0.54
1:D:326:ILE:HG22	1:D:328:PHE:CE1	2.42	0.54
1:E:120:LEU:O	1:E:120:LEU:HD13	2.06	0.54
1:E:173:ILE:C	1:E:175:LYS:N	2.60	0.54
1:E:230:ILE:HG13	1:E:237:PHE:CE2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ILE:HG13	1:F:237:PHE:CE2	2.43	0.54
1:F:271:LEU:HD23	1:F:275:GLY:HA3	1.90	0.54
1:F:671:ARG:O	1:F:674:SER:O	2.26	0.54
1:F:688:PHE:O	1:F:689:ALA:C	2.51	0.54
2:O:26:THR:HA	2:O:64:ASP:HA	1.90	0.54
2:Q:105:LEU:HD21	2:Q:124:MET:SD	2.48	0.54
2:T:49:GLN:H	2:T:49:GLN:NE2	2.03	0.54
1:A:186:LYS:O	1:A:189:ASP:HA	2.08	0.53
1:A:432:TYR:CE1	1:A:445:ARG:CZ	2.91	0.53
1:B:88:LYS:NZ	1:B:172:GLU:OE2	2.41	0.53
1:B:288:VAL:CG2	1:B:289:GLU:H	2.18	0.53
1:C:80:GLN:HG3	1:C:80:GLN:O	2.08	0.53
1:C:173:ILE:O	1:C:174:GLY:C	2.52	0.53
1:C:184:LYS:O	1:C:185:ASP:C	2.51	0.53
1:C:230:ILE:HG13	1:C:237:PHE:CE2	2.43	0.53
1:C:252:ASP:CG	1:C:253:HIS:N	2.65	0.53
1:C:550:SER:HB3	1:C:553:GLN:CB	2.38	0.53
1:D:410:ILE:HG22	1:D:411:GLU:N	2.23	0.53
1:D:722:ILE:HD13	1:D:764:LEU:CD2	2.38	0.53
1:E:165:GLN:OE1	1:E:252:ASP:HB3	2.08	0.53
1:E:234:LEU:O	1:E:238:GLN:HG3	2.07	0.53
1:E:246:SER:O	1:E:250:ALA:HB2	2.08	0.53
1:E:410:ILE:HD13	1:E:419:ILE:CD1	2.38	0.53
1:E:410:ILE:HG22	1:E:411:GLU:N	2.24	0.53
1:E:655:ASN:N	1:E:655:ASN:ND2	2.56	0.53
1:F:234:LEU:O	1:F:238:GLN:HG3	2.08	0.53
1:F:279:ILE:O	1:F:283:LEU:HD13	2.08	0.53
2:Q:26:THR:HA	2:Q:64:ASP:HA	1.90	0.53
2:Q:76:MET:HG3	2:Q:76:MET:O	2.06	0.53
2:T:11:GLU:C	2:T:13:LYS:H	2.16	0.53
2:T:136:VAL:HG23	2:T:136:VAL:O	2.08	0.53
1:A:165:GLN:OE1	1:A:252:ASP:HB3	2.07	0.53
1:A:252:ASP:O	1:A:254:ARG:HD2	2.07	0.53
1:A:410:ILE:HD13	1:A:419:ILE:CD1	2.38	0.53
1:B:175:LYS:HB2	1:B:175:LYS:HZ3	1.71	0.53
1:B:405:LEU:CD1	1:B:453:VAL:HG21	2.34	0.53
1:B:648:PRO:HA	1:B:651:LYS:HB2	1.89	0.53
1:C:410:ILE:HG22	1:C:411:GLU:N	2.23	0.53
1:C:552:TRP:O	1:C:555:GLN:HG2	2.09	0.53
1:D:334:LEU:HD12	1:D:334:LEU:N	2.23	0.53
1:D:508:ILE:HG12	1:D:536:TYR:CD2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:SER:O	1:D:696:LYS:HB2	2.08	0.53
1:E:137:PHE:O	1:E:138:ALA:C	2.51	0.53
1:E:184:LYS:O	1:E:185:ASP:C	2.51	0.53
1:E:252:ASP:CG	1:E:253:HIS:N	2.65	0.53
1:E:376:GLN:O	1:E:378:LEU:N	2.41	0.53
1:F:286:GLU:O	1:F:290:LYS:HE3	2.08	0.53
1:F:709:ASN:HB2	2:T:130:ILE:HG23	1.89	0.53
2:R:16:PHE:HA	2:R:35:VAL:CG1	2.37	0.53
2:S:84:GLU:OE2	2:S:84:GLU:N	2.39	0.53
2:T:93:ASP:OD1	2:T:97:ASN:ND2	2.41	0.53
1:A:271:LEU:HD23	1:A:275:GLY:HA3	1.90	0.53
1:B:130:SER:HB2	1:B:170:TYR:CE2	2.43	0.53
1:B:192:PHE:HB3	1:B:196:ILE:HD11	1.90	0.53
1:B:195:LEU:HD21	1:B:227:ILE:HG12	1.91	0.53
1:C:105:TYR:CB	1:C:153:ILE:HG12	2.37	0.53
1:C:295:VAL:HG21	1:C:603:ILE:CG2	2.38	0.53
1:C:671:ARG:O	1:C:674:SER:O	2.27	0.53
1:D:244:ALA:HB3	1:D:268:MET:HE3	1.90	0.53
1:D:248:TYR:C	1:D:248:TYR:HD2	2.16	0.53
1:D:376:GLN:O	1:D:378:LEU:N	2.42	0.53
1:D:609:GLU:OE2	1:D:609:GLU:N	2.34	0.53
1:D:680:LYS:H	1:D:687:GLU:HG3	1.73	0.53
1:D:730:ASN:O	1:D:733:GLU:N	2.41	0.53
1:D:746:LYS:HD3	1:D:750:GLN:HE21	1.74	0.53
1:E:405:LEU:HD12	1:E:405:LEU:N	2.23	0.53
1:E:557:LEU:HD11	1:E:575:VAL:HG12	1.89	0.53
1:E:680:LYS:H	1:E:687:GLU:HG3	1.72	0.53
1:F:697:ILE:HG21	1:F:732:ILE:HD11	1.90	0.53
1:F:742:ALA:HB1	1:F:743:PRO:HD2	1.90	0.53
2:S:65:PHE:CB	2:S:66:PRO:HD3	2.32	0.53
1:A:123:GLU:HG2	1:A:124:GLU:H	1.74	0.53
1:A:230:ILE:HG13	1:A:237:PHE:CE2	2.43	0.53
1:B:135:VAL:HG22	1:B:135:VAL:O	2.09	0.53
1:C:76:LEU:H	1:C:76:LEU:CD2	2.22	0.53
1:D:97:TYR:CD2	1:D:102:GLY:HA3	2.44	0.53
1:D:252:ASP:O	1:D:254:ARG:HD2	2.07	0.53
1:D:550:SER:HB3	1:D:553:GLN:CB	2.38	0.53
1:E:173:ILE:O	1:E:174:GLY:C	2.51	0.53
1:F:244:ALA:HB3	1:F:268:MET:HE3	1.91	0.53
1:F:246:SER:O	1:F:250:ALA:HB2	2.09	0.53
1:F:722:ILE:HD13	1:F:764:LEU:CD2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HB	1:A:491:ASP:HB3	1.90	0.53
1:B:179:LEU:HA	1:B:182:ILE:HG22	1.89	0.53
1:B:326:ILE:HG22	1:B:328:PHE:CE1	2.44	0.53
1:B:356:ASP:OD2	1:B:356:ASP:N	2.41	0.53
1:C:102:GLY:C	1:C:103:GLU:HG3	2.34	0.53
1:C:217:LYS:NZ	1:C:236:GLU:HB2	2.24	0.53
1:C:565:LYS:C	1:C:567:THR:H	2.17	0.53
1:C:621:GLY:HA2	2:Q:94:LYS:NZ	2.23	0.53
1:D:279:ILE:O	1:D:283:LEU:HD13	2.09	0.53
1:D:699:GLY:O	1:D:702:SER:N	2.42	0.53
1:E:214:PHE:HB3	1:E:218:LEU:HB3	1.90	0.53
1:E:699:GLY:O	1:E:702:SER:N	2.42	0.53
1:F:746:LYS:HD3	1:F:750:GLN:HE21	1.73	0.53
2:Q:64:ASP:OD1	2:Q:66:PRO:CD	2.56	0.53
2:Q:84:GLU:N	2:Q:84:GLU:OE2	2.39	0.53
2:R:12:PHE:CZ	2:R:76:MET:HE3	2.37	0.53
1:A:175:LYS:O	1:A:178:SER:N	2.38	0.53
1:A:192:PHE:HB3	1:A:196:ILE:HD11	1.90	0.53
1:A:700:TYR:CD1	1:A:727:GLN:HB3	2.43	0.53
1:B:173:ILE:O	1:B:174:GLY:C	2.52	0.53
1:B:234:LEU:O	1:B:238:GLN:HG3	2.07	0.53
1:B:722:ILE:HD13	1:B:764:LEU:CD2	2.38	0.53
1:C:697:ILE:HG21	1:C:732:ILE:HD11	1.90	0.53
1:C:699:GLY:O	1:C:702:SER:N	2.42	0.53
1:D:175:LYS:O	1:D:177:ILE:N	2.42	0.53
1:D:502:THR:HG22	2:R:111:ASN:O	2.08	0.53
1:E:97:TYR:CD2	1:E:102:GLY:HA3	2.43	0.53
1:E:557:LEU:HD11	1:E:575:VAL:CG1	2.38	0.53
1:F:135:VAL:O	1:F:135:VAL:HG22	2.08	0.53
1:F:225:ILE:HG12	1:F:229:PHE:HE2	1.74	0.53
2:O:146:THR:O	2:O:147:ALA:C	2.52	0.53
1:A:106:PHE:HA	1:A:154:ILE:O	2.09	0.53
1:A:376:GLN:O	1:A:378:LEU:N	2.42	0.53
1:A:746:LYS:HD3	1:A:750:GLN:HE21	1.73	0.53
1:C:375:GLY:O	1:C:377:GLN:N	2.42	0.53
1:C:410:ILE:HD13	1:C:419:ILE:CD1	2.38	0.53
1:C:722:ILE:HD13	1:C:764:LEU:CD2	2.38	0.53
1:D:217:LYS:NZ	1:D:236:GLU:HB2	2.24	0.53
1:E:609:GLU:H	1:E:609:GLU:CD	2.17	0.53
1:E:709:ASN:HB2	2:S:130:ILE:HG23	1.90	0.53
1:E:742:ALA:HB1	1:E:743:PRO:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:LYS:HE2	1:F:264:MET:HG2	1.91	0.53
2:Q:16:PHE:HA	2:Q:35:VAL:CG1	2.37	0.53
2:Q:146:THR:O	2:Q:147:ALA:C	2.52	0.53
2:S:105:LEU:HD21	2:S:124:MET:SD	2.48	0.53
1:B:165:GLN:OE1	1:B:252:ASP:HB3	2.08	0.53
1:B:481:VAL:O	1:B:484:VAL:HG23	2.07	0.53
1:B:700:TYR:CD1	1:B:727:GLN:HB3	2.43	0.53
1:C:165:GLN:OE1	1:C:252:ASP:HB3	2.08	0.53
1:C:680:LYS:H	1:C:687:GLU:HG3	1.73	0.53
1:D:195:LEU:HD21	1:D:227:ILE:HG12	1.90	0.53
1:D:495:PHE:O	1:D:496:ALA:HB2	2.09	0.53
1:D:628:PHE:CD1	1:D:645:TRP:CD1	2.97	0.53
1:E:135:VAL:HG22	1:E:135:VAL:O	2.09	0.53
1:E:184:LYS:HZ1	1:E:191:GLU:CB	2.21	0.53
1:E:271:LEU:HD23	1:E:275:GLY:HA3	1.90	0.53
1:F:133:GLU:O	1:F:133:GLU:HG3	2.08	0.53
1:F:179:LEU:HA	1:F:182:ILE:HG22	1.91	0.53
1:F:278:LYS:HE3	1:F:279:ILE:CD1	2.38	0.53
1:F:595:ILE:HG22	1:F:596:ILE:H	1.74	0.53
2:O:93:ASP:OD1	2:O:97:ASN:ND2	2.41	0.53
1:A:78:LYS:HG3	1:A:79:ILE:N	2.24	0.53
1:A:236:GLU:HA	1:A:239:HIS:HD2	1.74	0.53
1:A:661:ALA:O	1:A:665:LYS:HD3	2.08	0.53
1:C:135:VAL:O	1:C:135:VAL:HG22	2.07	0.53
1:C:334:LEU:HD12	1:C:334:LEU:N	2.23	0.53
1:C:442:TYR:CD1	1:C:455:TYR:HD1	2.25	0.53
1:D:286:GLU:O	1:D:290:LYS:HE3	2.09	0.53
1:D:405:LEU:HD12	1:D:405:LEU:N	2.23	0.53
1:D:442:TYR:CD1	1:D:455:TYR:HD1	2.25	0.53
1:E:195:LEU:HD21	1:E:227:ILE:HG12	1.91	0.53
1:E:632:TYR:O	1:E:633:ASN:HB2	2.08	0.53
1:E:755:ARG:O	1:E:756:ILE:C	2.51	0.53
1:F:78:LYS:HG3	1:F:79:ILE:N	2.23	0.53
1:F:171:TYR:O	1:F:175:LYS:NZ	2.42	0.53
1:F:565:LYS:C	1:F:567:THR:H	2.17	0.53
1:F:742:ALA:HB1	1:F:744:GLU:OE1	2.09	0.53
2:S:62:THR:OG1	2:S:63:ILE:N	2.42	0.53
1:A:186:LYS:HB2	1:A:190:PRO:CD	2.38	0.53
1:B:156:ILE:HD12	1:B:156:ILE:H	1.73	0.53
1:B:230:ILE:HG13	1:B:237:PHE:CE2	2.43	0.53
1:B:376:GLN:O	1:B:378:LEU:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ILE:C	1:B:604:LEU:HD12	2.34	0.53
1:B:688:PHE:O	1:B:689:ALA:C	2.52	0.53
1:B:699:GLY:O	1:B:702:SER:N	2.42	0.53
1:C:409:ARG:CD	1:C:413:LEU:HD21	2.39	0.53
1:D:165:GLN:OE1	1:D:252:ASP:HB3	2.07	0.53
1:D:214:PHE:CD1	1:D:218:LEU:HD23	2.44	0.53
1:D:405:LEU:CD1	1:D:453:VAL:HG21	2.34	0.53
1:D:742:ALA:HB1	1:D:743:PRO:HD2	1.91	0.53
1:E:495:PHE:O	1:E:496:ALA:HB2	2.09	0.53
1:F:165:GLN:HE21	1:F:251:PRO:HG2	1.74	0.53
1:F:178:SER:OG	1:F:179:LEU:CD2	2.56	0.53
1:F:217:LYS:NZ	1:F:236:GLU:HB2	2.24	0.53
1:F:635:ILE:H	1:F:635:ILE:CD1	2.16	0.53
2:P:93:ASP:OD1	2:P:97:ASN:ND2	2.42	0.53
2:T:6:GLU:O	2:T:9:ILE:N	2.38	0.53
1:A:185:ASP:O	1:A:190:PRO:CA	2.57	0.52
1:A:278:LYS:HE3	1:A:279:ILE:CD1	2.38	0.52
1:A:688:PHE:O	1:A:689:ALA:C	2.51	0.52
1:A:716:LYS:O	1:A:717:LYS:C	2.52	0.52
1:B:184:LYS:NZ	1:B:191:GLU:HB2	2.24	0.52
1:B:189:ASP:O	1:B:191:GLU:HG2	2.08	0.52
1:B:409:ARG:CD	1:B:413:LEU:HD21	2.39	0.52
1:B:742:ALA:HB1	1:B:743:PRO:HD2	1.91	0.52
1:C:161:ILE:CG2	1:C:168:GLU:HB2	2.39	0.52
1:C:742:ALA:HB1	1:C:744:GLU:OE1	2.09	0.52
1:D:178:SER:OG	1:D:179:LEU:CD2	2.58	0.52
1:D:595:ILE:HG22	1:D:596:ILE:H	1.73	0.52
1:E:105:TYR:CB	1:E:153:ILE:HG12	2.39	0.52
1:E:118:GLN:OE1	1:E:118:GLN:HA	2.09	0.52
1:E:217:LYS:NZ	1:E:236:GLU:HB2	2.24	0.52
1:E:595:ILE:HG22	1:E:596:ILE:H	1.74	0.52
1:E:722:ILE:HD13	1:E:764:LEU:CD2	2.38	0.52
1:E:730:ASN:O	1:E:733:GLU:N	2.42	0.52
1:E:746:LYS:HD3	1:E:750:GLN:HE21	1.74	0.52
1:F:105:TYR:CB	1:F:153:ILE:HG12	2.38	0.52
2:Q:63:ILE:HG13	2:Q:67:GLU:CB	2.39	0.52
2:Q:136:VAL:HG23	2:Q:136:VAL:O	2.08	0.52
2:R:105:LEU:HD21	2:R:124:MET:SD	2.48	0.52
2:T:26:THR:HA	2:T:64:ASP:HA	1.91	0.52
1:A:88:LYS:NZ	1:A:172:GLU:OE2	2.42	0.52
1:A:248:TYR:C	1:A:248:TYR:HD2	2.16	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:HG22	2:O:111:ASN:O	2.10	0.52
1:A:699:GLY:O	1:A:702:SER:N	2.42	0.52
1:B:217:LYS:NZ	1:B:236:GLU:HB2	2.24	0.52
1:B:345:THR:HB	1:B:491:ASP:HB3	1.90	0.52
1:B:470:ASN:O	1:B:472:ARG:HG3	2.08	0.52
1:C:118:GLN:OE1	1:C:118:GLN:HA	2.09	0.52
1:C:271:LEU:HD23	1:C:275:GLY:HA3	1.91	0.52
1:D:184:LYS:NZ	1:D:191:GLU:HB2	2.23	0.52
1:E:165:GLN:HE21	1:E:251:PRO:HG2	1.74	0.52
1:E:171:TYR:O	1:E:175:LYS:NZ	2.42	0.52
1:F:376:GLN:O	1:F:378:LEU:N	2.42	0.52
1:F:593:ILE:C	1:F:604:LEU:HD12	2.34	0.52
1:F:671:ARG:HH12	1:F:677:GLY:HA3	1.73	0.52
2:O:63:ILE:HG13	2:O:67:GLU:CB	2.39	0.52
2:P:63:ILE:HG13	2:P:67:GLU:CB	2.39	0.52
2:S:146:THR:O	2:S:147:ALA:C	2.51	0.52
1:A:171:TYR:O	1:A:175:LYS:NZ	2.43	0.52
1:B:557:LEU:HD11	1:B:575:VAL:CG1	2.39	0.52
1:B:730:ASN:O	1:B:733:GLU:N	2.42	0.52
1:C:324:THR:HB	1:C:499:PRO:CA	2.37	0.52
1:C:609:GLU:OE2	1:C:609:GLU:N	2.33	0.52
1:C:671:ARG:HH12	1:C:677:GLY:HA3	1.71	0.52
1:D:354:SER:OG	1:D:355:SER:N	2.42	0.52
1:E:356:ASP:OD2	1:E:356:ASP:N	2.42	0.52
1:F:611:THR:O	1:F:615:ILE:HG13	2.10	0.52
1:F:619:ILE:O	1:F:620:THR:C	2.53	0.52
2:Q:11:GLU:C	2:Q:13:LYS:H	2.17	0.52
2:Q:62:THR:OG1	2:Q:63:ILE:N	2.43	0.52
2:R:11:GLU:C	2:R:13:LYS:H	2.17	0.52
2:R:11:GLU:O	2:R:13:LYS:N	2.41	0.52
2:T:63:ILE:HG13	2:T:67:GLU:HB3	1.90	0.52
1:A:478:ALA:CB	1:A:486:LYS:O	2.57	0.52
1:A:501:LEU:HD22	2:O:112:LEU:HD21	1.92	0.52
1:B:78:LYS:HG3	1:B:79:ILE:N	2.24	0.52
1:C:248:TYR:C	1:C:248:TYR:HD2	2.16	0.52
1:C:257:LEU:O	1:C:261:ALA:O	2.28	0.52
1:C:742:ALA:HB1	1:C:743:PRO:HD2	1.91	0.52
1:D:76:LEU:N	1:D:76:LEU:HD22	2.25	0.52
1:D:165:GLN:HE21	1:D:251:PRO:HG2	1.74	0.52
1:D:275:GLY:CA	1:D:278:LYS:HG3	2.35	0.52
1:D:697:ILE:HG21	1:D:732:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:ALA:HB1	1:D:744:GLU:OE1	2.10	0.52
1:E:385:LEU:O	1:E:385:LEU:HD13	2.10	0.52
1:E:648:PRO:HA	1:E:651:LYS:HB2	1.90	0.52
1:E:693:SER:O	1:E:696:LYS:HB2	2.09	0.52
1:E:700:TYR:CD1	1:E:727:GLN:HB3	2.43	0.52
1:E:781:ASN:N	1:E:789:ASN:HD21	2.02	0.52
1:F:97:TYR:CD2	1:F:102:GLY:HA3	2.44	0.52
1:F:184:LYS:O	1:F:185:ASP:C	2.51	0.52
1:F:470:ASN:O	1:F:472:ARG:HG3	2.09	0.52
2:R:62:THR:OG1	2:R:63:ILE:N	2.42	0.52
2:R:97:ASN:ND2	2:R:97:ASN:N	2.37	0.52
2:R:146:THR:O	2:R:147:ALA:C	2.51	0.52
2:S:136:VAL:HG23	2:S:136:VAL:O	2.08	0.52
1:B:324:THR:HB	1:B:499:PRO:CA	2.38	0.52
1:B:327:LEU:O	1:B:495:PHE:N	2.42	0.52
1:B:630:ARG:NH1	2:P:83:GLU:HG2	2.25	0.52
1:D:173:ILE:O	1:D:174:GLY:C	2.52	0.52
1:D:218:LEU:HG	1:D:218:LEU:O	2.10	0.52
1:E:175:LYS:O	1:E:178:SER:N	2.38	0.52
1:E:565:LYS:C	1:E:567:THR:H	2.17	0.52
1:F:217:LYS:HB2	1:F:236:GLU:CG	2.40	0.52
1:F:305:SER:OG	1:F:307:LEU:HD13	2.09	0.52
1:F:405:LEU:CD1	1:F:453:VAL:HG21	2.33	0.52
1:F:781:ASN:N	1:F:789:ASN:HD21	2.03	0.52
2:O:105:LEU:HD21	2:O:124:MET:SD	2.50	0.52
2:S:63:ILE:HG13	2:S:67:GLU:HB3	1.90	0.52
1:A:80:GLN:HG3	1:A:80:GLN:O	2.09	0.52
1:A:120:LEU:HD13	1:A:120:LEU:O	2.06	0.52
1:A:464:VAL:CG2	1:A:465:LEU:HD12	2.33	0.52
1:B:118:GLN:OE1	1:B:118:GLN:HA	2.10	0.52
1:B:165:GLN:HE21	1:B:251:PRO:HG2	1.73	0.52
1:B:557:LEU:HD11	1:B:575:VAL:HG12	1.90	0.52
1:C:195:LEU:HD21	1:C:227:ILE:HG12	1.90	0.52
1:C:197:LYS:HE2	1:C:264:MET:HG2	1.91	0.52
1:D:102:GLY:C	1:D:103:GLU:HG3	2.34	0.52
1:D:128:MET:HE2	1:D:239:HIS:NE2	2.24	0.52
1:D:324:THR:HB	1:D:499:PRO:CA	2.38	0.52
1:D:565:LYS:C	1:D:567:THR:H	2.17	0.52
1:E:279:ILE:O	1:E:283:LEU:HD13	2.08	0.52
1:F:80:GLN:HG3	1:F:80:GLN:O	2.09	0.52
1:F:120:LEU:O	1:F:120:LEU:HD13	2.06	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:11:GLU:O	2:P:13:LYS:N	2.42	0.52
2:R:63:ILE:HG13	2:R:67:GLU:CB	2.39	0.52
1:A:102:GLY:C	1:A:103:GLU:HG3	2.35	0.52
1:A:413:LEU:HB2	1:A:419:ILE:HG12	1.92	0.52
1:A:565:LYS:C	1:A:567:THR:H	2.16	0.52
1:B:218:LEU:O	1:B:218:LEU:HG	2.10	0.52
1:B:565:LYS:C	1:B:567:THR:H	2.17	0.52
1:C:78:LYS:HG3	1:C:79:ILE:N	2.24	0.52
1:C:175:LYS:O	1:C:178:SER:N	2.38	0.52
1:C:217:LYS:HB2	1:C:236:GLU:CG	2.40	0.52
1:C:218:LEU:HG	1:C:218:LEU:O	2.10	0.52
1:C:326:ILE:HG22	1:C:328:PHE:CE1	2.44	0.52
1:C:480:ASN:HD22	1:C:481:VAL:N	2.07	0.52
1:C:781:ASN:N	1:C:789:ASN:HD21	2.03	0.52
1:D:161:ILE:CG2	1:D:168:GLU:HB2	2.39	0.52
1:D:409:ARG:CD	1:D:413:LEU:HD21	2.40	0.52
1:D:480:ASN:HD22	1:D:481:VAL:N	2.08	0.52
1:E:78:LYS:HG3	1:E:79:ILE:N	2.24	0.52
1:E:764:LEU:C	1:E:766:HIS:H	2.18	0.52
1:F:252:ASP:CG	1:F:253:HIS:N	2.67	0.52
1:F:271:LEU:HA	1:F:275:GLY:HA3	1.91	0.52
1:F:413:LEU:HB2	1:F:419:ILE:HG12	1.92	0.52
1:A:161:ILE:HG23	1:A:168:GLU:HB2	1.92	0.52
1:A:165:GLN:HE21	1:A:251:PRO:HG2	1.74	0.52
1:B:106:PHE:HA	1:B:154:ILE:O	2.10	0.52
1:C:648:PRO:HA	1:C:651:LYS:HB2	1.91	0.52
1:C:730:ASN:O	1:C:733:GLU:N	2.43	0.52
1:C:746:LYS:HD3	1:C:750:GLN:HE21	1.74	0.52
1:D:230:ILE:HG13	1:D:237:PHE:CE2	2.44	0.52
1:D:375:GLY:O	1:D:377:GLN:N	2.42	0.52
1:E:128:MET:O	1:E:128:MET:HG2	2.09	0.52
1:E:217:LYS:HB2	1:E:236:GLU:CG	2.39	0.52
1:E:288:VAL:CG2	1:E:289:GLU:H	2.19	0.52
1:E:470:ASN:O	1:E:472:ARG:HG3	2.10	0.52
1:F:409:ARG:CD	1:F:413:LEU:HD21	2.39	0.52
2:P:6:GLU:O	2:P:9:ILE:N	2.37	0.52
2:S:49:GLN:H	2:S:49:GLN:NE2	2.03	0.52
2:S:63:ILE:HG13	2:S:67:GLU:CB	2.40	0.52
2:T:97:ASN:ND2	2:T:97:ASN:N	2.37	0.52
1:A:105:TYR:CB	1:A:153:ILE:HG12	2.39	0.52
1:A:134:LYS:O	1:A:135:VAL:HG12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:NZ	1:A:236:GLU:HB2	2.24	0.52
1:A:305:SER:OG	1:A:307:LEU:HD13	2.09	0.52
1:A:730:ASN:O	1:A:733:GLU:N	2.43	0.52
1:B:246:SER:O	1:B:250:ALA:HB2	2.09	0.52
1:C:385:LEU:O	1:C:385:LEU:HD13	2.10	0.52
1:D:214:PHE:HB3	1:D:218:LEU:HB3	1.91	0.52
1:D:305:SER:OG	1:D:307:LEU:HD13	2.09	0.52
1:E:409:ARG:CD	1:E:413:LEU:HD21	2.40	0.52
1:E:502:THR:HG22	2:S:111:ASN:O	2.10	0.52
1:F:161:ILE:HG23	1:F:168:GLU:HB2	1.90	0.52
1:F:648:PRO:HA	1:F:651:LYS:HB2	1.91	0.52
2:O:11:GLU:O	2:O:13:LYS:N	2.42	0.52
2:O:102:ALA:HB2	2:O:125:ILE:HG13	1.92	0.52
2:P:136:VAL:HG23	2:P:136:VAL:O	2.09	0.52
2:S:64:ASP:OD1	2:S:66:PRO:CD	2.56	0.52
2:S:93:ASP:OD1	2:S:97:ASN:ND2	2.42	0.52
2:T:64:ASP:OD1	2:T:66:PRO:CD	2.57	0.52
1:A:214:PHE:HB3	1:A:218:LEU:HB3	1.91	0.52
1:B:120:LEU:O	1:B:120:LEU:HD13	2.06	0.52
1:B:501:LEU:HD22	2:P:112:LEU:HD21	1.92	0.52
1:B:742:ALA:HB1	1:B:744:GLU:OE1	2.09	0.52
1:C:156:ILE:HD12	1:C:156:ILE:H	1.75	0.52
1:C:192:PHE:HB3	1:C:196:ILE:HD11	1.92	0.52
1:C:716:LYS:O	1:C:717:LYS:C	2.52	0.52
1:D:78:LYS:HG3	1:D:79:ILE:N	2.25	0.52
1:D:106:PHE:HA	1:D:154:ILE:O	2.10	0.52
1:D:413:LEU:HB2	1:D:419:ILE:HG12	1.92	0.52
1:D:463:THR:HG22	1:D:465:LEU:H	1.75	0.52
1:E:102:GLY:C	1:E:103:GLU:HG3	2.35	0.52
1:F:118:GLN:OE1	1:F:118:GLN:HA	2.09	0.52
1:F:173:ILE:O	1:F:174:GLY:C	2.52	0.52
1:F:180:ASP:C	1:F:182:ILE:N	2.57	0.52
1:F:552:TRP:O	1:F:555:GLN:HG2	2.09	0.52
2:R:32:LEU:HD21	2:R:71:MET:HE1	1.92	0.52
2:R:102:ALA:HB2	2:R:125:ILE:HG13	1.92	0.52
2:T:62:THR:OG1	2:T:63:ILE:N	2.42	0.52
1:A:156:ILE:HD12	1:A:156:ILE:H	1.75	0.51
1:A:742:ALA:HB1	1:A:743:PRO:HD2	1.91	0.51
1:B:130:SER:O	1:B:132:GLY:O	2.28	0.51
1:B:197:LYS:HE2	1:B:264:MET:HG2	1.91	0.51
1:B:271:LEU:HD23	1:B:275:GLY:HA3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LYS:HB2	1:B:610:MET:HE1	1.92	0.51
1:C:305:SER:OG	1:C:307:LEU:HD13	2.09	0.51
1:D:180:ASP:C	1:D:182:ILE:N	2.63	0.51
1:D:621:GLY:HA2	2:R:94:LYS:NZ	2.25	0.51
1:D:781:ASN:N	1:D:789:ASN:HD21	2.03	0.51
1:E:124:GLU:OE2	1:E:129:ASN:ND2	2.42	0.51
1:E:197:LYS:HE3	1:E:264:MET:HA	1.92	0.51
1:E:286:GLU:O	1:E:290:LYS:HE3	2.10	0.51
1:E:550:SER:HG	1:E:552:TRP:CD1	2.28	0.51
1:F:275:GLY:HA2	1:F:278:LYS:CG	2.33	0.51
1:F:375:GLY:O	1:F:377:GLN:N	2.43	0.51
2:O:11:GLU:C	2:O:13:LYS:H	2.18	0.51
2:P:11:GLU:C	2:P:13:LYS:H	2.18	0.51
2:P:58:ASP:C	2:P:60:ASN:N	2.69	0.51
1:A:118:GLN:OE1	1:A:118:GLN:HA	2.09	0.51
1:A:184:LYS:HZ2	1:A:191:GLU:HG3	1.76	0.51
1:A:302:LEU:HA	1:A:305:SER:HB3	1.92	0.51
1:A:308:VAL:O	1:A:311:HIS:HB2	2.10	0.51
1:B:128:MET:CE	1:B:239:HIS:NE2	2.67	0.51
1:B:271:LEU:HA	1:B:275:GLY:HA3	1.92	0.51
1:B:521:ASN:HB3	1:B:524:GLU:HB3	1.92	0.51
1:C:214:PHE:CD1	1:C:218:LEU:HD23	2.46	0.51
1:C:413:LEU:HB2	1:C:419:ILE:HG12	1.93	0.51
1:D:76:LEU:H	1:D:76:LEU:HD22	1.75	0.51
1:F:128:MET:HE2	1:F:239:HIS:NE2	2.26	0.51
1:F:308:VAL:O	1:F:311:HIS:HB2	2.10	0.51
2:P:64:ASP:OD1	2:P:66:PRO:CD	2.56	0.51
1:A:552:TRP:O	1:A:555:GLN:HG2	2.10	0.51
1:B:173:ILE:O	1:B:175:LYS:N	2.43	0.51
1:B:385:LEU:O	1:B:385:LEU:HD13	2.11	0.51
1:B:724:ARG:HG3	1:B:724:ARG:NH1	2.26	0.51
1:B:746:LYS:HD3	1:B:750:GLN:HE21	1.74	0.51
1:C:308:VAL:O	1:C:311:HIS:HB2	2.11	0.51
1:C:356:ASP:OD2	1:C:356:ASP:N	2.42	0.51
1:C:619:ILE:O	1:C:620:THR:C	2.52	0.51
1:C:724:ARG:HG3	1:C:724:ARG:NH1	2.25	0.51
1:D:197:LYS:HE2	1:D:264:MET:HG2	1.91	0.51
1:D:257:LEU:O	1:D:261:ALA:O	2.28	0.51
1:D:619:ILE:O	1:D:620:THR:C	2.53	0.51
1:E:130:SER:O	1:E:132:GLY:O	2.28	0.51
1:E:229:PHE:O	1:E:229:PHE:CD1	2.64	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LYS:C	1:E:287:GLY:H	2.19	0.51
1:E:414:LYS:O	1:E:417:GLY:N	2.40	0.51
1:F:218:LEU:HG	1:F:218:LEU:O	2.11	0.51
1:F:229:PHE:O	1:F:229:PHE:CD1	2.64	0.51
1:F:405:LEU:HD12	1:F:405:LEU:H	1.75	0.51
2:O:62:THR:OG1	2:O:63:ILE:N	2.43	0.51
2:Q:93:ASP:OD1	2:Q:97:ASN:ND2	2.43	0.51
2:Q:111:ASN:C	2:Q:113:GLY:H	2.18	0.51
2:T:146:THR:O	2:T:147:ALA:C	2.53	0.51
1:A:375:GLY:O	1:A:377:GLN:N	2.43	0.51
1:A:693:SER:O	1:A:696:LYS:HB2	2.09	0.51
1:A:781:ASN:N	1:A:789:ASN:HD21	2.03	0.51
1:C:131:ARG:HB2	1:C:170:TYR:CE2	2.45	0.51
1:C:668:SER:CA	2:Q:14:GLU:HG3	2.32	0.51
1:D:385:LEU:O	1:D:385:LEU:HD13	2.11	0.51
1:E:128:MET:O	1:E:128:MET:CG	2.58	0.51
1:E:345:THR:HB	1:E:491:ASP:HB3	1.92	0.51
1:E:405:LEU:CD1	1:E:453:VAL:HG21	2.33	0.51
1:E:413:LEU:HB2	1:E:419:ILE:HG12	1.92	0.51
1:E:611:THR:O	1:E:615:ILE:HG13	2.10	0.51
1:F:74:GLU:HB2	1:F:78:LYS:CB	2.37	0.51
1:F:88:LYS:NZ	1:F:172:GLU:OE2	2.43	0.51
1:F:263:ASP:O	1:F:264:MET:C	2.54	0.51
1:F:442:TYR:CD1	1:F:455:TYR:HD1	2.26	0.51
1:A:308:VAL:HG22	1:A:336:THR:O	2.11	0.51
1:A:442:TYR:CD1	1:A:455:TYR:HD1	2.26	0.51
1:A:521:ASN:HB3	1:A:524:GLU:HB3	1.93	0.51
1:B:229:PHE:O	1:B:229:PHE:CD1	2.64	0.51
1:B:234:LEU:N	1:B:234:LEU:HD23	2.26	0.51
1:B:278:LYS:HE3	1:B:279:ILE:CD1	2.38	0.51
1:B:375:GLY:O	1:B:377:GLN:N	2.43	0.51
1:B:495:PHE:O	1:B:496:ALA:HB2	2.10	0.51
1:B:505:LYS:C	1:B:507:GLN:N	2.69	0.51
1:D:105:TYR:CB	1:D:153:ILE:HG12	2.39	0.51
1:D:217:LYS:HB2	1:D:236:GLU:CG	2.41	0.51
1:D:308:VAL:O	1:D:311:HIS:HB2	2.11	0.51
1:D:345:THR:HB	1:D:491:ASP:HB3	1.91	0.51
1:D:564:VAL:O	1:D:567:THR:HG22	2.10	0.51
1:E:90:PRO:HG2	1:E:93:VAL:CG1	2.40	0.51
1:E:154:ILE:HG13	1:E:171:TYR:CD1	2.44	0.51
1:E:173:ILE:O	1:E:175:LYS:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:O	1:E:218:LEU:HG	2.11	0.51
1:E:375:GLY:O	1:E:377:GLN:N	2.43	0.51
1:E:501:LEU:CD2	2:S:112:LEU:HD21	2.41	0.51
1:E:501:LEU:HD22	2:S:112:LEU:HD21	1.92	0.51
1:E:552:TRP:O	1:E:555:GLN:HG2	2.10	0.51
1:F:102:GLY:C	1:F:103:GLU:HG3	2.35	0.51
1:F:123:GLU:HG2	1:F:124:GLU:H	1.74	0.51
1:F:257:LEU:O	1:F:261:ALA:O	2.29	0.51
1:F:324:THR:HB	1:F:499:PRO:CA	2.37	0.51
1:F:463:THR:HG22	1:F:465:LEU:H	1.76	0.51
1:F:525:LYS:O	1:F:529:VAL:HG23	2.11	0.51
1:F:730:ASN:O	1:F:733:GLU:N	2.43	0.51
1:A:286:GLU:O	1:A:290:LYS:HE3	2.10	0.51
1:B:478:ALA:CB	1:B:486:LYS:O	2.57	0.51
1:B:552:TRP:O	1:B:555:GLN:HG2	2.10	0.51
1:C:165:GLN:HE21	1:C:251:PRO:HG2	1.75	0.51
1:C:229:PHE:O	1:C:229:PHE:CD1	2.64	0.51
1:C:354:SER:OG	1:C:355:SER:N	2.43	0.51
1:C:593:ILE:C	1:C:604:LEU:HD12	2.36	0.51
1:D:118:GLN:HA	1:D:118:GLN:OE1	2.09	0.51
1:D:456:LYS:HA	1:D:469:PHE:CD1	2.46	0.51
1:D:609:GLU:H	1:D:609:GLU:CD	2.19	0.51
1:E:90:PRO:O	1:E:91:LYS:C	2.54	0.51
1:E:156:ILE:HD12	1:E:156:ILE:H	1.75	0.51
1:E:234:LEU:N	1:E:234:LEU:HD23	2.26	0.51
1:F:90:PRO:O	1:F:91:LYS:C	2.54	0.51
1:F:189:ASP:O	1:F:191:GLU:N	2.44	0.51
1:F:741:ILE:O	1:F:741:ILE:HG13	2.11	0.51
2:P:62:THR:OG1	2:P:63:ILE:N	2.43	0.51
2:T:32:LEU:HD21	2:T:71:MET:HE1	1.93	0.51
1:A:99:GLU:C	1:A:101:GLY:N	2.68	0.51
1:A:505:LYS:C	1:A:507:GLN:N	2.69	0.51
1:B:105:TYR:CB	1:B:153:ILE:HG12	2.39	0.51
1:C:197:LYS:HE3	1:C:264:MET:HA	1.93	0.51
1:C:214:PHE:HB3	1:C:218:LEU:HB3	1.92	0.51
1:C:478:ALA:CB	1:C:486:LYS:O	2.58	0.51
1:E:175:LYS:CB	1:E:175:LYS:HZ3	2.23	0.51
1:E:214:PHE:CD1	1:E:218:LEU:HD23	2.46	0.51
1:E:680:LYS:H	1:E:687:GLU:CG	2.24	0.51
1:F:184:LYS:HE2	1:F:193:LEU:HD12	1.93	0.51
1:F:288:VAL:CG2	1:F:289:GLU:H	2.20	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:VAL:HG22	1:F:336:THR:O	2.11	0.51
1:F:495:PHE:O	1:F:496:ALA:HB2	2.11	0.51
2:P:111:ASN:C	2:P:113:GLY:H	2.18	0.51
2:R:76:MET:HA	2:R:79:THR:HG22	1.93	0.51
2:T:111:ASN:C	2:T:113:GLY:H	2.18	0.51
1:A:76:LEU:H	1:A:76:LEU:CD2	2.24	0.51
1:A:229:PHE:CD1	1:A:229:PHE:O	2.64	0.51
1:A:456:LYS:HA	1:A:469:PHE:CD1	2.46	0.51
1:B:197:LYS:HE3	1:B:264:MET:HA	1.92	0.51
1:B:413:LEU:HB2	1:B:419:ILE:HG12	1.92	0.51
1:B:564:VAL:O	1:B:567:THR:HG22	2.10	0.51
1:B:668:SER:CA	2:P:14:GLU:HG3	2.30	0.51
1:B:781:ASN:N	1:B:789:ASN:HD21	2.03	0.51
1:C:106:PHE:HA	1:C:154:ILE:O	2.09	0.51
1:C:301:ALA:HB1	1:C:604:LEU:HB2	1.92	0.51
1:C:405:LEU:HD12	1:C:405:LEU:H	1.75	0.51
1:C:606:LYS:HB2	1:C:610:MET:HE1	1.93	0.51
1:D:229:PHE:CD1	1:D:229:PHE:O	2.64	0.51
1:D:741:ILE:HG13	1:D:741:ILE:O	2.11	0.51
1:E:106:PHE:HA	1:E:154:ILE:O	2.11	0.51
1:E:184:LYS:HZ2	1:E:191:GLU:HG3	1.76	0.51
1:E:308:VAL:HG22	1:E:336:THR:O	2.11	0.51
1:E:593:ILE:C	1:E:604:LEU:HD12	2.35	0.51
1:E:636:ALA:O	1:E:640:LYS:HA	2.11	0.51
1:E:742:ALA:HB1	1:E:744:GLU:OE1	2.11	0.51
1:F:106:PHE:HA	1:F:154:ILE:O	2.10	0.51
1:F:195:LEU:HD21	1:F:227:ILE:HG12	1.91	0.51
1:F:197:LYS:HB3	1:F:197:LYS:HZ2	1.76	0.51
1:F:217:LYS:CB	1:F:236:GLU:HG3	2.41	0.51
2:Q:32:LEU:HD21	2:Q:71:MET:HE1	1.93	0.51
2:Q:76:MET:HA	2:Q:79:THR:HG22	1.92	0.51
2:T:63:ILE:HG13	2:T:67:GLU:CB	2.40	0.51
1:A:324:THR:HB	1:A:499:PRO:CA	2.38	0.51
1:A:593:ILE:C	1:A:604:LEU:HD12	2.36	0.51
1:B:217:LYS:HB2	1:B:236:GLU:CG	2.40	0.51
1:B:285:LYS:C	1:B:287:GLY:H	2.18	0.51
1:B:414:LYS:C	1:B:414:LYS:HD3	2.36	0.51
1:B:764:LEU:O	1:B:766:HIS:N	2.44	0.51
1:C:134:LYS:CG	1:C:136:PRO:HD3	2.34	0.51
1:C:184:LYS:HZ2	1:C:191:GLU:HG3	1.74	0.51
1:C:293:ILE:HD11	1:C:617:LYS:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:465:LEU:H	1.76	0.51
1:D:173:ILE:O	1:D:175:LYS:N	2.44	0.51
1:D:456:LYS:HA	1:D:469:PHE:CE1	2.46	0.51
1:D:593:ILE:C	1:D:604:LEU:HD12	2.36	0.51
1:D:668:SER:CA	2:R:14:GLU:HG3	2.33	0.51
1:E:80:GLN:HG3	1:E:80:GLN:O	2.09	0.51
1:E:564:VAL:O	1:E:567:THR:HG22	2.11	0.51
1:F:154:ILE:HG13	1:F:171:TYR:CD1	2.46	0.51
1:F:385:LEU:HD13	1:F:385:LEU:O	2.11	0.51
1:F:609:GLU:OE2	1:F:609:GLU:N	2.35	0.51
1:F:657:ILE:HD11	1:F:701:LEU:HD23	1.93	0.51
2:Q:58:ASP:C	2:Q:60:ASN:N	2.68	0.51
2:S:11:GLU:C	2:S:13:LYS:H	2.19	0.51
2:T:13:LYS:C	2:T:15:ALA:N	2.68	0.51
1:A:131:ARG:HG3	1:A:243:LEU:HD21	1.92	0.51
1:A:214:PHE:CD1	1:A:218:LEU:HD23	2.46	0.51
1:A:271:LEU:HA	1:A:275:GLY:HA3	1.92	0.51
1:A:405:LEU:HD12	1:A:405:LEU:H	1.75	0.51
1:A:611:THR:O	1:A:615:ILE:HG13	2.11	0.51
1:A:742:ALA:HB1	1:A:744:GLU:OE1	2.10	0.51
1:B:118:GLN:HE22	1:B:143:PHE:HD2	1.59	0.51
1:B:302:LEU:HA	1:B:305:SER:HB3	1.93	0.51
1:B:619:ILE:O	1:B:620:THR:C	2.54	0.51
1:B:741:ILE:HG13	1:B:741:ILE:O	2.11	0.51
1:D:185:ASP:O	1:D:190:PRO:CA	2.59	0.51
1:E:302:LEU:HA	1:E:305:SER:HB3	1.93	0.51
1:F:214:PHE:HB3	1:F:218:LEU:HB3	1.92	0.51
2:S:11:GLU:O	2:S:13:LYS:N	2.44	0.51
2:T:65:PHE:O	2:T:68:PHE:HB3	2.11	0.51
1:A:275:GLY:CA	1:A:278:LYS:HG3	2.36	0.50
1:A:409:ARG:CD	1:A:413:LEU:HD21	2.40	0.50
1:A:495:PHE:O	1:A:496:ALA:HB2	2.10	0.50
1:A:609:GLU:H	1:A:609:GLU:CD	2.19	0.50
1:B:409:ARG:HD2	1:B:413:LEU:HD21	1.93	0.50
1:C:74:GLU:HB2	1:C:78:LYS:CB	2.39	0.50
1:C:170:TYR:O	1:C:174:GLY:HA3	2.11	0.50
1:C:173:ILE:O	1:C:175:LYS:N	2.43	0.50
1:C:189:ASP:O	1:C:190:PRO:C	2.50	0.50
1:C:217:LYS:CB	1:C:236:GLU:HG3	2.41	0.50
1:C:288:VAL:CG2	1:C:289:GLU:H	2.20	0.50
1:C:502:THR:HG22	2:Q:111:ASN:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:PHE:N	1:C:602:PHE:HD2	2.09	0.50
1:C:657:ILE:HD11	1:C:701:LEU:HD23	1.93	0.50
1:D:80:GLN:HG3	1:D:80:GLN:O	2.10	0.50
1:D:118:GLN:HE22	1:D:143:PHE:HD2	1.59	0.50
1:D:192:PHE:HB3	1:D:196:ILE:HD11	1.92	0.50
1:D:197:LYS:HE3	1:D:264:MET:HA	1.93	0.50
1:D:356:ASP:OD2	1:D:356:ASP:N	2.41	0.50
1:E:263:ASP:O	1:E:264:MET:C	2.54	0.50
1:E:324:THR:HB	1:E:499:PRO:CA	2.38	0.50
1:E:405:LEU:HD12	1:E:405:LEU:H	1.76	0.50
1:F:192:PHE:HB3	1:F:196:ILE:HD11	1.92	0.50
1:F:234:LEU:N	1:F:234:LEU:HD23	2.26	0.50
1:F:345:THR:HB	1:F:491:ASP:HB3	1.93	0.50
1:F:499:PRO:CG	1:F:504:ILE:HD11	2.41	0.50
2:S:111:ASN:C	2:S:113:GLY:H	2.18	0.50
1:A:179:LEU:HA	1:A:182:ILE:HG22	1.93	0.50
1:A:197:LYS:HE2	1:A:264:MET:HG2	1.92	0.50
1:A:217:LYS:HB2	1:A:236:GLU:CG	2.41	0.50
1:A:218:LEU:HG	1:A:218:LEU:O	2.10	0.50
1:A:354:SER:OG	1:A:355:SER:N	2.44	0.50
1:B:170:TYR:O	1:B:174:GLY:HA3	2.11	0.50
1:B:286:GLU:O	1:B:290:LYS:HE3	2.12	0.50
1:B:301:ALA:HB1	1:B:604:LEU:HB2	1.94	0.50
1:B:308:VAL:HG22	1:B:336:THR:O	2.12	0.50
1:B:456:LYS:HA	1:B:469:PHE:CD1	2.46	0.50
1:B:463:THR:HG22	1:B:465:LEU:H	1.76	0.50
1:C:118:GLN:HE22	1:C:143:PHE:HD2	1.60	0.50
1:C:165:GLN:C	1:C:167:LYS:N	2.70	0.50
1:C:271:LEU:HA	1:C:275:GLY:HA3	1.92	0.50
1:C:275:GLY:CA	1:C:278:LYS:HG3	2.35	0.50
1:C:308:VAL:HG22	1:C:336:THR:O	2.10	0.50
1:C:345:THR:HB	1:C:491:ASP:HB3	1.92	0.50
1:D:175:LYS:HB2	1:D:175:LYS:HZ3	1.72	0.50
1:D:308:VAL:HG22	1:D:336:THR:O	2.11	0.50
1:D:499:PRO:CG	1:D:504:ILE:HD11	2.41	0.50
1:E:217:LYS:CB	1:E:236:GLU:HG3	2.40	0.50
1:E:271:LEU:HA	1:E:275:GLY:HA3	1.92	0.50
1:E:442:TYR:CD1	1:E:455:TYR:HD1	2.25	0.50
1:E:463:THR:HG22	1:E:465:LEU:H	1.76	0.50
1:E:480:ASN:HD22	1:E:481:VAL:N	2.09	0.50
1:F:156:ILE:HD12	1:F:156:ILE:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:ALA:CB	1:F:486:LYS:O	2.58	0.50
1:F:744:GLU:CD	1:F:744:GLU:H	2.19	0.50
2:Q:65:PHE:O	2:Q:68:PHE:HB3	2.12	0.50
1:A:173:ILE:O	1:A:175:LYS:N	2.44	0.50
1:B:102:GLY:C	1:B:103:GLU:HG3	2.36	0.50
1:B:308:VAL:O	1:B:311:HIS:HB2	2.11	0.50
1:B:480:ASN:HD22	1:B:481:VAL:N	2.10	0.50
1:B:657:ILE:HD11	1:B:701:LEU:HD23	1.93	0.50
1:B:716:LYS:O	1:B:717:LYS:C	2.54	0.50
1:C:456:LYS:HA	1:C:469:PHE:CD1	2.47	0.50
1:D:154:ILE:HG13	1:D:171:TYR:CD1	2.46	0.50
1:D:621:GLY:HA2	2:R:94:LYS:HZ3	1.77	0.50
1:E:409:ARG:HD2	1:E:413:LEU:HD21	1.94	0.50
1:F:173:ILE:O	1:F:175:LYS:N	2.44	0.50
1:F:197:LYS:HE3	1:F:264:MET:HA	1.93	0.50
1:F:497:LEU:CD1	1:F:556:MET:HG2	2.37	0.50
1:F:716:LYS:O	1:F:717:LYS:C	2.54	0.50
2:P:32:LEU:HD21	2:P:71:MET:HE1	1.93	0.50
1:A:197:LYS:HE3	1:A:264:MET:HA	1.92	0.50
1:A:238:GLN:C	1:A:240:ALA:N	2.69	0.50
1:A:384:ASN:O	1:A:386:GLU:N	2.45	0.50
1:A:519:THR:OG1	1:A:520:PRO:HD2	2.12	0.50
1:A:525:LYS:O	1:A:529:VAL:HG23	2.11	0.50
1:A:606:LYS:HB2	1:A:610:MET:HE1	1.93	0.50
1:C:285:LYS:C	1:C:287:GLY:H	2.19	0.50
1:C:409:ARG:HD2	1:C:413:LEU:HD21	1.93	0.50
1:C:797:ILE:O	1:C:797:ILE:HG13	2.11	0.50
1:D:90:PRO:O	1:D:91:LYS:C	2.53	0.50
1:D:288:VAL:CG2	1:D:289:GLU:H	2.20	0.50
1:E:657:ILE:HD11	1:E:701:LEU:HD23	1.94	0.50
1:F:217:LYS:HB2	1:F:236:GLU:HG3	1.93	0.50
1:F:285:LYS:C	1:F:287:GLY:H	2.19	0.50
1:F:301:ALA:HB1	1:F:604:LEU:HB2	1.94	0.50
1:A:480:ASN:HD22	1:A:481:VAL:N	2.09	0.50
1:A:619:ILE:O	1:A:620:THR:C	2.53	0.50
1:A:690:LYS:HD2	1:A:741:ILE:CG2	2.42	0.50
1:B:165:GLN:C	1:B:167:LYS:N	2.69	0.50
1:B:501:LEU:CD2	2:P:112:LEU:HD21	2.41	0.50
1:C:90:PRO:O	1:C:91:LYS:C	2.54	0.50
1:C:225:ILE:HG12	1:C:229:PHE:HE2	1.76	0.50
1:C:286:GLU:O	1:C:290:LYS:HE3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:PRO:CG	1:C:504:ILE:HD11	2.42	0.50
1:C:540:ARG:CZ	1:C:627:TYR:CE1	2.95	0.50
1:D:271:LEU:HA	1:D:275:GLY:HA3	1.92	0.50
1:E:738:SER:OG	1:E:739:LYS:N	2.38	0.50
1:F:118:GLN:HE22	1:F:143:PHE:HD2	1.60	0.50
1:F:327:LEU:O	1:F:495:PHE:N	2.40	0.50
1:F:797:ILE:O	1:F:797:ILE:HG13	2.12	0.50
2:O:65:PHE:O	2:O:68:PHE:HB3	2.11	0.50
2:R:65:PHE:O	2:R:68:PHE:HB3	2.12	0.50
2:S:32:LEU:HD21	2:S:71:MET:HE1	1.93	0.50
1:B:90:PRO:O	1:B:91:LYS:C	2.54	0.50
1:B:133:GLU:O	1:B:133:GLU:HG3	2.08	0.50
1:B:238:GLN:C	1:B:240:ALA:N	2.68	0.50
1:B:271:LEU:HB3	1:B:276:PHE:CE2	2.47	0.50
1:B:690:LYS:HD2	1:B:741:ILE:CG2	2.42	0.50
1:C:234:LEU:N	1:C:234:LEU:HD23	2.26	0.50
1:C:254:ARG:HD2	1:C:254:ARG:N	2.26	0.50
1:C:279:ILE:HD13	1:C:279:ILE:N	2.26	0.50
1:C:414:LYS:O	1:C:417:GLY:N	2.40	0.50
1:C:446:ILE:HA	1:C:453:VAL:HA	1.94	0.50
1:C:521:ASN:HB3	1:C:524:GLU:HB3	1.92	0.50
1:C:630:ARG:NH1	2:Q:83:GLU:HG2	2.26	0.50
1:D:384:ASN:C	1:D:386:GLU:N	2.69	0.50
1:D:384:ASN:O	1:D:386:GLU:N	2.44	0.50
1:D:505:LYS:C	1:D:507:GLN:N	2.69	0.50
1:E:192:PHE:HB3	1:E:196:ILE:HD11	1.92	0.50
1:E:473:ASN:N	1:E:473:ASN:OD1	2.45	0.50
1:E:521:ASN:HB3	1:E:524:GLU:HB3	1.93	0.50
1:E:619:ILE:O	1:E:620:THR:C	2.54	0.50
1:E:716:LYS:O	1:E:717:LYS:C	2.54	0.50
1:E:744:GLU:CD	1:E:744:GLU:H	2.20	0.50
1:E:797:ILE:O	1:E:797:ILE:HG13	2.12	0.50
1:F:271:LEU:HD13	1:F:276:PHE:HE2	1.77	0.50
1:F:295:VAL:HG21	1:F:603:ILE:CG2	2.42	0.50
1:F:502:THR:HG22	2:T:111:ASN:O	2.11	0.50
2:O:13:LYS:C	2:O:15:ALA:N	2.69	0.50
2:P:102:ALA:HB2	2:P:125:ILE:HG13	1.93	0.50
2:Q:13:LYS:C	2:Q:15:ALA:N	2.68	0.50
2:T:102:ALA:HB2	2:T:125:ILE:HG13	1.93	0.50
1:A:285:LYS:C	1:A:287:GLY:H	2.19	0.50
1:B:214:PHE:HB3	1:B:218:LEU:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:VAL:CG2	1:B:289:GLU:N	2.74	0.50
1:B:595:ILE:HG22	1:B:596:ILE:H	1.75	0.50
1:B:633:ASN:O	1:B:642:TYR:HE1	1.95	0.50
1:B:636:ALA:O	1:B:640:LYS:HA	2.12	0.50
1:B:680:LYS:H	1:B:687:GLU:CG	2.25	0.50
1:C:81:GLN:CD	1:C:156:ILE:HG21	2.37	0.50
1:C:99:GLU:C	1:C:101:GLY:N	2.68	0.50
1:C:178:SER:OG	1:C:179:LEU:N	2.44	0.50
1:C:217:LYS:HB2	1:C:236:GLU:HG3	1.93	0.50
1:C:302:LEU:HA	1:C:305:SER:HB3	1.93	0.50
1:C:497:LEU:CD1	1:C:556:MET:HG2	2.40	0.50
1:C:550:SER:HG	1:C:552:TRP:CD1	2.29	0.50
1:D:521:ASN:HB3	1:D:524:GLU:HB3	1.93	0.50
1:D:629:ASN:HB3	1:D:632:TYR:CD1	2.46	0.50
1:E:115:LYS:HZ1	1:E:117:LEU:HB2	1.77	0.50
1:E:185:ASP:O	1:E:190:PRO:HD3	2.11	0.50
1:E:238:GLN:C	1:E:240:ALA:N	2.68	0.50
1:E:301:ALA:HB1	1:E:604:LEU:HB2	1.93	0.50
1:E:666:ASN:O	1:E:670:ILE:HG13	2.12	0.50
1:F:271:LEU:HB3	1:F:276:PHE:CE2	2.46	0.50
1:F:302:LEU:HA	1:F:305:SER:HB3	1.92	0.50
1:F:409:ARG:HD2	1:F:413:LEU:HD21	1.94	0.50
1:F:680:LYS:H	1:F:687:GLU:CG	2.25	0.50
1:A:385:LEU:O	1:A:385:LEU:HD13	2.11	0.50
1:A:456:LYS:HA	1:A:469:PHE:CE1	2.47	0.50
1:A:564:VAL:O	1:A:567:THR:HG22	2.12	0.50
1:A:680:LYS:H	1:A:687:GLU:CG	2.25	0.50
1:A:741:ILE:HG13	1:A:741:ILE:O	2.11	0.50
1:B:525:LYS:O	1:B:529:VAL:HG23	2.11	0.50
1:C:130:SER:O	1:C:131:ARG:C	2.55	0.50
1:C:609:GLU:N	1:C:609:GLU:CD	2.70	0.50
1:D:196:ILE:O	1:D:199:LEU:HB2	2.12	0.50
1:D:217:LYS:CB	1:D:236:GLU:HG3	2.41	0.50
1:D:238:GLN:C	1:D:240:ALA:N	2.68	0.50
1:D:519:THR:OG1	1:D:520:PRO:HD2	2.11	0.50
1:D:606:LYS:HB2	1:D:610:MET:HE1	1.94	0.50
1:D:724:ARG:HG3	1:D:724:ARG:NH1	2.26	0.50
1:E:288:VAL:CG2	1:E:289:GLU:N	2.74	0.50
1:E:308:VAL:O	1:E:311:HIS:HB2	2.12	0.50
1:E:384:ASN:O	1:E:386:GLU:N	2.45	0.50
1:F:81:GLN:CD	1:F:156:ILE:HG21	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:LYS:HA	1:F:469:PHE:CD1	2.47	0.50
2:O:9:ILE:HD12	2:O:69:LEU:CD2	2.41	0.50
2:T:9:ILE:HD12	2:T:69:LEU:CD2	2.42	0.50
1:A:118:GLN:HE22	1:A:143:PHE:HD2	1.59	0.50
1:A:234:LEU:HD23	1:A:234:LEU:N	2.27	0.50
1:A:288:VAL:CG2	1:A:289:GLU:H	2.19	0.50
1:A:501:LEU:CD2	2:O:112:LEU:HD21	2.42	0.50
1:A:595:ILE:HG22	1:A:596:ILE:H	1.75	0.50
1:B:234:LEU:HD23	1:B:234:LEU:H	1.77	0.50
1:B:263:ASP:O	1:B:264:MET:C	2.53	0.50
1:B:293:ILE:HD11	1:B:617:LYS:HD3	1.94	0.50
1:D:263:ASP:O	1:D:264:MET:C	2.55	0.50
1:D:302:LEU:HA	1:D:305:SER:HB3	1.93	0.50
1:D:730:ASN:C	1:D:732:ILE:N	2.70	0.50
1:E:81:GLN:CD	1:E:156:ILE:HG21	2.37	0.50
1:E:278:LYS:HE3	1:E:279:ILE:CD1	2.39	0.50
1:F:99:GLU:C	1:F:101:GLY:N	2.69	0.50
1:F:214:PHE:CD1	1:F:218:LEU:HD23	2.47	0.50
1:F:354:SER:OG	1:F:355:SER:N	2.45	0.50
2:O:65:PHE:CB	2:O:66:PRO:HD3	2.32	0.50
2:P:146:THR:O	2:P:147:ALA:C	2.52	0.50
2:R:58:ASP:C	2:R:60:ASN:N	2.68	0.50
1:A:81:GLN:CD	1:A:156:ILE:HG21	2.37	0.49
1:A:90:PRO:HG2	1:A:93:VAL:CG1	2.42	0.49
1:A:263:ASP:O	1:A:264:MET:C	2.54	0.49
1:A:463:THR:HG22	1:A:465:LEU:H	1.76	0.49
1:A:797:ILE:HG13	1:A:797:ILE:O	2.12	0.49
1:B:405:LEU:HD12	1:B:405:LEU:H	1.76	0.49
1:B:414:LYS:O	1:B:417:GLY:N	2.41	0.49
1:B:442:TYR:HD1	1:B:455:TYR:CD1	2.26	0.49
1:B:502:THR:HG22	2:P:111:ASN:O	2.12	0.49
1:B:764:LEU:C	1:B:766:HIS:N	2.70	0.49
1:B:776:LEU:HD23	1:B:776:LEU:C	2.37	0.49
1:C:456:LYS:HA	1:C:469:PHE:CE1	2.47	0.49
1:C:564:VAL:O	1:C:567:THR:HG22	2.11	0.49
1:D:156:ILE:HD12	1:D:156:ILE:H	1.75	0.49
1:D:238:GLN:C	1:D:240:ALA:H	2.20	0.49
1:F:629:ASN:HB3	1:F:632:TYR:CD1	2.47	0.49
2:O:111:ASN:C	2:O:113:GLY:H	2.18	0.49
2:T:58:ASP:C	2:T:60:ASN:N	2.68	0.49
1:A:76:LEU:HD22	1:A:76:LEU:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:HB1	1:A:604:LEU:HB2	1.93	0.49
1:A:621:GLY:HA2	2:O:94:LYS:NZ	2.27	0.49
1:A:630:ARG:NH1	2:O:83:GLU:HG2	2.28	0.49
1:B:88:LYS:NZ	1:B:172:GLU:CD	2.70	0.49
1:B:214:PHE:CD1	1:B:218:LEU:HD23	2.46	0.49
1:B:279:ILE:HD13	1:B:279:ILE:N	2.27	0.49
1:B:797:ILE:HG13	1:B:797:ILE:O	2.12	0.49
1:C:76:LEU:HD22	1:C:76:LEU:N	2.28	0.49
1:C:271:LEU:HB3	1:C:276:PHE:CE2	2.48	0.49
1:C:384:ASN:O	1:C:386:GLU:N	2.44	0.49
1:C:495:PHE:O	1:C:496:ALA:HB2	2.12	0.49
1:D:187:SER:O	1:D:188:LEU:C	2.50	0.49
1:E:217:LYS:HB2	1:E:236:GLU:HG3	1.92	0.49
1:E:442:TYR:HD1	1:E:455:TYR:CD1	2.26	0.49
1:F:254:ARG:HD2	1:F:254:ARG:N	2.26	0.49
1:F:323:ASN:HD22	1:F:598:PRO:HB3	1.78	0.49
1:F:384:ASN:O	1:F:386:GLU:N	2.45	0.49
2:O:32:LEU:HD21	2:O:71:MET:HE1	1.94	0.49
2:P:49:GLN:H	2:P:49:GLN:NE2	2.03	0.49
2:S:6:GLU:O	2:S:9:ILE:N	2.38	0.49
1:B:81:GLN:CD	1:B:156:ILE:HG21	2.37	0.49
1:B:666:ASN:O	1:B:670:ILE:HG13	2.12	0.49
1:B:736:LEU:HD11	1:B:750:GLN:NE2	2.26	0.49
1:C:218:LEU:C	1:C:220:LEU:N	2.69	0.49
1:C:223:LYS:HD3	1:C:224:SER:H	1.77	0.49
1:C:244:ALA:CB	1:C:264:MET:HE3	2.43	0.49
1:C:735:VAL:O	1:C:738:SER:HB3	2.11	0.49
1:D:178:SER:OG	1:D:179:LEU:N	2.44	0.49
1:D:234:LEU:HD23	1:D:234:LEU:N	2.26	0.49
1:E:165:GLN:C	1:E:167:LYS:N	2.70	0.49
1:E:271:LEU:HB3	1:E:276:PHE:CE2	2.47	0.49
1:E:609:GLU:CD	1:E:609:GLU:N	2.71	0.49
1:F:618:ASN:O	1:F:622:LYS:HB2	2.11	0.49
1:A:223:LYS:HD3	1:A:224:SER:H	1.76	0.49
1:A:384:ASN:C	1:A:386:GLU:N	2.69	0.49
1:B:128:MET:O	1:B:128:MET:HG2	2.12	0.49
1:C:238:GLN:C	1:C:240:ALA:N	2.68	0.49
1:C:680:LYS:H	1:C:687:GLU:CG	2.26	0.49
1:D:170:TYR:O	1:D:174:GLY:HA3	2.12	0.49
1:D:540:ARG:CZ	1:D:627:TYR:CE1	2.95	0.49
1:D:680:LYS:H	1:D:687:GLU:CG	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:LYS:NZ	1:E:172:GLU:CD	2.69	0.49
1:E:170:TYR:O	1:E:174:GLY:HA3	2.12	0.49
1:E:609:GLU:OE2	1:E:609:GLU:N	2.37	0.49
1:E:724:ARG:HG3	1:E:724:ARG:NH1	2.27	0.49
1:F:165:GLN:C	1:F:167:LYS:N	2.70	0.49
1:F:296:LEU:CD2	1:F:296:LEU:N	2.38	0.49
1:F:442:TYR:HD1	1:F:455:TYR:CD1	2.26	0.49
1:F:606:LYS:HB2	1:F:610:MET:HE1	1.94	0.49
2:P:65:PHE:O	2:P:68:PHE:HB3	2.12	0.49
2:T:101:SER:OG	2:T:104:GLU:HG2	2.13	0.49
1:A:133:GLU:O	1:A:133:GLU:HG3	2.08	0.49
1:A:187:SER:O	1:A:188:LEU:C	2.50	0.49
1:A:473:ASN:OD1	1:A:473:ASN:N	2.44	0.49
1:B:616:GLU:HA	1:B:620:THR:HB	1.94	0.49
1:C:234:LEU:HD23	1:C:234:LEU:H	1.77	0.49
1:C:414:LYS:HD3	1:C:414:LYS:C	2.37	0.49
1:D:74:GLU:HB2	1:D:78:LYS:CB	2.39	0.49
1:D:234:LEU:HD23	1:D:234:LEU:H	1.77	0.49
1:D:285:LYS:C	1:D:287:GLY:H	2.19	0.49
1:D:322:LEU:HD13	1:D:556:MET:CE	2.42	0.49
1:D:473:ASN:OD1	1:D:473:ASN:N	2.45	0.49
1:D:686:ASP:O	1:D:689:ALA:HB3	2.12	0.49
1:E:76:LEU:HD22	1:E:76:LEU:N	2.27	0.49
1:E:456:LYS:HA	1:E:469:PHE:CD1	2.47	0.49
1:E:690:LYS:HD2	1:E:741:ILE:CG2	2.42	0.49
1:F:76:LEU:H	1:F:76:LEU:CD2	2.25	0.49
1:F:76:LEU:HD22	1:F:76:LEU:N	2.27	0.49
1:F:134:LYS:O	1:F:135:VAL:HG12	2.13	0.49
1:F:210:PHE:HZ	1:F:221:ASN:OD1	1.95	0.49
1:F:217:LYS:CG	1:F:236:GLU:HG3	2.43	0.49
1:F:602:PHE:N	1:F:602:PHE:HD2	2.10	0.49
2:R:6:GLU:O	2:R:9:ILE:N	2.38	0.49
2:S:13:LYS:C	2:S:15:ALA:N	2.69	0.49
2:S:65:PHE:O	2:S:68:PHE:HB3	2.12	0.49
1:A:88:LYS:NZ	1:A:172:GLU:CD	2.71	0.49
1:A:609:GLU:N	1:A:609:GLU:CD	2.71	0.49
1:B:217:LYS:CB	1:B:236:GLU:HG3	2.42	0.49
1:B:244:ALA:CB	1:B:268:MET:HE3	2.42	0.49
1:B:275:GLY:CA	1:B:278:LYS:HG3	2.37	0.49
1:B:442:TYR:CD1	1:B:455:TYR:HD1	2.25	0.49
1:B:473:ASN:OD1	1:B:473:ASN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:THR:O	1:B:615:ILE:HG13	2.12	0.49
1:C:131:ARG:HB2	1:C:170:TYR:CZ	2.48	0.49
1:C:327:LEU:HG	1:C:595:ILE:HG23	1.93	0.49
1:C:595:ILE:HG22	1:C:596:ILE:H	1.75	0.49
1:D:81:GLN:CD	1:D:156:ILE:HG21	2.38	0.49
1:D:295:VAL:HG21	1:D:603:ILE:CG2	2.42	0.49
1:D:405:LEU:HD12	1:D:405:LEU:H	1.77	0.49
1:D:716:LYS:O	1:D:717:LYS:C	2.54	0.49
1:D:765:THR:HG22	1:D:769:SER:HB2	1.95	0.49
1:E:384:ASN:C	1:E:386:GLU:N	2.69	0.49
1:E:499:PRO:CG	1:E:504:ILE:HD11	2.42	0.49
1:E:540:ARG:CZ	1:E:627:TYR:CE1	2.96	0.49
1:F:88:LYS:NZ	1:F:172:GLU:CD	2.71	0.49
1:F:90:PRO:HG2	1:F:93:VAL:CG1	2.42	0.49
1:F:164:GLU:C	1:F:166:SER:N	2.70	0.49
1:F:521:ASN:HB3	1:F:524:GLU:HB3	1.93	0.49
1:F:552:TRP:HA	1:F:555:GLN:HG2	1.95	0.49
1:F:633:ASN:O	1:F:642:TYR:HE1	1.96	0.49
2:O:64:ASP:OD1	2:O:66:PRO:CD	2.56	0.49
2:Q:97:ASN:ND2	2:Q:97:ASN:N	2.38	0.49
2:Q:102:ALA:HB2	2:Q:125:ILE:HG13	1.93	0.49
1:B:76:LEU:HD22	1:B:76:LEU:N	2.27	0.49
1:C:327:LEU:O	1:C:495:PHE:N	2.41	0.49
1:C:629:ASN:HB3	1:C:632:TYR:CD1	2.48	0.49
1:D:134:LYS:O	1:D:135:VAL:HG12	2.13	0.49
1:D:254:ARG:HD2	1:D:254:ARG:N	2.27	0.49
1:D:666:ASN:O	1:D:670:ILE:HG13	2.11	0.49
1:D:797:ILE:HG13	1:D:797:ILE:O	2.13	0.49
1:E:184:LYS:NZ	1:E:191:GLU:HG3	2.27	0.49
1:E:322:LEU:HD13	1:E:556:MET:CE	2.43	0.49
1:E:606:LYS:HB2	1:E:610:MET:HE1	1.95	0.49
1:E:659:THR:O	1:E:660:SER:C	2.55	0.49
1:E:730:ASN:C	1:E:732:ILE:N	2.70	0.49
1:E:764:LEU:O	1:E:766:HIS:N	2.46	0.49
1:F:736:LEU:HD11	1:F:750:GLN:NE2	2.27	0.49
2:Q:12:PHE:HE1	2:Q:72:MET:CE	2.25	0.49
1:A:165:GLN:C	1:A:167:LYS:N	2.70	0.49
1:A:175:LYS:CB	1:A:175:LYS:HZ3	2.25	0.49
1:A:210:PHE:HZ	1:A:221:ASN:OD1	1.96	0.49
1:A:271:LEU:HB3	1:A:276:PHE:CE2	2.47	0.49
1:A:356:ASP:OD2	1:A:356:ASP:N	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:HD3	1:A:414:LYS:C	2.38	0.49
1:A:629:ASN:HB3	1:A:632:TYR:CD1	2.47	0.49
1:B:529:VAL:O	1:B:532:LEU:HB2	2.13	0.49
1:B:609:GLU:H	1:B:609:GLU:CD	2.19	0.49
1:B:744:GLU:H	1:B:744:GLU:CD	2.19	0.49
1:C:88:LYS:NZ	1:C:172:GLU:OE2	2.46	0.49
1:C:308:VAL:O	1:C:311:HIS:N	2.42	0.49
1:C:323:ASN:HD22	1:C:598:PRO:HB3	1.78	0.49
1:C:736:LEU:HD11	1:C:750:GLN:NE2	2.27	0.49
1:D:197:LYS:O	1:D:197:LYS:HD2	2.13	0.49
1:D:279:ILE:HD13	1:D:279:ILE:N	2.28	0.49
1:D:609:GLU:N	1:D:609:GLU:CD	2.71	0.49
1:E:182:ILE:O	1:E:187:SER:HB2	2.13	0.49
1:E:741:ILE:HG13	1:E:741:ILE:O	2.12	0.49
1:F:189:ASP:O	1:F:191:GLU:HG2	2.12	0.49
1:F:238:GLN:C	1:F:240:ALA:N	2.69	0.49
1:F:293:ILE:HD11	1:F:617:LYS:HD3	1.94	0.49
1:F:473:ASN:OD1	1:F:473:ASN:N	2.45	0.49
1:F:609:GLU:N	1:F:609:GLU:CD	2.71	0.49
2:R:73:ALA:O	2:R:75:LYS:N	2.46	0.49
1:A:122:GLU:CG	1:A:147:ARG:HB2	2.43	0.49
1:A:217:LYS:CB	1:A:236:GLU:HG3	2.42	0.49
1:A:657:ILE:HD11	1:A:701:LEU:HD23	1.94	0.49
1:B:99:GLU:C	1:B:101:GLY:N	2.67	0.49
1:B:164:GLU:C	1:B:166:SER:N	2.71	0.49
1:B:178:SER:OG	1:B:179:LEU:CD2	2.60	0.49
1:B:210:PHE:HZ	1:B:221:ASN:OD1	1.96	0.49
1:B:561:ASN:OD1	1:B:574:VAL:N	2.41	0.49
1:B:706:ASN:O	2:P:130:ILE:HG23	2.13	0.49
1:C:122:GLU:CG	1:C:147:ARG:HB2	2.43	0.49
1:C:384:ASN:C	1:C:386:GLU:N	2.69	0.49
1:C:433:TYR:HE1	1:C:448:ASP:OD2	1.96	0.49
1:C:666:ASN:O	1:C:670:ILE:HG13	2.13	0.49
1:D:164:GLU:O	1:D:166:SER:N	2.46	0.49
1:D:525:LYS:O	1:D:529:VAL:HG23	2.13	0.49
1:D:628:PHE:CE2	2:R:90:ARG:HD3	2.35	0.49
1:D:636:ALA:O	1:D:640:LYS:HA	2.12	0.49
1:D:764:LEU:C	1:D:766:HIS:H	2.21	0.49
1:E:519:THR:OG1	1:E:520:PRO:HD2	2.13	0.49
1:E:525:LYS:O	1:E:529:VAL:HG23	2.13	0.49
1:E:602:PHE:N	1:E:602:PHE:HD2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:736:LEU:HD11	1:E:750:GLN:NE2	2.27	0.49
1:F:456:LYS:HA	1:F:469:PHE:CE1	2.48	0.49
1:F:480:ASN:HD22	1:F:481:VAL:N	2.10	0.49
2:P:120:GLU:HA	2:P:123:GLN:HB2	1.95	0.49
2:Q:73:ALA:O	2:Q:75:LYS:N	2.46	0.49
1:A:552:TRP:HA	1:A:555:GLN:HG2	1.94	0.49
1:A:744:GLU:H	1:A:744:GLU:CD	2.20	0.49
1:B:323:ASN:C	1:B:324:THR:CG2	2.86	0.49
1:B:384:ASN:O	1:B:386:GLU:N	2.46	0.49
1:B:456:LYS:HA	1:B:469:PHE:CE1	2.47	0.49
1:B:499:PRO:CG	1:B:504:ILE:HD11	2.42	0.49
1:C:323:ASN:C	1:C:323:ASN:ND2	2.71	0.49
1:C:616:GLU:HA	1:C:620:THR:HB	1.95	0.49
1:C:735:VAL:HA	1:C:738:SER:HB2	1.95	0.49
1:C:776:LEU:HD23	1:C:776:LEU:C	2.37	0.49
1:D:164:GLU:C	1:D:166:SER:N	2.70	0.49
1:D:217:LYS:HB2	1:D:236:GLU:HG3	1.93	0.49
1:D:223:LYS:HD3	1:D:224:SER:H	1.78	0.49
1:D:327:LEU:O	1:D:495:PHE:N	2.42	0.49
1:D:611:THR:O	1:D:615:ILE:HG13	2.12	0.49
1:D:630:ARG:NH1	2:R:83:GLU:HG2	2.28	0.49
1:E:133:GLU:O	1:E:133:GLU:HG3	2.08	0.49
1:E:164:GLU:C	1:E:166:SER:N	2.70	0.49
1:E:414:LYS:C	1:E:414:LYS:HD3	2.38	0.49
1:E:433:TYR:HE1	1:E:448:ASP:OD2	1.96	0.49
1:F:130:SER:O	1:F:131:ARG:C	2.56	0.49
1:F:234:LEU:HD23	1:F:234:LEU:H	1.77	0.49
1:F:716:LYS:O	1:F:720:ILE:HG22	2.13	0.49
2:P:65:PHE:CB	2:P:66:PRO:HD3	2.34	0.49
2:Q:9:ILE:HD12	2:Q:69:LEU:CD2	2.43	0.49
2:Q:120:GLU:HA	2:Q:123:GLN:HB2	1.95	0.49
2:R:13:LYS:C	2:R:15:ALA:N	2.68	0.49
2:R:111:ASN:C	2:R:113:GLY:H	2.19	0.49
1:A:189:ASP:O	1:A:191:GLU:HG2	2.13	0.48
1:A:445:ARG:HG2	1:A:471:TRP:CZ3	2.48	0.48
1:A:609:GLU:O	1:A:610:MET:C	2.56	0.48
1:B:122:GLU:CG	1:B:147:ARG:HB2	2.43	0.48
1:B:184:LYS:NZ	1:B:191:GLU:HG3	2.27	0.48
1:C:271:LEU:HD13	1:C:276:PHE:HE2	1.78	0.48
1:C:322:LEU:HD13	1:C:556:MET:CE	2.41	0.48
1:C:730:ASN:C	1:C:732:ILE:N	2.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:735:VAL:O	1:C:738:SER:CB	2.61	0.48
1:D:271:LEU:HB3	1:D:276:PHE:CE2	2.48	0.48
1:D:301:ALA:HB1	1:D:604:LEU:HB2	1.93	0.48
1:D:368:GLN:OE1	1:D:368:GLN:HA	2.13	0.48
1:D:391:ILE:HG23	1:D:398:ILE:O	2.13	0.48
1:D:409:ARG:HD2	1:D:413:LEU:HD21	1.94	0.48
1:D:445:ARG:HG2	1:D:471:TRP:CZ3	2.48	0.48
1:D:446:ILE:HA	1:D:453:VAL:HA	1.95	0.48
1:D:690:LYS:HD3	1:D:741:ILE:HG23	1.95	0.48
1:E:118:GLN:HE22	1:E:143:PHE:HD2	1.61	0.48
1:E:199:LEU:HG	1:E:225:ILE:O	2.13	0.48
1:E:630:ARG:NH1	2:S:83:GLU:HG2	2.25	0.48
1:F:122:GLU:CG	1:F:147:ARG:HB2	2.43	0.48
1:F:564:VAL:O	1:F:567:THR:HG22	2.13	0.48
1:F:735:VAL:O	1:F:738:SER:HB3	2.12	0.48
2:R:13:LYS:HZ1	2:R:65:PHE:HB3	1.76	0.48
2:R:65:PHE:CB	2:R:66:PRO:HD3	2.34	0.48
1:A:90:PRO:O	1:A:91:LYS:C	2.55	0.48
1:A:170:TYR:O	1:A:174:GLY:HA3	2.12	0.48
1:A:178:SER:OG	1:A:179:LEU:CD2	2.61	0.48
1:A:196:ILE:O	1:A:199:LEU:HB2	2.14	0.48
1:B:144:GLU:CG	1:B:177:ILE:HD11	2.41	0.48
1:B:445:ARG:HG2	1:B:471:TRP:CZ3	2.48	0.48
1:C:173:ILE:HG23	1:C:174:GLY:H	1.77	0.48
1:C:187:SER:O	1:C:188:LEU:C	2.51	0.48
1:C:238:GLN:C	1:C:240:ALA:H	2.21	0.48
1:C:263:ASP:O	1:C:264:MET:C	2.54	0.48
1:C:473:ASN:OD1	1:C:473:ASN:N	2.45	0.48
1:C:744:GLU:CD	1:C:744:GLU:H	2.20	0.48
1:D:199:LEU:HG	1:D:225:ILE:O	2.13	0.48
1:D:433:TYR:HE1	1:D:448:ASP:OD2	1.95	0.48
1:D:501:LEU:HD22	2:R:112:LEU:HD21	1.96	0.48
1:D:671:ARG:HH12	1:D:677:GLY:HA3	1.74	0.48
1:D:736:LEU:HD11	1:D:750:GLN:NE2	2.27	0.48
1:E:89:ILE:HG22	1:E:90:PRO:HD2	1.95	0.48
1:E:130:SER:O	1:E:131:ARG:C	2.54	0.48
1:E:164:GLU:HG2	1:E:166:SER:HB3	1.95	0.48
1:E:178:SER:OG	1:E:179:LEU:CD2	2.60	0.48
1:E:497:LEU:CD1	1:E:556:MET:HG2	2.40	0.48
1:F:79:ILE:C	1:F:81:GLN:N	2.70	0.48
1:F:437:SER:O	1:F:439:ASN:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:117:THR:CG2	2:P:120:GLU:HB2	2.43	0.48
1:A:173:ILE:HG23	1:A:174:GLY:H	1.78	0.48
1:A:234:LEU:HD23	1:A:234:LEU:H	1.78	0.48
1:A:540:ARG:CZ	1:A:627:TYR:CE1	2.96	0.48
1:A:629:ASN:HD22	1:A:630:ARG:N	2.11	0.48
1:B:182:ILE:O	1:B:187:SER:HB2	2.12	0.48
1:B:663:PHE:O	1:B:664:ILE:C	2.57	0.48
1:B:665:LYS:HE2	2:P:11:GLU:OE2	2.14	0.48
1:C:501:LEU:CD2	2:Q:112:LEU:HD21	2.44	0.48
1:C:665:LYS:HE2	2:Q:11:GLU:OE2	2.14	0.48
1:C:741:ILE:O	1:C:741:ILE:HG13	2.12	0.48
1:D:88:LYS:NZ	1:D:172:GLU:OE2	2.46	0.48
1:D:293:ILE:HD11	1:D:617:LYS:HD3	1.95	0.48
1:D:713:SER:O	1:D:714:GLN:C	2.55	0.48
1:D:776:LEU:HD23	1:D:776:LEU:C	2.37	0.48
1:E:207:ASP:C	1:E:209:LEU:H	2.22	0.48
1:E:391:ILE:HG23	1:E:398:ILE:O	2.13	0.48
1:E:456:LYS:HA	1:E:469:PHE:CE1	2.48	0.48
1:F:170:TYR:O	1:F:174:GLY:HA3	2.13	0.48
1:F:384:ASN:C	1:F:386:GLU:N	2.69	0.48
1:F:414:LYS:HD3	1:F:414:LYS:C	2.38	0.48
1:F:472:ARG:HB3	1:F:472:ARG:NH1	2.29	0.48
1:F:517:VAL:C	1:F:519:THR:H	2.21	0.48
2:P:9:ILE:HD12	2:P:69:LEU:CD2	2.43	0.48
2:Q:11:GLU:C	2:Q:13:LYS:N	2.71	0.48
2:Q:13:LYS:HA	2:Q:16:PHE:HB3	1.95	0.48
2:S:12:PHE:HE1	2:S:72:MET:CE	2.25	0.48
2:S:102:ALA:HB2	2:S:125:ILE:HG13	1.94	0.48
2:T:12:PHE:HE1	2:T:72:MET:CE	2.25	0.48
1:A:279:ILE:N	1:A:279:ILE:HD13	2.28	0.48
1:B:384:ASN:C	1:B:386:GLU:N	2.70	0.48
1:B:486:LYS:HE3	1:B:570:THR:O	2.13	0.48
1:B:581:GLN:HE21	1:B:629:ASN:H	1.61	0.48
1:C:169:VAL:O	1:C:172:GLU:HB2	2.14	0.48
1:C:480:ASN:HD22	1:C:480:ASN:C	2.21	0.48
1:C:686:ASP:O	1:C:689:ALA:HB3	2.14	0.48
1:D:495:PHE:O	1:D:581:GLN:HG2	2.13	0.48
1:D:602:PHE:N	1:D:602:PHE:HD2	2.11	0.48
1:E:217:LYS:CG	1:E:236:GLU:HG3	2.44	0.48
1:E:254:ARG:HD2	1:E:254:ARG:N	2.26	0.48
1:E:296:LEU:CD2	1:E:296:LEU:N	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ASN:HD22	1:E:598:PRO:HB3	1.79	0.48
1:E:368:GLN:HA	1:E:368:GLN:OE1	2.14	0.48
1:F:334:LEU:H	1:F:334:LEU:CD1	2.26	0.48
1:F:581:GLN:HE21	1:F:629:ASN:H	1.61	0.48
2:O:6:GLU:O	2:O:9:ILE:N	2.39	0.48
2:R:12:PHE:HE1	2:R:72:MET:CE	2.25	0.48
2:S:120:GLU:HA	2:S:123:GLN:HB2	1.95	0.48
1:A:504:ILE:N	1:A:504:ILE:HD12	2.29	0.48
1:A:736:LEU:HD11	1:A:750:GLN:NE2	2.27	0.48
1:B:115:LYS:HZ1	1:B:117:LEU:HB2	1.78	0.48
1:B:325:TYR:CD1	1:B:598:PRO:HD3	2.49	0.48
1:B:334:LEU:H	1:B:334:LEU:CD1	2.27	0.48
1:B:409:ARG:CZ	1:B:413:LEU:HD21	2.44	0.48
1:B:609:GLU:CD	1:B:609:GLU:N	2.72	0.48
1:B:609:GLU:O	1:B:610:MET:C	2.56	0.48
1:B:730:ASN:C	1:B:732:ILE:N	2.70	0.48
1:C:525:LYS:O	1:C:529:VAL:HG23	2.12	0.48
1:C:765:THR:HG22	1:C:769:SER:HB2	1.96	0.48
1:D:79:ILE:C	1:D:81:GLN:N	2.71	0.48
1:D:414:LYS:C	1:D:414:LYS:HD3	2.38	0.48
1:D:478:ALA:CB	1:D:486:LYS:O	2.58	0.48
1:D:480:ASN:HD22	1:D:480:ASN:C	2.22	0.48
1:D:609:GLU:O	1:D:610:MET:C	2.56	0.48
1:E:107:THR:HG21	1:E:115:LYS:CD	2.36	0.48
1:E:325:TYR:CD1	1:E:598:PRO:HD3	2.49	0.48
1:E:517:VAL:C	1:E:519:THR:H	2.21	0.48
1:E:597:ASN:O	1:E:599:GLU:N	2.46	0.48
1:E:690:LYS:HD3	1:E:741:ILE:HG23	1.94	0.48
1:F:199:LEU:HG	1:F:225:ILE:O	2.13	0.48
1:F:323:ASN:C	1:F:323:ASN:ND2	2.71	0.48
1:F:630:ARG:NH1	2:T:83:GLU:HG2	2.26	0.48
1:F:735:VAL:HA	1:F:738:SER:HB2	1.96	0.48
2:P:101:SER:OG	2:P:104:GLU:HG2	2.14	0.48
1:A:323:ASN:C	1:A:323:ASN:ND2	2.72	0.48
1:A:376:GLN:C	1:A:378:LEU:N	2.72	0.48
1:A:636:ALA:O	1:A:640:LYS:HA	2.12	0.48
1:A:776:LEU:HD23	1:A:776:LEU:C	2.38	0.48
1:B:164:GLU:O	1:B:166:SER:N	2.47	0.48
1:B:184:LYS:HE2	1:B:193:LEU:HD12	1.96	0.48
1:B:196:ILE:O	1:B:199:LEU:HB2	2.14	0.48
1:B:354:SER:OG	1:B:355:SER:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:TYR:HE1	1:B:448:ASP:OD2	1.96	0.48
1:D:244:ALA:CB	1:D:264:MET:HE3	2.44	0.48
1:D:339:ILE:O	1:D:342:GLY:N	2.47	0.48
1:D:376:GLN:C	1:D:378:LEU:N	2.72	0.48
1:D:744:GLU:H	1:D:744:GLU:CD	2.21	0.48
1:E:173:ILE:HG23	1:E:174:GLY:H	1.78	0.48
1:E:218:LEU:C	1:E:220:LEU:N	2.70	0.48
1:E:234:LEU:HD23	1:E:234:LEU:H	1.77	0.48
1:E:279:ILE:HD13	1:E:279:ILE:N	2.28	0.48
1:E:552:TRP:HA	1:E:555:GLN:HG2	1.94	0.48
1:F:184:LYS:HE2	1:F:193:LEU:CD1	2.43	0.48
1:F:207:ASP:C	1:F:209:LEU:H	2.22	0.48
1:F:730:ASN:C	1:F:732:ILE:N	2.71	0.48
2:T:58:ASP:HB3	2:T:62:THR:CG2	2.44	0.48
1:A:326:ILE:CG2	1:A:328:PHE:CE1	2.97	0.48
1:A:334:LEU:H	1:A:334:LEU:CD1	2.26	0.48
1:B:223:LYS:HD3	1:B:224:SER:H	1.76	0.48
1:B:540:ARG:CZ	1:B:627:TYR:CE1	2.97	0.48
1:B:629:ASN:HB3	1:B:632:TYR:CD1	2.49	0.48
1:B:686:ASP:O	1:B:689:ALA:HB3	2.13	0.48
1:C:611:THR:O	1:C:615:ILE:HG13	2.13	0.48
1:D:210:PHE:HZ	1:D:221:ASN:OD1	1.97	0.48
1:D:217:LYS:CG	1:D:236:GLU:HG3	2.44	0.48
1:E:122:GLU:CG	1:E:147:ARG:HB2	2.43	0.48
1:E:275:GLY:CA	1:E:278:LYS:HG3	2.37	0.48
1:E:293:ILE:HD11	1:E:617:LYS:HD3	1.94	0.48
1:F:414:LYS:O	1:F:417:GLY:N	2.39	0.48
1:F:540:ARG:CZ	1:F:627:TYR:CE1	2.97	0.48
1:F:636:ALA:O	1:F:640:LYS:HA	2.13	0.48
1:F:713:SER:O	1:F:714:GLN:C	2.56	0.48
1:F:776:LEU:HD23	1:F:776:LEU:C	2.38	0.48
2:T:117:THR:CG2	2:T:120:GLU:HB2	2.42	0.48
1:A:164:GLU:C	1:A:166:SER:N	2.71	0.48
1:A:319:ALA:O	1:A:323:ASN:HA	2.14	0.48
1:A:338:LEU:HD21	1:A:409:ARG:NE	2.29	0.48
1:A:409:ARG:HD2	1:A:413:LEU:HD21	1.95	0.48
1:A:414:LYS:O	1:A:417:GLY:N	2.40	0.48
1:A:602:PHE:N	1:A:602:PHE:HD2	2.11	0.48
1:A:764:LEU:O	1:A:766:HIS:N	2.46	0.48
1:B:217:LYS:HB2	1:B:236:GLU:HG3	1.93	0.48
1:C:208:LEU:H	1:C:208:LEU:HD12	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:THR:OG1	1:C:520:PRO:HD2	2.13	0.48
1:C:636:ALA:O	1:C:640:LYS:HA	2.13	0.48
1:D:300:LYS:O	1:D:303:LYS:HB2	2.14	0.48
1:D:338:LEU:HD21	1:D:409:ARG:NE	2.29	0.48
1:D:472:ARG:HB3	1:D:472:ARG:NH1	2.29	0.48
1:D:486:LYS:HE3	1:D:570:THR:O	2.14	0.48
1:D:501:LEU:CD2	2:R:112:LEU:HD21	2.43	0.48
1:E:244:ALA:CB	1:E:264:MET:HE3	2.44	0.48
1:F:324:THR:CB	1:F:499:PRO:HA	2.41	0.48
1:F:391:ILE:HG23	1:F:398:ILE:O	2.14	0.48
1:F:666:ASN:O	1:F:670:ILE:HG13	2.13	0.48
1:F:715:GLU:OE1	1:F:767:GLN:NE2	2.47	0.48
2:O:101:SER:OG	2:O:104:GLU:HG2	2.13	0.48
1:A:238:GLN:C	1:A:240:ALA:H	2.22	0.48
1:A:293:ILE:HD11	1:A:617:LYS:HD3	1.95	0.48
1:A:300:LYS:O	1:A:303:LYS:HB2	2.14	0.48
1:A:306:GLY:O	1:A:336:THR:HG23	2.14	0.48
1:A:472:ARG:HB3	1:A:472:ARG:NH1	2.28	0.48
1:A:690:LYS:HD3	1:A:741:ILE:HG23	1.96	0.48
1:A:797:ILE:O	1:A:798:ASP:OD1	2.32	0.48
1:B:271:LEU:HD13	1:B:276:PHE:HE2	1.79	0.48
1:B:495:PHE:O	1:B:581:GLN:HG2	2.14	0.48
1:B:730:ASN:O	1:B:732:ILE:N	2.46	0.48
1:C:609:GLU:CD	1:C:609:GLU:H	2.18	0.48
1:D:271:LEU:HD13	1:D:276:PHE:HE2	1.79	0.48
1:D:552:TRP:HA	1:D:555:GLN:HG2	1.94	0.48
1:D:564:VAL:C	1:D:567:THR:HG22	2.39	0.48
1:D:635:ILE:H	1:D:635:ILE:CD1	2.15	0.48
1:E:257:LEU:O	1:E:261:ALA:O	2.32	0.48
1:E:327:LEU:HG	1:E:595:ILE:HG12	1.96	0.48
1:E:431:LYS:O	1:E:432:TYR:HD2	1.97	0.48
1:E:616:GLU:HA	1:E:620:THR:HB	1.95	0.48
1:F:279:ILE:HD13	1:F:279:ILE:N	2.28	0.48
1:F:338:LEU:HD21	1:F:409:ARG:NE	2.29	0.48
1:F:514:ASP:C	1:F:516:VAL:N	2.71	0.48
2:P:12:PHE:HE1	2:P:72:MET:CE	2.26	0.48
2:T:120:GLU:HA	2:T:123:GLN:HB2	1.95	0.48
1:A:217:LYS:HB2	1:A:236:GLU:HG3	1.94	0.48
1:A:271:LEU:HD13	1:A:276:PHE:HE2	1.78	0.48
1:A:730:ASN:C	1:A:732:ILE:N	2.70	0.48
1:B:217:LYS:HZ2	1:B:217:LYS:CB	2.24	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASN:HD22	1:B:598:PRO:HB3	1.79	0.48
1:B:437:SER:O	1:B:439:ASN:N	2.43	0.48
1:B:519:THR:OG1	1:B:520:PRO:HD2	2.14	0.48
1:C:256:VAL:O	1:C:260:TYR:HB2	2.14	0.48
1:C:749:PHE:O	1:C:750:GLN:C	2.57	0.48
1:D:131:ARG:HB2	1:D:170:TYR:CE2	2.49	0.48
1:D:323:ASN:HD22	1:D:598:PRO:HB3	1.79	0.48
1:D:616:GLU:HA	1:D:620:THR:HB	1.95	0.48
1:E:210:PHE:HZ	1:E:221:ASN:OD1	1.97	0.48
1:E:495:PHE:O	1:E:581:GLN:HG2	2.14	0.48
1:E:713:SER:O	1:E:714:GLN:C	2.57	0.48
1:E:743:PRO:O	1:E:746:LYS:N	2.47	0.48
1:F:175:LYS:CB	1:F:175:LYS:HZ3	2.26	0.48
1:F:616:GLU:HA	1:F:620:THR:HB	1.95	0.48
2:O:9:ILE:O	2:O:10:ALA:C	2.55	0.48
2:R:9:ILE:O	2:R:10:ALA:C	2.57	0.48
2:R:120:GLU:HA	2:R:123:GLN:HB2	1.96	0.48
1:A:164:GLU:O	1:A:166:SER:N	2.47	0.47
1:A:529:VAL:O	1:A:532:LEU:HB2	2.13	0.47
1:A:713:SER:O	1:A:714:GLN:C	2.56	0.47
1:B:217:LYS:HZ1	1:B:236:GLU:HB2	1.79	0.47
1:B:238:GLN:C	1:B:240:ALA:H	2.21	0.47
1:B:254:ARG:HD2	1:B:254:ARG:N	2.26	0.47
1:B:391:ILE:HG23	1:B:398:ILE:O	2.14	0.47
1:B:500:SER:HG	1:B:502:THR:HG1	1.61	0.47
1:C:79:ILE:C	1:C:81:GLN:N	2.72	0.47
1:C:90:PRO:HG2	1:C:93:VAL:CG1	2.44	0.47
1:C:148:GLU:HG3	1:C:149:THR:H	1.78	0.47
1:C:197:LYS:HD2	1:C:197:LYS:O	2.14	0.47
1:C:431:LYS:O	1:C:432:TYR:HD2	1.97	0.47
1:C:472:ARG:HB3	1:C:472:ARG:NH1	2.29	0.47
1:C:495:PHE:O	1:C:581:GLN:HG2	2.13	0.47
1:C:552:TRP:HA	1:C:555:GLN:HG2	1.95	0.47
1:D:122:GLU:CG	1:D:147:ARG:HB2	2.43	0.47
1:D:323:ASN:C	1:D:323:ASN:ND2	2.70	0.47
1:D:517:VAL:C	1:D:519:THR:H	2.22	0.47
1:D:743:PRO:O	1:D:746:LYS:N	2.47	0.47
1:E:164:GLU:O	1:E:166:SER:N	2.47	0.47
1:E:238:GLN:C	1:E:240:ALA:H	2.21	0.47
1:E:529:VAL:O	1:E:532:LEU:HB2	2.14	0.47
1:F:208:LEU:H	1:F:208:LEU:HD12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:PHE:O	1:F:581:GLN:HG2	2.14	0.47
1:F:514:ASP:C	1:F:516:VAL:H	2.22	0.47
2:O:8:GLN:O	2:O:12:PHE:HD2	1.97	0.47
2:P:109:MET:HG3	2:P:116:LEU:CD1	2.44	0.47
2:Q:73:ALA:O	2:Q:74:ARG:C	2.57	0.47
2:R:9:ILE:HD12	2:R:69:LEU:CD2	2.43	0.47
2:S:101:SER:OG	2:S:104:GLU:HG2	2.13	0.47
1:A:169:VAL:O	1:A:172:GLU:HB2	2.14	0.47
1:A:207:ASP:C	1:A:209:LEU:H	2.21	0.47
1:A:472:ARG:HB3	1:A:472:ARG:HH11	1.79	0.47
1:B:199:LEU:HG	1:B:225:ILE:O	2.14	0.47
1:C:191:GLU:C	1:C:193:LEU:N	2.72	0.47
1:C:244:ALA:CB	1:C:268:MET:HE3	2.44	0.47
1:C:432:TYR:CD2	1:C:447:SER:HA	2.49	0.47
1:C:711:ILE:C	1:C:712:PHE:HD2	2.22	0.47
1:C:713:SER:O	1:C:714:GLN:C	2.56	0.47
1:D:90:PRO:HG2	1:D:93:VAL:CG1	2.44	0.47
1:D:169:VAL:O	1:D:172:GLU:HB2	2.15	0.47
1:E:79:ILE:C	1:E:81:GLN:N	2.70	0.47
1:E:409:ARG:CZ	1:E:413:LEU:HD21	2.44	0.47
1:E:431:LYS:O	1:E:432:TYR:CD2	2.67	0.47
1:E:437:SER:O	1:E:439:ASN:N	2.43	0.47
1:E:486:LYS:HE3	1:E:570:THR:O	2.13	0.47
1:F:79:ILE:O	1:F:81:GLN:N	2.47	0.47
1:F:433:TYR:HE1	1:F:448:ASP:OD2	1.97	0.47
1:F:523:LEU:HD22	2:T:127:GLU:CD	2.39	0.47
1:F:665:LYS:HE2	2:T:11:GLU:OE2	2.14	0.47
1:F:749:PHE:O	1:F:750:GLN:C	2.57	0.47
2:O:120:GLU:HA	2:O:123:GLN:HB2	1.95	0.47
2:P:13:LYS:HA	2:P:16:PHE:HB3	1.95	0.47
2:S:58:ASP:HB3	2:S:62:THR:CG2	2.44	0.47
2:S:117:THR:CG2	2:S:120:GLU:HB2	2.42	0.47
2:T:13:LYS:HA	2:T:16:PHE:HB3	1.96	0.47
1:A:197:LYS:O	1:A:197:LYS:HD2	2.14	0.47
1:A:431:LYS:O	1:A:432:TYR:HD2	1.98	0.47
1:A:499:PRO:CG	1:A:504:ILE:HD11	2.43	0.47
1:A:517:VAL:C	1:A:519:THR:H	2.21	0.47
1:B:207:ASP:C	1:B:209:LEU:H	2.22	0.47
1:B:244:ALA:CB	1:B:264:MET:HE3	2.44	0.47
1:B:690:LYS:HD3	1:B:741:ILE:HG23	1.96	0.47
1:C:133:GLU:O	1:C:133:GLU:HG3	2.08	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:C	1:C:166:SER:N	2.71	0.47
1:C:325:TYR:CD1	1:C:598:PRO:HD3	2.50	0.47
1:D:133:GLU:HG3	1:D:133:GLU:O	2.08	0.47
1:D:184:LYS:HZ2	1:D:191:GLU:HG3	1.79	0.47
1:D:368:GLN:C	1:D:370:LEU:H	2.22	0.47
1:D:437:SER:O	1:D:439:ASN:N	2.42	0.47
1:E:300:LYS:O	1:E:303:LYS:HB2	2.14	0.47
1:E:306:GLY:O	1:E:336:THR:HG23	2.14	0.47
1:E:338:LEU:HD21	1:E:409:ARG:NE	2.29	0.47
1:E:522:SER:O	2:S:124:MET:HE2	2.15	0.47
1:E:663:PHE:O	1:E:664:ILE:C	2.57	0.47
1:E:665:LYS:HE2	2:S:11:GLU:OE2	2.14	0.47
1:E:706:ASN:O	2:S:130:ILE:HG23	2.14	0.47
1:E:776:LEU:HD23	1:E:776:LEU:C	2.39	0.47
1:F:197:LYS:HD2	1:F:197:LYS:O	2.15	0.47
1:F:431:LYS:O	1:F:432:TYR:CD2	2.67	0.47
1:F:690:LYS:HD2	1:F:741:ILE:CG2	2.43	0.47
2:P:9:ILE:O	2:P:10:ALA:C	2.57	0.47
2:T:76:MET:HA	2:T:79:THR:HG22	1.95	0.47
1:A:254:ARG:HD2	1:A:254:ARG:N	2.27	0.47
1:A:288:VAL:C	1:A:290:LYS:N	2.72	0.47
1:A:391:ILE:HG23	1:A:398:ILE:O	2.14	0.47
1:A:433:TYR:HE1	1:A:448:ASP:OD2	1.97	0.47
1:B:339:ILE:O	1:B:342:GLY:N	2.48	0.47
1:B:376:GLN:C	1:B:378:LEU:N	2.72	0.47
1:B:523:LEU:HD22	2:P:127:GLU:CD	2.40	0.47
1:C:76:LEU:H	1:C:76:LEU:HD22	1.79	0.47
1:C:154:ILE:HG13	1:C:171:TYR:CD1	2.49	0.47
1:C:173:ILE:HD12	1:C:243:LEU:HD21	1.96	0.47
1:C:288:VAL:C	1:C:290:LYS:N	2.72	0.47
1:C:663:PHE:O	1:C:664:ILE:C	2.57	0.47
1:D:173:ILE:HG23	1:D:174:GLY:H	1.79	0.47
1:D:175:LYS:CB	1:D:175:LYS:HZ3	2.28	0.47
1:D:431:LYS:O	1:D:432:TYR:HD2	1.97	0.47
1:D:472:ARG:HB3	1:D:472:ARG:HH11	1.79	0.47
1:D:504:ILE:N	1:D:504:ILE:HD12	2.29	0.47
1:D:690:LYS:HD2	1:D:741:ILE:CG2	2.44	0.47
1:E:88:LYS:NZ	1:E:172:GLU:OE1	2.48	0.47
1:E:354:SER:OG	1:E:355:SER:N	2.47	0.47
1:E:730:ASN:O	1:E:732:ILE:N	2.47	0.47
1:F:729:TYR:HB2	1:F:756:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:76:MET:HA	2:O:79:THR:HG22	1.96	0.47
2:P:13:LYS:C	2:P:15:ALA:N	2.69	0.47
2:Q:30:LYS:H	2:Q:30:LYS:CD	2.13	0.47
2:Q:101:SER:OG	2:Q:104:GLU:HG2	2.14	0.47
2:S:109:MET:HG3	2:S:116:LEU:CD1	2.44	0.47
2:T:27:ILE:HD12	2:T:32:LEU:HA	1.96	0.47
2:T:89:PHE:O	2:T:90:ARG:C	2.55	0.47
1:A:218:LEU:C	1:A:220:LEU:N	2.68	0.47
1:A:339:ILE:O	1:A:342:GLY:N	2.48	0.47
1:A:384:ASN:C	1:A:386:GLU:H	2.23	0.47
1:A:486:LYS:HE3	1:A:570:THR:O	2.15	0.47
1:A:555:GLN:HG3	1:A:556:MET:N	2.29	0.47
1:A:633:ASN:O	1:A:642:TYR:HE1	1.96	0.47
1:B:173:ILE:HG23	1:B:174:GLY:H	1.78	0.47
1:B:564:VAL:C	1:B:567:THR:HG22	2.40	0.47
1:B:610:MET:O	1:B:614:PHE:N	2.43	0.47
1:C:115:LYS:HZ1	1:C:117:LEU:HB2	1.80	0.47
1:C:210:PHE:HZ	1:C:221:ASN:OD1	1.97	0.47
1:C:295:VAL:HG12	1:C:605:THR:HA	1.95	0.47
1:C:621:GLY:HA2	2:Q:94:LYS:HZ3	1.78	0.47
1:D:295:VAL:HG12	1:D:605:THR:HA	1.96	0.47
1:D:555:GLN:HG3	1:D:556:MET:N	2.29	0.47
1:E:311:HIS:CD2	1:E:564:VAL:HB	2.49	0.47
1:E:686:ASP:O	1:E:689:ALA:HB3	2.14	0.47
1:E:711:ILE:C	1:E:712:PHE:HD2	2.22	0.47
1:F:322:LEU:HD13	1:F:556:MET:CE	2.43	0.47
1:F:409:ARG:CZ	1:F:413:LEU:HD21	2.44	0.47
1:F:431:LYS:O	1:F:432:TYR:HD2	1.97	0.47
1:F:519:THR:OG1	1:F:520:PRO:HD2	2.14	0.47
1:F:609:GLU:O	1:F:610:MET:C	2.56	0.47
2:O:117:THR:CG2	2:O:120:GLU:HB2	2.42	0.47
2:T:138:TYR:O	2:T:142:VAL:HG23	2.14	0.47
1:A:173:ILE:HD12	1:A:243:LEU:HD21	1.97	0.47
1:A:181:ILE:O	1:A:181:ILE:HG12	2.15	0.47
1:A:561:ASN:OD1	1:A:574:VAL:N	2.41	0.47
1:A:711:ILE:C	1:A:712:PHE:HD2	2.23	0.47
1:B:311:HIS:CD2	1:B:564:VAL:HB	2.49	0.47
1:B:711:ILE:C	1:B:712:PHE:HD2	2.22	0.47
1:D:207:ASP:C	1:D:209:LEU:H	2.22	0.47
1:D:447:SER:OG	1:D:448:ASP:N	2.45	0.47
1:D:711:ILE:C	1:D:712:PHE:HD2	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:ILE:O	1:D:798:ASP:OD1	2.32	0.47
1:E:220:LEU:HG	1:E:223:LYS:HB2	1.96	0.47
1:E:323:ASN:C	1:E:324:THR:CG2	2.88	0.47
1:E:376:GLN:C	1:E:378:LEU:N	2.72	0.47
1:E:445:ARG:HG2	1:E:471:TRP:CZ3	2.49	0.47
1:E:629:ASN:HB3	1:E:632:TYR:CD1	2.50	0.47
1:F:88:LYS:NZ	1:F:172:GLU:OE1	2.47	0.47
1:F:325:TYR:CD1	1:F:598:PRO:HD3	2.49	0.47
1:F:472:ARG:HB3	1:F:472:ARG:HH11	1.80	0.47
1:F:501:LEU:HD22	2:T:112:LEU:HD21	1.96	0.47
1:F:691:LYS:O	1:F:692:GLU:C	2.55	0.47
2:O:109:MET:HG3	2:O:116:LEU:CD1	2.45	0.47
2:Q:117:THR:CG2	2:Q:120:GLU:HB2	2.42	0.47
2:R:49:GLN:HA	2:R:52:ILE:HG22	1.96	0.47
2:S:58:ASP:C	2:S:60:ASN:N	2.68	0.47
2:T:30:LYS:H	2:T:30:LYS:CD	2.12	0.47
2:T:109:MET:HG3	2:T:116:LEU:CD1	2.45	0.47
1:A:208:LEU:H	1:A:208:LEU:HD12	1.80	0.47
1:A:225:ILE:HG12	1:A:229:PHE:CE2	2.48	0.47
1:A:323:ASN:C	1:A:324:THR:CG2	2.88	0.47
1:A:442:TYR:HD1	1:A:455:TYR:CD1	2.26	0.47
1:A:495:PHE:O	1:A:581:GLN:HG2	2.15	0.47
1:A:497:LEU:CD1	1:A:556:MET:HG2	2.38	0.47
1:A:743:PRO:O	1:A:746:LYS:N	2.48	0.47
1:B:90:PRO:HG2	1:B:93:VAL:CG1	2.44	0.47
1:B:306:GLY:O	1:B:336:THR:HG23	2.14	0.47
1:B:327:LEU:HG	1:B:595:ILE:HG12	1.96	0.47
1:B:368:GLN:C	1:B:370:LEU:H	2.23	0.47
1:B:431:LYS:O	1:B:432:TYR:HD2	1.97	0.47
1:B:472:ARG:NH1	1:B:472:ARG:HB3	2.29	0.47
1:B:517:VAL:C	1:B:519:THR:H	2.22	0.47
1:B:621:GLY:HA2	2:P:94:LYS:NZ	2.29	0.47
1:B:636:ALA:O	1:B:640:LYS:N	2.47	0.47
1:B:756:ILE:O	1:B:760:VAL:HG23	2.15	0.47
1:C:181:ILE:O	1:C:181:ILE:HG12	2.15	0.47
1:C:207:ASP:C	1:C:209:LEU:H	2.22	0.47
1:C:220:LEU:HG	1:C:223:LYS:HB2	1.96	0.47
1:C:472:ARG:HB3	1:C:472:ARG:HH11	1.79	0.47
1:C:514:ASP:C	1:C:516:VAL:H	2.22	0.47
1:C:517:VAL:C	1:C:519:THR:H	2.22	0.47
1:C:597:ASN:O	1:C:599:GLU:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD13	1:D:120:LEU:O	2.06	0.47
1:D:164:GLU:HG2	1:D:166:SER:HB3	1.97	0.47
1:D:189:ASP:O	1:D:191:GLU:HG2	2.15	0.47
1:D:409:ARG:CZ	1:D:413:LEU:HD21	2.44	0.47
1:D:636:ALA:O	1:D:640:LYS:N	2.47	0.47
1:D:729:TYR:HB2	1:D:756:ILE:HG21	1.96	0.47
1:E:79:ILE:O	1:E:81:GLN:N	2.48	0.47
1:E:169:VAL:O	1:E:172:GLU:HB2	2.14	0.47
1:E:225:ILE:HG23	1:E:229:PHE:CE2	2.49	0.47
1:E:244:ALA:CB	1:E:268:MET:HE3	2.45	0.47
1:E:334:LEU:H	1:E:334:LEU:CD1	2.27	0.47
1:E:480:ASN:HD22	1:E:480:ASN:C	2.23	0.47
1:E:677:GLY:HA2	1:E:745:TYR:OH	2.15	0.47
1:E:797:ILE:O	1:E:798:ASP:OD1	2.33	0.47
1:F:164:GLU:O	1:F:166:SER:N	2.47	0.47
1:F:196:ILE:O	1:F:199:LEU:HB2	2.14	0.47
1:F:220:LEU:HG	1:F:223:LYS:HB2	1.97	0.47
1:F:244:ALA:CB	1:F:264:MET:HE3	2.44	0.47
1:F:288:VAL:C	1:F:290:LYS:N	2.72	0.47
1:F:597:ASN:O	1:F:599:GLU:N	2.46	0.47
1:F:636:ALA:O	1:F:640:LYS:N	2.48	0.47
1:F:686:ASP:O	1:F:689:ALA:HB3	2.14	0.47
1:F:724:ARG:HG3	1:F:724:ARG:NH1	2.27	0.47
2:O:11:GLU:C	2:O:13:LYS:N	2.73	0.47
2:O:13:LYS:HA	2:O:16:PHE:HB3	1.96	0.47
2:P:111:ASN:C	2:P:113:GLY:N	2.73	0.47
2:Q:3:GLN:N	2:Q:77:LYS:HD3	2.30	0.47
2:Q:49:GLN:HA	2:Q:52:ILE:HG22	1.96	0.47
2:Q:138:TYR:CZ	2:Q:142:VAL:HG21	2.50	0.47
2:R:138:TYR:CZ	2:R:142:VAL:HG21	2.50	0.47
2:S:27:ILE:HD12	2:S:32:LEU:HA	1.97	0.47
1:A:130:SER:O	1:A:132:GLY:O	2.33	0.47
1:A:244:ALA:CB	1:A:264:MET:HE3	2.44	0.47
1:A:322:LEU:HD13	1:A:556:MET:CE	2.44	0.47
1:A:409:ARG:CZ	1:A:413:LEU:HD21	2.43	0.47
1:A:663:PHE:O	1:A:664:ILE:C	2.58	0.47
1:A:691:LYS:O	1:A:692:GLU:C	2.57	0.47
1:B:152:LEU:CD2	1:B:154:ILE:HG12	2.45	0.47
1:B:208:LEU:H	1:B:208:LEU:HD12	1.80	0.47
1:B:523:LEU:HD22	2:P:127:GLU:HG2	1.97	0.47
1:B:743:PRO:O	1:B:746:LYS:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:MET:CE	1:C:239:HIS:NE2	2.76	0.47
1:C:199:LEU:HG	1:C:225:ILE:O	2.14	0.47
1:D:181:ILE:O	1:D:181:ILE:HG12	2.14	0.47
1:D:432:TYR:CD2	1:D:447:SER:HA	2.50	0.47
1:D:514:ASP:C	1:D:516:VAL:H	2.22	0.47
1:D:529:VAL:O	1:D:532:LEU:HB2	2.14	0.47
1:E:223:LYS:HD3	1:E:224:SER:H	1.77	0.47
1:E:327:LEU:HG	1:E:595:ILE:HG23	1.97	0.47
1:F:102:GLY:HA2	1:F:150:PRO:O	2.15	0.47
1:F:275:GLY:CA	1:F:278:LYS:HG3	2.37	0.47
1:F:711:ILE:C	1:F:712:PHE:HD2	2.23	0.47
2:O:12:PHE:HE1	2:O:72:MET:CE	2.26	0.47
2:O:73:ALA:O	2:O:74:ARG:C	2.58	0.47
2:P:27:ILE:HD12	2:P:32:LEU:HA	1.97	0.47
2:P:73:ALA:O	2:P:74:ARG:C	2.57	0.47
2:Q:25:GLY:HA3	2:Q:65:PHE:CZ	2.50	0.47
2:S:73:ALA:O	2:S:74:ARG:C	2.58	0.47
2:T:9:ILE:O	2:T:10:ALA:C	2.57	0.47
1:A:184:LYS:HE2	1:A:193:LEU:HD12	1.97	0.47
1:A:217:LYS:CG	1:A:236:GLU:HG3	2.44	0.47
1:A:332:ASN:OD1	1:A:334:LEU:N	2.46	0.47
1:A:368:GLN:C	1:A:370:LEU:H	2.23	0.47
1:A:666:ASN:O	1:A:670:ILE:HG13	2.13	0.47
1:B:181:ILE:O	1:B:181:ILE:HG12	2.14	0.47
1:B:368:GLN:OE1	1:B:368:GLN:HA	2.15	0.47
1:C:196:ILE:O	1:C:199:LEU:HB2	2.14	0.47
1:C:501:LEU:HD22	2:Q:112:LEU:HD21	1.97	0.47
1:C:514:ASP:O	1:C:516:VAL:N	2.48	0.47
1:C:636:ALA:O	1:C:640:LYS:N	2.48	0.47
1:D:173:ILE:HD12	1:D:243:LEU:HD21	1.96	0.47
1:D:325:TYR:CD1	1:D:598:PRO:HD3	2.50	0.47
1:D:442:TYR:HD1	1:D:455:TYR:CD1	2.26	0.47
1:D:550:SER:HG	1:D:552:TRP:CD1	2.33	0.47
1:E:181:ILE:O	1:E:181:ILE:HG12	2.15	0.47
1:E:427:ASP:C	1:E:429:GLY:H	2.23	0.47
1:E:514:ASP:C	1:E:516:VAL:N	2.73	0.47
1:F:238:GLN:C	1:F:240:ALA:H	2.22	0.47
1:F:327:LEU:HG	1:F:595:ILE:HG23	1.97	0.47
1:F:501:LEU:CD2	2:T:112:LEU:HD21	2.45	0.47
1:F:609:GLU:CD	1:F:609:GLU:H	2.19	0.47
1:F:735:VAL:O	1:F:738:SER:CB	2.63	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:114:GLU:HA	2:P:114:GLU:OE2	2.15	0.47
2:Q:9:ILE:O	2:Q:10:ALA:C	2.58	0.47
2:R:109:MET:HG3	2:R:116:LEU:CD1	2.44	0.47
2:S:13:LYS:HA	2:S:16:PHE:HB3	1.95	0.47
2:S:114:GLU:HA	2:S:114:GLU:OE2	2.15	0.47
1:A:686:ASP:O	1:A:689:ALA:HB3	2.14	0.47
1:A:730:ASN:O	1:A:732:ILE:N	2.47	0.47
1:A:764:LEU:C	1:A:766:HIS:N	2.72	0.47
1:B:197:LYS:HD2	1:B:197:LYS:O	2.14	0.47
1:B:327:LEU:HG	1:B:595:ILE:HG23	1.97	0.47
1:C:217:LYS:CG	1:C:236:GLU:HG3	2.44	0.47
1:C:523:LEU:HD22	2:Q:127:GLU:CD	2.40	0.47
1:D:165:GLN:C	1:D:167:LYS:N	2.70	0.47
1:D:176:GLY:O	1:D:180:ASP:OD1	2.32	0.47
1:D:431:LYS:O	1:D:432:TYR:CD2	2.68	0.47
1:D:633:ASN:O	1:D:642:TYR:HE1	1.98	0.47
1:D:657:ILE:HD11	1:D:701:LEU:HD23	1.97	0.47
1:D:659:THR:O	1:D:660:SER:C	2.57	0.47
1:E:208:LEU:HD12	1:E:208:LEU:H	1.79	0.47
1:E:368:GLN:C	1:E:370:LEU:H	2.23	0.47
1:E:504:ILE:HD12	1:E:504:ILE:N	2.30	0.47
1:E:580:GLU:C	1:E:582:ASP:H	2.23	0.47
1:E:674:SER:C	1:E:676:VAL:H	2.23	0.47
1:F:218:LEU:C	1:F:220:LEU:N	2.69	0.47
1:F:256:VAL:O	1:F:260:TYR:HB2	2.15	0.47
1:F:629:ASN:HD22	1:F:630:ARG:N	2.13	0.47
2:Q:109:MET:HG3	2:Q:116:LEU:CD1	2.45	0.47
2:Q:114:GLU:HA	2:Q:114:GLU:OE2	2.15	0.47
2:S:8:GLN:O	2:S:12:PHE:HD2	1.98	0.47
2:S:9:ILE:HD12	2:S:69:LEU:CD2	2.45	0.47
1:A:323:ASN:HD22	1:A:598:PRO:HB3	1.79	0.46
1:B:130:SER:O	1:B:131:ARG:C	2.57	0.46
1:B:225:ILE:HG12	1:B:229:PHE:CE2	2.49	0.46
1:B:319:ALA:O	1:B:323:ASN:HA	2.15	0.46
1:B:384:ASN:C	1:B:386:GLU:H	2.24	0.46
1:B:504:ILE:HD12	1:B:504:ILE:N	2.30	0.46
1:C:164:GLU:O	1:C:166:SER:N	2.48	0.46
1:C:409:ARG:CZ	1:C:413:LEU:HD21	2.44	0.46
1:C:529:VAL:O	1:C:532:LEU:HB2	2.14	0.46
1:D:99:GLU:C	1:D:101:GLY:N	2.68	0.46
1:D:427:ASP:C	1:D:429:GLY:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:ASN:C	1:E:386:GLU:H	2.23	0.46
1:E:478:ALA:CB	1:E:486:LYS:O	2.59	0.46
1:E:635:ILE:H	1:E:635:ILE:CD1	2.16	0.46
1:F:173:ILE:HG23	1:F:174:GLY:H	1.79	0.46
1:F:327:LEU:HG	1:F:595:ILE:HG12	1.96	0.46
1:F:368:GLN:C	1:F:370:LEU:H	2.23	0.46
1:F:427:ASP:C	1:F:429:GLY:H	2.23	0.46
1:F:529:VAL:O	1:F:532:LEU:HB2	2.15	0.46
1:F:699:GLY:O	1:F:700:TYR:C	2.58	0.46
2:O:27:ILE:HD12	2:O:32:LEU:HA	1.97	0.46
2:P:138:TYR:CZ	2:P:142:VAL:HG21	2.50	0.46
2:R:13:LYS:HA	2:R:16:PHE:HB3	1.95	0.46
2:S:49:GLN:HA	2:S:52:ILE:HG22	1.96	0.46
1:A:88:LYS:NZ	1:A:172:GLU:OE1	2.48	0.46
1:A:152:LEU:CD2	1:A:154:ILE:HG12	2.45	0.46
1:A:199:LEU:HG	1:A:225:ILE:O	2.14	0.46
1:A:225:ILE:HG23	1:A:229:PHE:CE2	2.50	0.46
1:A:368:GLN:OE1	1:A:368:GLN:HA	2.14	0.46
1:A:636:ALA:O	1:A:640:LYS:N	2.47	0.46
1:B:300:LYS:O	1:B:303:LYS:HB2	2.15	0.46
1:B:497:LEU:CD1	1:B:556:MET:HG2	2.40	0.46
1:C:300:LYS:O	1:C:303:LYS:HB2	2.15	0.46
1:C:338:LEU:HD21	1:C:409:ARG:NE	2.31	0.46
1:C:442:TYR:HD1	1:C:455:TYR:CD1	2.26	0.46
1:C:445:ARG:HG2	1:C:471:TRP:CZ3	2.50	0.46
1:C:514:ASP:C	1:C:516:VAL:N	2.72	0.46
1:C:555:GLN:HG3	1:C:556:MET:N	2.30	0.46
1:D:218:LEU:C	1:D:220:LEU:N	2.68	0.46
1:D:327:LEU:HG	1:D:595:ILE:HG12	1.97	0.46
1:E:197:LYS:HD2	1:E:197:LYS:O	2.14	0.46
1:E:472:ARG:NH1	1:E:472:ARG:HB3	2.30	0.46
2:S:111:ASN:C	2:S:113:GLY:N	2.73	0.46
2:T:49:GLN:HA	2:T:52:ILE:HG22	1.97	0.46
1:A:191:GLU:C	1:A:193:LEU:N	2.73	0.46
1:A:427:ASP:C	1:A:429:GLY:H	2.23	0.46
1:A:431:LYS:O	1:A:432:TYR:CD2	2.68	0.46
1:A:564:VAL:C	1:A:567:THR:HG22	2.41	0.46
1:A:581:GLN:HE21	1:A:629:ASN:H	1.61	0.46
1:A:674:SER:C	1:A:676:VAL:H	2.24	0.46
1:B:522:SER:O	2:P:124:MET:HE2	2.15	0.46
1:B:797:ILE:O	1:B:798:ASP:OD1	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HB2	1:C:190:PRO:CD	2.44	0.46
1:C:243:LEU:HA	1:C:246:SER:OG	2.16	0.46
1:C:368:GLN:OE1	1:C:368:GLN:HA	2.14	0.46
1:C:564:VAL:C	1:C:567:THR:HG22	2.40	0.46
1:C:674:SER:C	1:C:676:VAL:H	2.23	0.46
1:D:185:ASP:O	1:D:190:PRO:CD	2.63	0.46
1:D:256:VAL:O	1:D:260:TYR:HB2	2.15	0.46
1:D:288:VAL:C	1:D:290:LYS:N	2.72	0.46
1:D:319:ALA:O	1:D:323:ASN:HA	2.15	0.46
1:D:324:THR:CB	1:D:499:PRO:HA	2.41	0.46
1:D:384:ASN:C	1:D:386:GLU:H	2.23	0.46
1:D:514:ASP:O	1:D:516:VAL:N	2.48	0.46
1:E:191:GLU:C	1:E:193:LEU:N	2.73	0.46
1:E:271:LEU:HD13	1:E:276:PHE:HE2	1.79	0.46
1:E:288:VAL:C	1:E:290:LYS:N	2.72	0.46
1:F:182:ILE:C	1:F:183:SER:O	2.57	0.46
1:F:339:ILE:O	1:F:342:GLY:N	2.48	0.46
1:F:446:ILE:HA	1:F:453:VAL:HA	1.97	0.46
1:F:663:PHE:O	1:F:664:ILE:C	2.58	0.46
1:F:759:GLN:HA	1:F:759:GLN:NE2	2.21	0.46
2:R:6:GLU:O	2:R:9:ILE:HB	2.15	0.46
2:R:11:GLU:C	2:R:13:LYS:N	2.72	0.46
2:R:101:SER:OG	2:R:104:GLU:HG2	2.15	0.46
2:T:73:ALA:O	2:T:74:ARG:C	2.58	0.46
1:A:115:LYS:HZ1	1:A:117:LEU:HB2	1.80	0.46
1:A:514:ASP:C	1:A:516:VAL:H	2.24	0.46
1:A:616:GLU:HA	1:A:620:THR:HB	1.96	0.46
1:A:620:THR:HG22	1:A:621:GLY:N	2.31	0.46
1:B:79:ILE:C	1:B:81:GLN:N	2.71	0.46
1:B:173:ILE:HD12	1:B:243:LEU:HD21	1.98	0.46
1:B:431:LYS:O	1:B:432:TYR:CD2	2.68	0.46
1:B:514:ASP:C	1:B:516:VAL:H	2.24	0.46
1:B:597:ASN:O	1:B:599:GLU:N	2.48	0.46
1:B:602:PHE:N	1:B:602:PHE:HD2	2.11	0.46
1:C:743:PRO:O	1:C:746:LYS:N	2.48	0.46
1:D:131:ARG:HB2	1:D:170:TYR:CZ	2.51	0.46
1:D:308:VAL:O	1:D:311:HIS:N	2.42	0.46
1:E:196:ILE:O	1:E:199:LEU:HB2	2.14	0.46
1:E:514:ASP:C	1:E:516:VAL:H	2.24	0.46
1:F:514:ASP:O	1:F:516:VAL:N	2.48	0.46
1:F:550:SER:HG	1:F:552:TRP:CD1	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:797:ILE:O	1:F:798:ASP:OD1	2.32	0.46
2:R:73:ALA:O	2:R:74:ARG:C	2.58	0.46
2:R:117:THR:CG2	2:R:120:GLU:HB2	2.42	0.46
2:S:9:ILE:O	2:S:10:ALA:C	2.57	0.46
2:S:89:PHE:O	2:S:90:ARG:C	2.55	0.46
2:S:138:TYR:O	2:S:142:VAL:HG23	2.16	0.46
1:A:79:ILE:C	1:A:81:GLN:N	2.72	0.46
1:A:164:GLU:HG2	1:A:166:SER:HB3	1.98	0.46
1:A:443:GLU:HG3	1:A:458:LYS:HE3	1.98	0.46
1:A:567:THR:HG23	1:A:568:GLY:N	2.30	0.46
1:A:756:ILE:O	1:A:760:VAL:HG23	2.16	0.46
1:B:79:ILE:O	1:B:81:GLN:N	2.48	0.46
1:B:144:GLU:HG2	1:B:177:ILE:CD1	2.44	0.46
1:B:169:VAL:O	1:B:172:GLU:HB2	2.16	0.46
1:B:220:LEU:HG	1:B:223:LYS:HB2	1.97	0.46
1:B:338:LEU:HD21	1:B:409:ARG:NE	2.30	0.46
1:C:427:ASP:C	1:C:429:GLY:H	2.23	0.46
1:D:326:ILE:CG2	1:D:328:PHE:CE1	2.99	0.46
1:D:674:SER:C	1:D:676:VAL:H	2.24	0.46
1:D:730:ASN:O	1:D:732:ILE:N	2.48	0.46
1:E:161:ILE:HG21	1:E:168:GLU:HB2	1.96	0.46
1:E:555:GLN:HG3	1:E:556:MET:N	2.30	0.46
1:F:107:THR:HG21	1:F:115:LYS:CD	2.38	0.46
1:F:164:GLU:HG2	1:F:166:SER:HB3	1.98	0.46
1:F:445:ARG:HG2	1:F:471:TRP:CZ3	2.50	0.46
1:F:523:LEU:HD22	2:T:127:GLU:HG2	1.97	0.46
2:O:6:GLU:O	2:O:9:ILE:HB	2.16	0.46
2:R:8:GLN:O	2:R:12:PHE:HD2	1.98	0.46
2:R:55:VAL:CG2	2:R:67:GLU:OE1	2.63	0.46
2:S:58:ASP:O	2:S:60:ASN:N	2.47	0.46
1:A:296:LEU:CD2	1:A:296:LEU:N	2.38	0.46
1:A:311:HIS:CD2	1:A:564:VAL:HB	2.51	0.46
1:A:628:PHE:CE2	2:O:90:ARG:HD3	2.34	0.46
1:B:161:ILE:HG21	1:B:168:GLU:HB2	1.96	0.46
1:B:443:GLU:HG3	1:B:458:LYS:HE3	1.97	0.46
1:B:550:SER:HG	1:B:552:TRP:CD1	2.33	0.46
1:B:609:GLU:O	1:B:613:ARG:N	2.46	0.46
1:B:659:THR:O	1:B:660:SER:C	2.56	0.46
1:C:140:ARG:NH1	1:C:141:PHE:HE1	2.14	0.46
1:C:180:ASP:C	1:C:182:ILE:N	2.62	0.46
1:C:391:ILE:HG23	1:C:398:ILE:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:LYS:HD2	1:C:741:ILE:CG2	2.45	0.46
1:C:729:TYR:HB2	1:C:756:ILE:HG21	1.96	0.46
1:D:663:PHE:O	1:D:664:ILE:C	2.58	0.46
1:D:665:LYS:HE2	2:R:11:GLU:OE2	2.16	0.46
1:E:308:VAL:O	1:E:311:HIS:N	2.43	0.46
1:E:326:ILE:CG2	1:E:328:PHE:CE1	2.99	0.46
1:E:339:ILE:O	1:E:342:GLY:N	2.48	0.46
1:E:636:ALA:O	1:E:640:LYS:N	2.47	0.46
1:E:715:GLU:OE1	1:E:767:GLN:NE2	2.47	0.46
1:F:140:ARG:NH1	1:F:141:PHE:HE1	2.14	0.46
1:F:173:ILE:HD12	1:F:243:LEU:HD21	1.97	0.46
1:F:300:LYS:O	1:F:303:LYS:HB2	2.15	0.46
1:F:730:ASN:O	1:F:732:ILE:N	2.49	0.46
2:P:11:GLU:C	2:P:13:LYS:N	2.73	0.46
1:A:659:THR:O	1:A:660:SER:C	2.58	0.46
1:B:123:GLU:HG2	1:B:124:GLU:H	1.80	0.46
1:B:427:ASP:C	1:B:429:GLY:H	2.24	0.46
1:B:552:TRP:HA	1:B:555:GLN:HG2	1.96	0.46
1:C:437:SER:O	1:C:439:ASN:N	2.42	0.46
1:C:443:GLU:HG3	1:C:458:LYS:HE3	1.97	0.46
1:D:133:GLU:OE1	1:D:134:LYS:N	2.49	0.46
1:D:208:LEU:H	1:D:208:LEU:HD12	1.80	0.46
1:D:334:LEU:H	1:D:334:LEU:CD1	2.28	0.46
1:D:501:LEU:HB2	1:D:623:ASP:O	2.16	0.46
1:E:140:ARG:NH1	1:E:141:PHE:HE1	2.14	0.46
1:E:185:ASP:O	1:E:190:PRO:HG3	2.16	0.46
1:E:319:ALA:O	1:E:323:ASN:HA	2.15	0.46
1:F:169:VAL:O	1:F:172:GLU:HB2	2.15	0.46
1:F:311:HIS:CD2	1:F:564:VAL:HB	2.51	0.46
2:P:49:GLN:HA	2:P:52:ILE:HG22	1.96	0.46
2:T:81:SER:O	2:T:82:GLU:C	2.59	0.46
1:A:257:LEU:O	1:A:261:ALA:O	2.33	0.46
1:A:716:LYS:O	1:A:720:ILE:HG22	2.16	0.46
1:A:724:ARG:HG3	1:A:724:ARG:NH1	2.27	0.46
1:B:100:LEU:CD1	1:B:182:ILE:HG21	2.45	0.46
1:B:505:LYS:HE3	1:B:513:TRP:CD2	2.51	0.46
1:B:691:LYS:O	1:B:692:GLU:C	2.59	0.46
1:C:89:ILE:HG22	1:C:90:PRO:HD2	1.97	0.46
1:C:133:GLU:OE1	1:C:134:LYS:N	2.49	0.46
1:C:161:ILE:HG23	1:C:168:GLU:HB2	1.97	0.46
1:C:323:ASN:C	1:C:324:THR:CG2	2.88	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:LYS:O	1:C:432:TYR:CD2	2.68	0.46
1:C:504:ILE:HD12	1:C:504:ILE:N	2.30	0.46
1:D:140:ARG:NH1	1:D:141:PHE:HE1	2.14	0.46
1:D:620:THR:HG22	1:D:621:GLY:N	2.31	0.46
1:E:699:GLY:O	1:E:700:TYR:C	2.58	0.46
1:E:729:TYR:HB2	1:E:756:ILE:HG21	1.97	0.46
1:E:743:PRO:HA	1:E:746:LYS:CB	2.46	0.46
1:F:306:GLY:O	1:F:336:THR:HG23	2.14	0.46
1:F:546:LYS:NZ	1:F:554:LYS:HE2	2.30	0.46
1:F:555:GLN:HG3	1:F:556:MET:N	2.30	0.46
1:F:743:PRO:O	1:F:746:LYS:N	2.48	0.46
2:O:39:LEU:HD23	2:O:39:LEU:HA	1.84	0.46
2:O:49:GLN:HA	2:O:52:ILE:HG22	1.96	0.46
2:O:81:SER:O	2:O:82:GLU:C	2.59	0.46
2:O:138:TYR:CZ	2:O:142:VAL:HG21	2.51	0.46
2:P:58:ASP:HB3	2:P:62:THR:CG2	2.44	0.46
2:Q:97:ASN:HD22	2:Q:98:GLY:N	2.13	0.46
2:Q:111:ASN:C	2:Q:113:GLY:N	2.73	0.46
2:T:11:GLU:C	2:T:13:LYS:N	2.71	0.46
1:B:76:LEU:H	1:B:76:LEU:CD2	2.27	0.46
1:B:140:ARG:NH1	1:B:141:PHE:HE1	2.13	0.46
1:B:185:ASP:O	1:B:190:PRO:CD	2.64	0.46
1:B:514:ASP:C	1:B:516:VAL:N	2.73	0.46
1:B:609:GLU:OE2	1:B:609:GLU:N	2.36	0.46
1:C:148:GLU:CG	1:C:149:THR:N	2.73	0.46
1:C:323:ASN:ND2	1:C:598:PRO:CB	2.79	0.46
1:C:690:LYS:HD3	1:C:741:ILE:HG23	1.97	0.46
1:D:152:LEU:CD2	1:D:154:ILE:HG12	2.46	0.46
1:D:580:GLU:C	1:D:582:ASP:H	2.23	0.46
1:D:743:PRO:HA	1:D:746:LYS:CB	2.45	0.46
1:E:133:GLU:OE1	1:E:134:LYS:N	2.49	0.46
1:E:173:ILE:HD12	1:E:243:LEU:HD21	1.97	0.46
1:E:236:GLU:HA	1:E:239:HIS:HD2	1.74	0.46
1:E:323:ASN:C	1:E:323:ASN:ND2	2.73	0.46
1:E:564:VAL:C	1:E:567:THR:HG22	2.40	0.46
1:F:236:GLU:HA	1:F:239:HIS:HD2	1.75	0.46
1:F:244:ALA:CB	1:F:268:MET:HE3	2.46	0.46
1:F:323:ASN:C	1:F:324:THR:CG2	2.88	0.46
1:F:323:ASN:ND2	1:F:598:PRO:CB	2.79	0.46
1:F:376:GLN:C	1:F:378:LEU:N	2.72	0.46
2:O:3:GLN:N	2:O:77:LYS:NZ	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:73:ALA:O	2:O:75:LYS:N	2.48	0.46
2:R:25:GLY:HA3	2:R:65:PHE:CZ	2.51	0.46
1:A:244:ALA:CB	1:A:268:MET:HE3	2.45	0.46
1:A:480:ASN:HD22	1:A:480:ASN:C	2.23	0.46
1:A:567:THR:CG2	1:A:568:GLY:N	2.79	0.46
1:A:746:LYS:CD	1:A:750:GLN:HE21	2.29	0.46
1:A:749:PHE:O	1:A:750:GLN:C	2.56	0.46
1:A:765:THR:HG22	1:A:769:SER:HB2	1.97	0.46
1:B:133:GLU:OE1	1:B:134:LYS:N	2.49	0.46
1:B:288:VAL:C	1:B:290:LYS:N	2.72	0.46
1:B:699:GLY:O	1:B:700:TYR:C	2.58	0.46
1:C:319:ALA:O	1:C:323:ASN:HA	2.15	0.46
1:C:339:ILE:O	1:C:342:GLY:N	2.48	0.46
1:C:659:THR:O	1:C:660:SER:C	2.57	0.46
1:C:797:ILE:O	1:C:798:ASP:OD1	2.32	0.46
1:D:191:GLU:C	1:D:193:LEU:N	2.74	0.46
1:D:220:LEU:HG	1:D:223:LYS:HB2	1.97	0.46
1:D:514:ASP:C	1:D:516:VAL:N	2.71	0.46
1:D:735:VAL:O	1:D:738:SER:HB3	2.16	0.46
1:D:743:PRO:O	1:D:744:GLU:C	2.59	0.46
1:D:749:PHE:O	1:D:750:GLN:C	2.57	0.46
1:E:102:GLY:HA2	1:E:150:PRO:O	2.16	0.46
1:E:472:ARG:HB3	1:E:472:ARG:HH11	1.81	0.46
2:R:39:LEU:HD23	2:R:39:LEU:HA	1.86	0.46
2:T:3:GLN:N	2:T:77:LYS:HD3	2.31	0.46
1:A:220:LEU:HG	1:A:223:LYS:HB2	1.97	0.45
1:A:256:VAL:O	1:A:260:TYR:HB2	2.16	0.45
1:A:327:LEU:HG	1:A:595:ILE:HG23	1.98	0.45
1:A:609:GLU:O	1:A:613:ARG:N	2.48	0.45
1:B:185:ASP:O	1:B:190:PRO:CG	2.64	0.45
1:B:509:PRO:O	1:B:511:LYS:N	2.49	0.45
1:C:79:ILE:O	1:C:81:GLN:N	2.50	0.45
1:C:88:LYS:NZ	1:C:172:GLU:CD	2.74	0.45
1:C:743:PRO:O	1:C:744:GLU:C	2.59	0.45
1:D:244:ALA:CB	1:D:268:MET:HE3	2.45	0.45
1:D:288:VAL:CG2	1:D:289:GLU:N	2.75	0.45
1:D:323:ASN:C	1:D:324:THR:CG2	2.89	0.45
1:D:756:ILE:O	1:D:760:VAL:HG23	2.16	0.45
1:E:137:PHE:O	1:E:140:ARG:HB2	2.16	0.45
1:E:152:LEU:CD2	1:E:154:ILE:HG12	2.46	0.45
1:E:256:VAL:O	1:E:260:TYR:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:609:GLU:O	1:E:610:MET:C	2.58	0.45
1:E:633:ASN:O	1:E:642:TYR:HE1	1.99	0.45
1:F:326:ILE:CG2	1:F:328:PHE:CE1	2.99	0.45
1:F:368:GLN:OE1	1:F:368:GLN:HA	2.15	0.45
1:F:443:GLU:HG3	1:F:458:LYS:HE3	1.97	0.45
1:F:659:THR:O	1:F:660:SER:C	2.58	0.45
2:P:109:MET:HG3	2:P:116:LEU:HD11	1.97	0.45
2:Q:138:TYR:CZ	2:Q:142:VAL:CG2	2.99	0.45
2:S:25:GLY:HA3	2:S:65:PHE:CZ	2.51	0.45
2:T:114:GLU:HA	2:T:114:GLU:OE2	2.16	0.45
1:A:77:ASP:O	1:A:81:GLN:HB2	2.16	0.45
1:A:197:LYS:HD3	1:A:263:ASP:CB	2.44	0.45
1:B:161:ILE:O	1:B:165:GLN:HA	2.17	0.45
1:B:480:ASN:HD22	1:B:480:ASN:C	2.24	0.45
1:B:713:SER:O	1:B:714:GLN:C	2.58	0.45
1:C:185:ASP:O	1:C:190:PRO:CA	2.64	0.45
1:C:730:ASN:O	1:C:732:ILE:N	2.49	0.45
1:D:443:GLU:HG3	1:D:458:LYS:HE3	1.98	0.45
1:D:735:VAL:HA	1:D:738:SER:HB2	1.98	0.45
1:E:184:LYS:HE2	1:E:193:LEU:HD12	1.98	0.45
1:E:501:LEU:HD22	2:S:112:LEU:CD2	2.46	0.45
1:E:505:LYS:HE3	1:E:513:TRP:CD2	2.51	0.45
1:E:621:GLY:HA2	2:S:94:LYS:NZ	2.30	0.45
1:F:217:LYS:HZ2	1:F:236:GLU:HB2	1.80	0.45
1:F:515:LYS:HB3	1:F:515:LYS:HZ3	1.80	0.45
1:F:674:SER:C	1:F:676:VAL:H	2.23	0.45
2:O:89:PHE:O	2:O:90:ARG:C	2.58	0.45
2:O:102:ALA:CB	2:O:125:ILE:HG13	2.47	0.45
2:P:6:GLU:O	2:P:9:ILE:HB	2.16	0.45
2:R:114:GLU:OE2	2:R:114:GLU:HA	2.15	0.45
2:T:25:GLY:HA3	2:T:65:PHE:CZ	2.51	0.45
2:T:138:TYR:CZ	2:T:142:VAL:HG21	2.51	0.45
1:A:130:SER:O	1:A:131:ARG:C	2.60	0.45
1:A:325:TYR:CD1	1:A:598:PRO:HD3	2.51	0.45
1:A:678:VAL:HG13	1:A:745:TYR:CD2	2.52	0.45
1:B:137:PHE:O	1:B:140:ARG:HB2	2.17	0.45
1:B:164:GLU:HG2	1:B:166:SER:HB3	1.97	0.45
1:B:192:PHE:HB3	1:B:196:ILE:CD1	2.46	0.45
1:B:567:THR:CG2	1:B:568:GLY:N	2.80	0.45
1:B:629:ASN:HD22	1:B:630:ARG:N	2.14	0.45
1:B:674:SER:C	1:B:676:VAL:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLY:O	1:C:180:ASP:OD1	2.34	0.45
1:C:334:LEU:H	1:C:334:LEU:CD1	2.28	0.45
1:C:523:LEU:HD22	2:Q:127:GLU:HG2	1.99	0.45
1:C:633:ASN:O	1:C:642:TYR:HE1	1.98	0.45
1:C:670:ILE:CG2	1:C:744:GLU:HB2	2.46	0.45
1:C:706:ASN:O	2:Q:130:ILE:HG23	2.17	0.45
1:C:756:ILE:O	1:C:760:VAL:HG23	2.16	0.45
1:D:88:LYS:NZ	1:D:172:GLU:CD	2.74	0.45
1:D:197:LYS:HD3	1:D:263:ASP:CB	2.45	0.45
1:D:509:PRO:O	1:D:511:LYS:N	2.49	0.45
1:D:566:TYR:N	1:D:566:TYR:CD2	2.84	0.45
1:E:505:LYS:C	1:E:507:GLN:N	2.69	0.45
1:E:523:LEU:HD22	2:S:127:GLU:CD	2.41	0.45
1:E:743:PRO:O	1:E:744:GLU:C	2.59	0.45
1:F:462:ILE:CG1	1:F:463:THR:N	2.78	0.45
2:O:65:PHE:H	2:O:65:PHE:HD1	1.65	0.45
2:Q:6:GLU:O	2:Q:9:ILE:HB	2.16	0.45
2:Q:27:ILE:HD12	2:Q:32:LEU:HA	1.97	0.45
2:R:102:ALA:CB	2:R:125:ILE:HG13	2.46	0.45
2:R:138:TYR:O	2:R:142:VAL:HG23	2.17	0.45
1:A:597:ASN:O	1:A:599:GLU:N	2.48	0.45
1:B:90:PRO:HD3	1:B:249:PHE:CE2	2.51	0.45
1:B:197:LYS:HD3	1:B:263:ASP:CB	2.44	0.45
1:B:217:LYS:CG	1:B:236:GLU:HG3	2.44	0.45
1:B:243:LEU:HA	1:B:246:SER:OG	2.16	0.45
1:B:322:LEU:HD13	1:B:556:MET:CE	2.44	0.45
1:B:683:GLY:O	1:B:684:ASP:C	2.60	0.45
1:C:102:GLY:HA2	1:C:150:PRO:O	2.17	0.45
1:C:173:ILE:HG23	1:C:174:GLY:N	2.32	0.45
1:C:609:GLU:O	1:C:610:MET:C	2.57	0.45
1:C:620:THR:HG22	1:C:621:GLY:N	2.31	0.45
1:E:240:ALA:O	1:E:241:PHE:C	2.60	0.45
1:E:243:LEU:HA	1:E:246:SER:OG	2.16	0.45
1:F:89:ILE:HG22	1:F:90:PRO:HD2	1.98	0.45
1:F:223:LYS:HD3	1:F:224:SER:H	1.77	0.45
1:F:243:LEU:HA	1:F:246:SER:OG	2.16	0.45
2:P:25:GLY:HA3	2:P:65:PHE:CZ	2.51	0.45
2:P:138:TYR:CZ	2:P:142:VAL:CG2	2.99	0.45
2:Q:55:VAL:CG2	2:Q:67:GLU:OE1	2.64	0.45
2:T:65:PHE:H	2:T:65:PHE:HD1	1.65	0.45
1:A:391:ILE:O	1:A:392:THR:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASP:C	1:A:516:VAL:N	2.73	0.45
1:B:225:ILE:HG23	1:B:229:PHE:CE2	2.51	0.45
1:B:472:ARG:HB3	1:B:472:ARG:HH11	1.80	0.45
1:B:743:PRO:HA	1:B:746:LYS:CB	2.46	0.45
1:C:179:LEU:HA	1:C:182:ILE:HG22	1.98	0.45
1:C:275:GLY:CA	1:C:278:LYS:HE2	2.47	0.45
1:C:324:THR:CB	1:C:499:PRO:HA	2.40	0.45
1:C:458:LYS:C	1:C:460:GLY:H	2.25	0.45
1:C:580:GLU:C	1:C:582:ASP:H	2.24	0.45
1:C:581:GLN:HE21	1:C:629:ASN:H	1.63	0.45
1:C:746:LYS:CD	1:C:750:GLN:HE21	2.30	0.45
1:D:79:ILE:O	1:D:81:GLN:N	2.50	0.45
1:D:243:LEU:HA	1:D:246:SER:OG	2.16	0.45
1:D:461:LYS:HD2	1:D:461:LYS:HA	1.79	0.45
1:D:670:ILE:CG2	1:D:744:GLU:HB2	2.47	0.45
1:E:275:GLY:CA	1:E:278:LYS:HE2	2.47	0.45
1:E:756:ILE:O	1:E:760:VAL:HG23	2.16	0.45
1:F:187:SER:O	1:F:188:LEU:C	2.51	0.45
1:F:678:VAL:HG13	1:F:745:TYR:CD2	2.51	0.45
1:F:743:PRO:O	1:F:744:GLU:C	2.59	0.45
2:P:138:TYR:O	2:P:142:VAL:HG23	2.17	0.45
2:Q:81:SER:O	2:Q:82:GLU:C	2.59	0.45
2:S:39:LEU:HD23	2:S:39:LEU:HA	1.84	0.45
2:T:73:ALA:O	2:T:75:LYS:N	2.50	0.45
1:A:85:LEU:HD12	1:A:168:GLU:OE1	2.17	0.45
1:A:133:GLU:OE1	1:A:134:LYS:N	2.49	0.45
1:A:501:LEU:HD22	2:O:112:LEU:CD2	2.46	0.45
1:A:514:ASP:O	1:A:516:VAL:N	2.50	0.45
1:A:743:PRO:HA	1:A:746:LYS:CB	2.47	0.45
1:B:88:LYS:NZ	1:B:172:GLU:OE1	2.49	0.45
1:B:323:ASN:C	1:B:323:ASN:ND2	2.72	0.45
1:B:580:GLU:C	1:B:582:ASP:H	2.23	0.45
1:B:604:LEU:HG	1:B:605:THR:O	2.17	0.45
1:C:88:LYS:NZ	1:C:172:GLU:OE1	2.50	0.45
1:C:164:GLU:HG2	1:C:166:SER:HB3	1.98	0.45
1:C:195:LEU:CD1	1:C:230:ILE:HG21	2.46	0.45
1:D:148:GLU:CG	1:D:149:THR:N	2.73	0.45
1:D:365:PRO:HB2	1:D:367:ASP:O	2.17	0.45
1:D:735:VAL:O	1:D:738:SER:CB	2.65	0.45
1:E:192:PHE:HB3	1:E:196:ILE:CD1	2.47	0.45
1:E:372:LYS:HG3	1:E:373:LYS:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:LYS:NZ	1:F:117:LEU:HB2	2.32	0.45
1:F:133:GLU:OE1	1:F:134:LYS:N	2.49	0.45
1:F:192:PHE:H	1:F:192:PHE:HD1	1.65	0.45
1:F:349:ASN:HD22	1:F:350:VAL:N	2.15	0.45
1:F:609:GLU:O	1:F:613:ARG:N	2.48	0.45
1:F:639:ASN:C	1:F:639:ASN:ND2	2.75	0.45
1:F:690:LYS:HD3	1:F:741:ILE:HG23	1.97	0.45
2:O:5:THR:O	2:O:6:GLU:C	2.60	0.45
2:O:25:GLY:HA3	2:O:65:PHE:CZ	2.51	0.45
2:O:58:ASP:HB3	2:O:62:THR:CG2	2.43	0.45
2:O:58:ASP:O	2:O:60:ASN:N	2.49	0.45
2:P:8:GLN:O	2:P:12:PHE:HD2	2.00	0.45
2:R:3:GLN:N	2:R:77:LYS:HD3	2.31	0.45
2:R:27:ILE:HD12	2:R:32:LEU:HA	1.98	0.45
2:R:81:SER:O	2:R:82:GLU:C	2.59	0.45
1:A:102:GLY:HA2	1:A:150:PRO:O	2.17	0.45
1:A:365:PRO:HB2	1:A:367:ASP:O	2.17	0.45
1:A:493:ASP:OD2	1:A:577:HIS:CE1	2.70	0.45
1:A:580:GLU:C	1:A:582:ASP:H	2.23	0.45
1:A:729:TYR:HB2	1:A:756:ILE:HG21	1.97	0.45
1:B:77:ASP:O	1:B:81:GLN:HB2	2.17	0.45
1:B:332:ASN:OD1	1:B:334:LEU:N	2.47	0.45
1:B:555:GLN:HG3	1:B:556:MET:N	2.31	0.45
1:B:597:ASN:CB	1:B:598:PRO:HD2	2.46	0.45
1:B:620:THR:HG22	1:B:621:GLY:N	2.31	0.45
1:B:743:PRO:O	1:B:744:GLU:C	2.60	0.45
1:C:152:LEU:CD2	1:C:154:ILE:HG12	2.46	0.45
1:C:443:GLU:O	1:C:455:TYR:HA	2.16	0.45
1:D:480:ASN:C	1:D:480:ASN:ND2	2.75	0.45
1:D:595:ILE:CG2	1:D:596:ILE:N	2.79	0.45
1:D:639:ASN:C	1:D:639:ASN:ND2	2.75	0.45
1:D:719:LYS:O	1:D:720:ILE:C	2.60	0.45
1:E:180:ASP:CG	1:E:181:ILE:N	2.67	0.45
1:E:189:ASP:O	1:E:190:PRO:C	2.59	0.45
1:E:621:GLY:HA2	2:S:94:LYS:HZ3	1.82	0.45
1:E:671:ARG:HD2	2:S:14:GLU:HG2	1.99	0.45
1:E:749:PHE:O	1:E:750:GLN:C	2.56	0.45
1:E:764:LEU:C	1:E:766:HIS:N	2.75	0.45
1:F:319:ALA:O	1:F:323:ASN:HA	2.15	0.45
1:F:384:ASN:C	1:F:386:GLU:H	2.23	0.45
1:F:567:THR:HG23	1:F:568:GLY:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:756:ILE:O	1:F:760:VAL:HG23	2.16	0.45
2:P:65:PHE:H	2:P:65:PHE:HD1	1.65	0.45
2:Q:58:ASP:HB3	2:Q:62:THR:CG2	2.43	0.45
2:S:138:TYR:CZ	2:S:142:VAL:HG21	2.52	0.45
2:T:109:MET:HG3	2:T:116:LEU:HD11	1.98	0.45
1:A:100:LEU:CD1	1:A:182:ILE:HG21	2.47	0.45
1:A:243:LEU:HA	1:A:246:SER:OG	2.16	0.45
1:A:372:LYS:HG3	1:A:373:LYS:N	2.32	0.45
1:A:549:LEU:HB3	1:A:578:GLY:HA3	1.99	0.45
1:A:719:LYS:O	1:A:720:ILE:C	2.60	0.45
1:A:722:ILE:HD13	1:A:764:LEU:HD21	1.99	0.45
1:A:743:PRO:O	1:A:744:GLU:C	2.60	0.45
1:B:501:LEU:HD22	2:P:112:LEU:CD2	2.47	0.45
1:B:566:TYR:N	1:B:566:TYR:CD2	2.85	0.45
1:B:639:ASN:C	1:B:639:ASN:ND2	2.74	0.45
1:B:665:LYS:HE2	2:P:11:GLU:CD	2.41	0.45
1:B:749:PHE:O	1:B:750:GLN:C	2.57	0.45
1:C:279:ILE:CD1	1:C:279:ILE:H	2.28	0.45
1:C:327:LEU:HG	1:C:595:ILE:HG12	1.98	0.45
1:C:486:LYS:HE3	1:C:570:THR:O	2.17	0.45
1:C:699:GLY:O	1:C:700:TYR:C	2.59	0.45
1:D:195:LEU:CD1	1:D:230:ILE:HG21	2.47	0.45
1:D:372:LYS:HG3	1:D:373:LYS:N	2.32	0.45
1:D:691:LYS:O	1:D:692:GLU:C	2.58	0.45
1:E:77:ASP:O	1:E:81:GLN:HB2	2.17	0.45
1:E:197:LYS:HD3	1:E:263:ASP:CB	2.44	0.45
1:E:567:THR:HG23	1:E:568:GLY:N	2.31	0.45
1:E:671:ARG:NH1	1:E:671:ARG:HG3	2.32	0.45
1:F:131:ARG:HB2	1:F:170:TYR:CE2	2.52	0.45
1:F:152:LEU:CD2	1:F:154:ILE:HG12	2.46	0.45
1:F:270:LYS:O	1:F:273:LYS:HB2	2.16	0.45
1:F:325:TYR:HB2	1:F:498:ALA:HB3	1.99	0.45
1:F:706:ASN:O	2:T:130:ILE:HG23	2.17	0.45
2:Q:28:THR:HB	2:Q:30:LYS:HZ3	1.82	0.45
2:T:5:THR:O	2:T:6:GLU:C	2.60	0.45
2:T:6:GLU:O	2:T:9:ILE:HB	2.16	0.45
1:A:76:LEU:H	1:A:76:LEU:HD22	1.82	0.45
1:A:192:PHE:HB3	1:A:196:ILE:CD1	2.46	0.45
1:A:443:GLU:O	1:A:455:TYR:HA	2.17	0.45
1:A:446:ILE:HA	1:A:453:VAL:HA	1.98	0.45
1:A:523:LEU:HD22	2:O:127:GLU:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HB2	1:B:183:SER:HB2	1.98	0.45
1:B:324:THR:CB	1:B:499:PRO:HA	2.41	0.45
1:B:725:GLY:O	1:B:728:ALA:HB3	2.17	0.45
1:B:759:GLN:HA	1:B:759:GLN:NE2	2.20	0.45
1:C:288:VAL:CG2	1:C:289:GLU:N	2.75	0.45
1:C:368:GLN:C	1:C:370:LEU:H	2.24	0.45
1:C:567:THR:CG2	1:C:568:GLY:N	2.80	0.45
1:D:102:GLY:HA2	1:D:150:PRO:O	2.16	0.45
1:D:414:LYS:O	1:D:417:GLY:N	2.40	0.45
1:D:604:LEU:HG	1:D:605:THR:O	2.17	0.45
1:D:716:LYS:O	1:D:720:ILE:HG22	2.17	0.45
1:E:405:LEU:CD1	1:E:405:LEU:H	2.30	0.45
1:E:493:ASP:OD2	1:E:577:HIS:CE1	2.70	0.45
1:E:515:LYS:HB3	1:E:515:LYS:HZ3	1.82	0.45
1:E:630:ARG:CD	2:S:83:GLU:HG2	2.47	0.45
1:E:670:ILE:CG2	1:E:744:GLU:HB2	2.46	0.45
1:F:153:ILE:C	1:F:154:ILE:HD13	2.42	0.45
1:F:505:LYS:HE3	1:F:513:TRP:CD2	2.52	0.45
1:F:580:GLU:C	1:F:582:ASP:H	2.23	0.45
2:Q:39:LEU:HD23	2:Q:39:LEU:HA	1.85	0.45
2:R:94:LYS:NZ	2:R:94:LYS:HB3	2.31	0.45
2:S:3:GLN:N	2:S:77:LYS:HD3	2.31	0.45
2:T:111:ASN:C	2:T:113:GLY:N	2.73	0.45
1:A:458:LYS:C	1:A:460:GLY:H	2.25	0.45
1:A:639:ASN:C	1:A:639:ASN:ND2	2.75	0.45
1:A:665:LYS:HE2	2:O:11:GLU:OE2	2.17	0.45
1:B:368:GLN:HG3	1:B:384:ASN:N	2.32	0.45
1:B:372:LYS:HG3	1:B:373:LYS:N	2.32	0.45
1:B:480:ASN:HD21	1:B:483:GLY:CA	2.29	0.45
1:B:678:VAL:HG13	1:B:745:TYR:CD2	2.52	0.45
1:C:236:GLU:HA	1:C:239:HIS:HD2	1.75	0.45
1:D:368:GLN:HG3	1:D:384:ASN:N	2.32	0.45
1:D:529:VAL:O	1:D:532:LEU:N	2.49	0.45
1:E:567:THR:CG2	1:E:568:GLY:N	2.80	0.45
1:F:405:LEU:CD1	1:F:405:LEU:H	2.30	0.45
1:F:567:THR:CG2	1:F:568:GLY:N	2.79	0.45
1:F:610:MET:O	1:F:614:PHE:N	2.43	0.45
1:F:620:THR:HG22	1:F:621:GLY:N	2.32	0.45
2:O:111:ASN:C	2:O:113:GLY:N	2.73	0.45
2:P:3:GLN:N	2:P:77:LYS:HD3	2.32	0.45
2:Q:58:ASP:O	2:Q:60:ASN:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:65:PHE:H	2:Q:65:PHE:HD1	1.65	0.45
2:S:6:GLU:O	2:S:9:ILE:HB	2.17	0.45
1:A:509:PRO:O	1:A:511:LYS:N	2.50	0.44
1:A:566:TYR:N	1:A:566:TYR:CD2	2.84	0.44
1:A:604:LEU:HG	1:A:605:THR:O	2.17	0.44
1:A:722:ILE:HD13	1:A:764:LEU:HD23	1.99	0.44
1:B:323:ASN:C	1:B:324:THR:HG22	2.42	0.44
1:B:337:ASN:C	1:B:339:ILE:N	2.75	0.44
1:B:567:THR:HG23	1:B:568:GLY:N	2.31	0.44
1:C:120:LEU:HD13	1:C:120:LEU:O	2.06	0.44
1:C:137:PHE:O	1:C:140:ARG:HB2	2.16	0.44
1:C:376:GLN:C	1:C:378:LEU:N	2.71	0.44
1:C:509:PRO:O	1:C:511:LYS:N	2.50	0.44
1:C:629:ASN:HD22	1:C:630:ARG:N	2.15	0.44
1:C:759:GLN:HA	1:C:759:GLN:NE2	2.19	0.44
1:D:135:VAL:N	1:D:136:PRO:CD	2.81	0.44
1:D:391:ILE:O	1:D:392:THR:C	2.60	0.44
1:E:76:LEU:CD2	1:E:76:LEU:H	2.29	0.44
1:E:349:ASN:HD22	1:E:350:VAL:N	2.15	0.44
1:E:443:GLU:HG3	1:E:458:LYS:HE3	1.97	0.44
1:E:509:PRO:O	1:E:511:LYS:N	2.50	0.44
1:E:566:TYR:CD2	1:E:566:TYR:N	2.84	0.44
1:E:610:MET:O	1:E:614:PHE:N	2.44	0.44
1:F:137:PHE:O	1:F:140:ARG:HB2	2.17	0.44
1:F:192:PHE:HB3	1:F:196:ILE:CD1	2.47	0.44
1:F:504:ILE:HD12	1:F:504:ILE:N	2.32	0.44
1:F:529:VAL:O	1:F:532:LEU:N	2.50	0.44
2:O:3:GLN:N	2:O:77:LYS:HD3	2.32	0.44
2:O:13:LYS:HZ1	2:O:65:PHE:HB3	1.79	0.44
2:R:92:PHE:C	2:R:94:LYS:N	2.75	0.44
2:R:109:MET:HG3	2:R:116:LEU:HD11	1.99	0.44
1:A:349:ASN:HD22	1:A:350:VAL:N	2.15	0.44
1:A:677:GLY:HA2	1:A:745:TYR:OH	2.16	0.44
1:B:135:VAL:N	1:B:136:PRO:CD	2.81	0.44
1:B:690:LYS:CD	1:B:741:ILE:HG23	2.47	0.44
1:C:192:PHE:HB3	1:C:196:ILE:CD1	2.47	0.44
1:C:306:GLY:O	1:C:336:THR:HG23	2.17	0.44
1:C:457:THR:CG2	1:C:468:LYS:HA	2.42	0.44
1:C:719:LYS:O	1:C:720:ILE:C	2.59	0.44
1:D:115:LYS:HZ1	1:D:117:LEU:HB2	1.82	0.44
1:D:161:ILE:HG23	1:D:168:GLU:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ASN:HD22	1:D:350:VAL:N	2.15	0.44
1:D:610:MET:O	1:D:614:PHE:N	2.44	0.44
1:E:295:VAL:HG21	1:E:603:ILE:CG2	2.47	0.44
1:F:372:LYS:HG3	1:F:373:LYS:N	2.32	0.44
1:F:457:THR:CG2	1:F:468:LYS:HA	2.43	0.44
1:F:458:LYS:C	1:F:460:GLY:H	2.25	0.44
1:F:564:VAL:C	1:F:567:THR:HG22	2.41	0.44
1:F:677:GLY:HA2	1:F:745:TYR:OH	2.17	0.44
2:P:81:SER:O	2:P:82:GLU:C	2.60	0.44
2:Q:5:THR:O	2:Q:6:GLU:C	2.61	0.44
2:Q:89:PHE:O	2:Q:90:ARG:C	2.59	0.44
2:R:65:PHE:H	2:R:65:PHE:HD1	1.65	0.44
2:S:11:GLU:C	2:S:13:LYS:N	2.74	0.44
1:A:137:PHE:O	1:A:140:ARG:HB2	2.17	0.44
1:A:450:ASN:O	1:A:452:GLU:N	2.48	0.44
1:A:690:LYS:CD	1:A:741:ILE:HG23	2.47	0.44
1:B:102:GLY:HA2	1:B:150:PRO:O	2.17	0.44
1:B:192:PHE:HD1	1:B:192:PHE:H	1.65	0.44
1:B:729:TYR:HB2	1:B:756:ILE:HG21	1.99	0.44
1:C:372:LYS:HG3	1:C:373:LYS:N	2.32	0.44
1:C:447:SER:OG	1:C:448:ASP:N	2.46	0.44
1:C:610:MET:O	1:C:614:PHE:N	2.44	0.44
1:C:716:LYS:O	1:C:720:ILE:HG22	2.17	0.44
1:C:723:PHE:O	1:C:724:ARG:C	2.60	0.44
1:D:185:ASP:O	1:D:190:PRO:HD3	2.16	0.44
1:D:270:LYS:O	1:D:273:LYS:HB2	2.18	0.44
1:D:581:GLN:HE21	1:D:629:ASN:H	1.64	0.44
1:E:443:GLU:CG	1:E:458:LYS:HE3	2.47	0.44
1:E:480:ASN:HD21	1:E:483:GLY:CA	2.30	0.44
1:F:622:LYS:HA	1:F:622:LYS:HD3	1.20	0.44
1:F:683:GLY:O	1:F:684:ASP:C	2.59	0.44
1:F:725:GLY:O	1:F:728:ALA:HB3	2.17	0.44
2:O:114:GLU:OE2	2:O:114:GLU:HA	2.17	0.44
2:O:146:THR:O	2:O:148:LYS:N	2.51	0.44
2:P:58:ASP:O	2:P:60:ASN:N	2.50	0.44
2:P:89:PHE:O	2:P:90:ARG:C	2.58	0.44
2:R:110:THR:O	2:R:113:GLY:N	2.47	0.44
2:R:111:ASN:C	2:R:113:GLY:N	2.73	0.44
1:A:71:PHE:HD1	1:A:108:ASP:OD1	2.00	0.44
1:A:480:ASN:HD21	1:A:483:GLY:CA	2.30	0.44
1:B:85:LEU:HD12	1:B:168:GLU:OE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:HG22	1:B:90:PRO:HD2	1.99	0.44
1:B:153:ILE:C	1:B:154:ILE:HD13	2.43	0.44
1:C:140:ARG:NE	1:C:140:ARG:CA	2.78	0.44
1:C:391:ILE:O	1:C:393:GLU:N	2.51	0.44
1:C:579:THR:O	1:C:581:GLN:N	2.51	0.44
1:C:604:LEU:HG	1:C:605:THR:O	2.17	0.44
1:D:240:ALA:O	1:D:241:PHE:C	2.60	0.44
1:D:323:ASN:ND2	1:D:598:PRO:CB	2.81	0.44
1:D:443:GLU:O	1:D:455:TYR:HA	2.18	0.44
1:D:567:THR:HG23	1:D:568:GLY:N	2.32	0.44
1:D:629:ASN:HD22	1:D:630:ARG:N	2.15	0.44
1:D:746:LYS:CD	1:D:750:GLN:HE21	2.30	0.44
1:E:234:LEU:H	1:E:234:LEU:CD2	2.31	0.44
1:E:443:GLU:O	1:E:455:TYR:HA	2.18	0.44
1:E:639:ASN:C	1:E:639:ASN:ND2	2.74	0.44
1:E:683:GLY:O	1:E:684:ASP:C	2.60	0.44
1:E:691:LYS:O	1:E:692:GLU:C	2.59	0.44
1:F:549:LEU:HB3	1:F:578:GLY:HA3	1.99	0.44
2:O:26:THR:HB	2:O:62:THR:OG1	2.18	0.44
2:O:138:TYR:CZ	2:O:142:VAL:CG2	3.00	0.44
2:R:89:PHE:O	2:R:90:ARG:C	2.60	0.44
2:S:65:PHE:H	2:S:65:PHE:HD1	1.66	0.44
1:A:178:SER:OG	1:A:179:LEU:N	2.50	0.44
1:A:546:LYS:NZ	1:A:554:LYS:HE2	2.33	0.44
1:A:579:THR:O	1:A:581:GLN:N	2.51	0.44
1:B:195:LEU:CD1	1:B:230:ILE:HG21	2.48	0.44
1:B:240:ALA:O	1:B:241:PHE:C	2.61	0.44
1:B:443:GLU:CG	1:B:458:LYS:HE3	2.48	0.44
1:B:514:ASP:O	1:B:516:VAL:N	2.51	0.44
1:B:549:LEU:HB3	1:B:578:GLY:HA3	2.00	0.44
1:B:621:GLY:HA2	2:P:94:LYS:HZ3	1.81	0.44
1:B:746:LYS:CD	1:B:750:GLN:HE21	2.30	0.44
1:C:115:LYS:NZ	1:C:117:LEU:HB2	2.33	0.44
1:C:270:LYS:O	1:C:273:LYS:HB2	2.18	0.44
1:C:325:TYR:HB2	1:C:498:ALA:HB3	1.99	0.44
1:C:439:ASN:OD1	1:C:440:GLN:N	2.51	0.44
1:C:567:THR:HG23	1:C:568:GLY:N	2.30	0.44
1:D:275:GLY:CA	1:D:278:LYS:HE2	2.47	0.44
1:D:327:LEU:HG	1:D:595:ILE:HG23	1.99	0.44
1:E:71:PHE:HD1	1:E:108:ASP:OD1	2.00	0.44
1:E:323:ASN:ND2	1:E:598:PRO:CB	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:LYS:HA	1:E:461:LYS:HD2	1.79	0.44
1:E:514:ASP:O	1:E:516:VAL:N	2.50	0.44
1:F:169:VAL:CG2	1:F:246:SER:HB2	2.48	0.44
1:F:195:LEU:CD1	1:F:230:ILE:HG21	2.48	0.44
1:F:368:GLN:HG3	1:F:384:ASN:N	2.31	0.44
2:P:102:ALA:CB	2:P:125:ILE:HG13	2.48	0.44
2:Q:26:THR:HB	2:Q:62:THR:OG1	2.17	0.44
2:R:3:GLN:N	2:R:77:LYS:NZ	2.60	0.44
2:R:138:TYR:CZ	2:R:142:VAL:CG2	3.00	0.44
2:T:94:LYS:HB3	2:T:94:LYS:NZ	2.31	0.44
2:T:138:TYR:CZ	2:T:142:VAL:CG2	3.01	0.44
1:A:135:VAL:N	1:A:136:PRO:CD	2.81	0.44
1:A:195:LEU:CD1	1:A:230:ILE:HG21	2.48	0.44
1:A:270:LYS:O	1:A:273:LYS:HB2	2.18	0.44
1:A:522:SER:O	2:O:124:MET:HE2	2.17	0.44
1:B:256:VAL:O	1:B:260:TYR:HB2	2.18	0.44
1:B:257:LEU:O	1:B:261:ALA:O	2.36	0.44
1:B:279:ILE:HD13	1:B:279:ILE:H	1.83	0.44
1:B:405:LEU:CD1	1:B:405:LEU:H	2.31	0.44
1:B:538:ILE:HG21	2:P:87:GLU:HB2	1.99	0.44
1:C:349:ASN:HD22	1:C:350:VAL:N	2.16	0.44
1:C:368:GLN:HG3	1:C:384:ASN:N	2.32	0.44
1:C:691:LYS:O	1:C:692:GLU:C	2.60	0.44
1:D:71:PHE:HD1	1:D:108:ASP:OD1	2.00	0.44
1:D:311:HIS:CD2	1:D:564:VAL:HB	2.53	0.44
1:D:706:ASN:O	2:R:130:ILE:HG23	2.18	0.44
1:D:725:GLY:O	1:D:728:ALA:HB3	2.17	0.44
1:E:135:VAL:N	1:E:136:PRO:CD	2.81	0.44
1:E:217:LYS:HZ2	1:E:236:GLU:HB2	1.81	0.44
1:E:579:THR:O	1:E:581:GLN:N	2.51	0.44
1:E:735:VAL:HA	1:E:738:SER:HB2	2.00	0.44
1:F:97:TYR:O	1:F:100:LEU:N	2.50	0.44
1:F:332:ASN:OD1	1:F:334:LEU:N	2.47	0.44
2:P:146:THR:O	2:P:148:LYS:N	2.51	0.44
2:Q:44:THR:HG23	2:Q:47:GLU:OE2	2.18	0.44
2:Q:109:MET:HG3	2:Q:116:LEU:HD11	2.00	0.44
2:R:26:THR:HB	2:R:62:THR:OG1	2.17	0.44
2:R:97:ASN:HD22	2:R:98:GLY:N	2.15	0.44
2:T:26:THR:HB	2:T:62:THR:OG1	2.18	0.44
2:T:102:ALA:CB	2:T:125:ILE:HG13	2.48	0.44
1:A:184:LYS:NZ	1:A:191:GLU:HG3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:O	1:A:241:PHE:C	2.61	0.44
1:A:327:LEU:HG	1:A:595:ILE:HG12	1.98	0.44
1:A:462:ILE:CG1	1:A:463:THR:N	2.79	0.44
1:A:523:LEU:HD22	2:O:127:GLU:CD	2.43	0.44
1:A:635:ILE:N	1:A:635:ILE:CD1	2.78	0.44
1:B:115:LYS:NZ	1:B:117:LEU:HB2	2.32	0.44
1:B:332:ASN:OD1	1:B:334:LEU:CD1	2.65	0.44
1:B:435:LEU:HG	1:B:446:ILE:HG22	1.99	0.44
1:B:443:GLU:O	1:B:455:TYR:HA	2.18	0.44
1:B:622:LYS:HA	1:B:622:LYS:HD3	1.34	0.44
1:C:135:VAL:N	1:C:136:PRO:CD	2.81	0.44
1:C:240:ALA:O	1:C:241:PHE:C	2.60	0.44
1:C:278:LYS:HB2	1:C:279:ILE:HD13	2.00	0.44
1:C:311:HIS:CD2	1:C:564:VAL:HB	2.52	0.44
1:C:384:ASN:C	1:C:386:GLU:H	2.23	0.44
1:C:462:ILE:CG1	1:C:463:THR:N	2.79	0.44
1:C:715:GLU:OE1	1:C:767:GLN:NE2	2.51	0.44
1:C:725:GLY:O	1:C:728:ALA:HB3	2.17	0.44
1:D:225:ILE:HG12	1:D:229:PHE:CE2	2.51	0.44
1:D:305:SER:C	1:D:307:LEU:H	2.26	0.44
1:D:505:LYS:HE3	1:D:513:TRP:CD2	2.51	0.44
1:D:567:THR:CG2	1:D:568:GLY:N	2.81	0.44
1:D:665:LYS:HE2	2:R:11:GLU:CD	2.43	0.44
1:E:173:ILE:HG23	1:E:174:GLY:N	2.33	0.44
1:E:195:LEU:CD1	1:E:230:ILE:HG21	2.48	0.44
1:E:327:LEU:N	1:E:327:LEU:HD12	2.32	0.44
1:E:368:GLN:HG3	1:E:384:ASN:N	2.32	0.44
1:E:549:LEU:HB3	1:E:578:GLY:HA3	2.00	0.44
1:E:620:THR:HG22	1:E:621:GLY:N	2.31	0.44
1:F:509:PRO:O	1:F:511:LYS:N	2.50	0.44
1:F:743:PRO:HA	1:F:746:LYS:CB	2.46	0.44
1:F:746:LYS:CD	1:F:750:GLN:HE21	2.30	0.44
1:A:169:VAL:CG2	1:A:246:SER:HB2	2.47	0.44
1:A:337:ASN:C	1:A:339:ILE:N	2.75	0.44
1:B:97:TYR:HD2	1:B:102:GLY:HA3	1.83	0.44
1:B:124:GLU:OE2	1:B:129:ASN:ND2	2.51	0.44
1:B:323:ASN:ND2	1:B:598:PRO:CB	2.81	0.44
1:B:326:ILE:CG2	1:B:328:PHE:CE1	3.00	0.44
1:B:458:LYS:C	1:B:460:GLY:H	2.25	0.44
1:C:292:ARG:NE	1:C:617:LYS:NZ	2.66	0.44
1:C:391:ILE:O	1:C:392:THR:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:LEU:HB3	1:C:578:GLY:HA3	1.99	0.44
1:D:137:PHE:O	1:D:140:ARG:HB2	2.17	0.44
1:D:179:LEU:HA	1:D:182:ILE:HG22	1.99	0.44
1:D:225:ILE:HG23	1:D:229:PHE:CD2	2.53	0.44
1:D:225:ILE:HG23	1:D:229:PHE:CE2	2.53	0.44
1:D:292:ARG:NE	1:D:617:LYS:NZ	2.66	0.44
1:D:306:GLY:O	1:D:336:THR:HG23	2.17	0.44
1:D:663:PHE:CE1	1:D:752:LEU:HD11	2.53	0.44
1:D:699:GLY:O	1:D:700:TYR:C	2.60	0.44
1:E:91:LYS:O	1:E:94:LEU:HB2	2.17	0.44
1:E:725:GLY:O	1:E:728:ALA:HB3	2.17	0.44
1:F:115:LYS:HZ1	1:F:117:LEU:HB2	1.82	0.44
1:F:364:ILE:O	1:F:365:PRO:C	2.61	0.44
1:F:411:GLU:O	1:F:414:LYS:HB3	2.18	0.44
1:F:462:ILE:CD1	1:F:466:GLY:HA2	2.44	0.44
1:F:480:ASN:HD22	1:F:480:ASN:C	2.24	0.44
1:F:480:ASN:HD21	1:F:483:GLY:CA	2.30	0.44
2:O:44:THR:HG23	2:O:47:GLU:OE2	2.18	0.44
2:Q:8:GLN:O	2:Q:12:PHE:HD2	1.99	0.44
2:Q:13:LYS:NZ	2:Q:65:PHE:CB	2.74	0.44
2:R:58:ASP:O	2:R:60:ASN:N	2.48	0.44
2:S:30:LYS:H	2:S:30:LYS:CD	2.13	0.44
2:T:8:GLN:O	2:T:12:PHE:HD2	2.00	0.44
2:T:55:VAL:CG2	2:T:67:GLU:OE1	2.65	0.44
2:T:97:ASN:HD22	2:T:98:GLY:N	2.16	0.44
1:A:115:LYS:NZ	1:A:117:LEU:HB2	2.33	0.44
1:A:144:GLU:CG	1:A:177:ILE:HD11	2.45	0.44
1:A:391:ILE:O	1:A:393:GLU:N	2.51	0.44
1:A:706:ASN:O	2:O:130:ILE:HG23	2.18	0.44
1:B:173:ILE:HG23	1:B:174:GLY:N	2.33	0.44
1:B:344:ALA:HB3	1:B:488:LEU:HD23	2.00	0.44
1:B:482:GLU:O	1:B:484:VAL:HG23	2.17	0.44
1:C:92:ASP:C	1:C:94:LEU:N	2.75	0.44
1:C:131:ARG:CB	1:C:170:TYR:OH	2.65	0.44
1:C:169:VAL:CG2	1:C:246:SER:HB2	2.48	0.44
1:C:326:ILE:CG2	1:C:328:PHE:CE1	3.01	0.44
1:C:480:ASN:C	1:C:480:ASN:ND2	2.75	0.44
1:C:517:VAL:HG23	1:C:518:ASN:ND2	2.33	0.44
1:C:683:GLY:O	1:C:684:ASP:C	2.61	0.44
1:C:764:LEU:C	1:C:766:HIS:H	2.26	0.44
1:D:501:LEU:HD22	2:R:112:LEU:CD2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:LEU:HB3	1:D:578:GLY:HA3	2.00	0.44
1:D:551:ASN:HD22	1:D:551:ASN:HA	1.58	0.44
1:D:607:ASN:HB2	1:D:610:MET:H	1.83	0.44
1:E:71:PHE:CG	1:E:73:ASN:HB2	2.53	0.44
1:E:746:LYS:CD	1:E:750:GLN:HE21	2.31	0.44
1:F:135:VAL:N	1:F:136:PRO:CD	2.81	0.44
1:F:432:TYR:CD2	1:F:447:SER:HA	2.53	0.44
1:F:443:GLU:O	1:F:455:TYR:HA	2.18	0.44
1:F:614:PHE:CD2	1:F:614:PHE:O	2.71	0.44
1:F:670:ILE:CG2	1:F:744:GLU:HB2	2.47	0.44
2:P:94:LYS:NZ	2:P:94:LYS:HB3	2.32	0.44
2:S:26:THR:HB	2:S:62:THR:OG1	2.18	0.44
2:S:102:ALA:CB	2:S:125:ILE:HG13	2.48	0.44
1:A:173:ILE:HG23	1:A:174:GLY:N	2.33	0.43
1:A:275:GLY:CA	1:A:278:LYS:HE2	2.48	0.43
1:A:343:VAL:HG12	1:A:344:ALA:N	2.33	0.43
1:B:169:VAL:CG2	1:B:246:SER:HB2	2.48	0.43
1:B:234:LEU:H	1:B:234:LEU:CD2	2.31	0.43
1:B:270:LYS:O	1:B:273:LYS:HB2	2.17	0.43
1:B:322:LEU:O	1:B:323:ASN:HB3	2.18	0.43
1:B:391:ILE:O	1:B:392:THR:C	2.61	0.43
1:B:391:ILE:O	1:B:393:GLU:N	2.51	0.43
1:B:461:LYS:HD2	1:B:461:LYS:HA	1.79	0.43
1:B:656:THR:O	1:B:755:ARG:NH1	2.51	0.43
1:C:327:LEU:HD12	1:C:327:LEU:N	2.33	0.43
1:C:482:GLU:O	1:C:484:VAL:HG23	2.18	0.43
1:C:500:SER:OG	1:C:502:THR:OG1	2.34	0.43
1:D:458:LYS:C	1:D:460:GLY:H	2.26	0.43
1:D:683:GLY:O	1:D:684:ASP:C	2.60	0.43
1:E:85:LEU:HD12	1:E:168:GLU:OE1	2.18	0.43
1:E:99:GLU:C	1:E:101:GLY:N	2.68	0.43
1:E:153:ILE:C	1:E:154:ILE:HD13	2.42	0.43
1:E:411:GLU:O	1:E:414:LYS:HB3	2.18	0.43
1:E:517:VAL:HG23	1:E:518:ASN:ND2	2.33	0.43
1:F:71:PHE:CG	1:F:73:ASN:HB2	2.53	0.43
1:F:178:SER:OG	1:F:179:LEU:N	2.48	0.43
1:F:275:GLY:CA	1:F:278:LYS:HE2	2.47	0.43
1:F:665:LYS:HE2	2:T:11:GLU:CD	2.43	0.43
1:F:777:TYR:O	1:F:778:LYS:C	2.61	0.43
2:S:44:THR:HG23	2:S:47:GLU:OE2	2.18	0.43
2:S:109:MET:HG3	2:S:116:LEU:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ALA:HB3	1:A:488:LEU:HD23	2.00	0.43
1:A:671:ARG:NH1	1:A:671:ARG:HG3	2.33	0.43
1:B:517:VAL:HG23	1:B:518:ASN:ND2	2.33	0.43
1:B:677:GLY:HA2	1:B:745:TYR:OH	2.18	0.43
1:B:708:ALA:C	1:B:710:HIS:H	2.26	0.43
1:C:71:PHE:HD1	1:C:108:ASP:OD1	2.00	0.43
1:C:175:LYS:HB2	1:C:175:LYS:HZ3	1.77	0.43
1:C:243:LEU:O	1:C:247:TYR:HB2	2.18	0.43
1:C:463:THR:O	1:C:466:GLY:N	2.50	0.43
1:D:71:PHE:CG	1:D:73:ASN:HB2	2.53	0.43
1:D:97:TYR:O	1:D:100:LEU:N	2.52	0.43
1:D:173:ILE:HG23	1:D:174:GLY:N	2.33	0.43
1:D:234:LEU:H	1:D:234:LEU:CD2	2.31	0.43
1:D:279:ILE:CD1	1:D:279:ILE:H	2.30	0.43
1:D:446:ILE:CG1	1:D:447:SER:N	2.81	0.43
1:D:523:LEU:HD22	2:R:127:GLU:CD	2.43	0.43
1:D:777:TYR:O	1:D:778:LYS:C	2.60	0.43
1:E:97:TYR:HD2	1:E:102:GLY:HA3	1.84	0.43
1:E:187:SER:O	1:E:188:LEU:C	2.50	0.43
1:E:225:ILE:HG12	1:E:229:PHE:CE2	2.51	0.43
1:E:324:THR:CB	1:E:499:PRO:HA	2.41	0.43
1:E:457:THR:CG2	1:E:468:LYS:HA	2.42	0.43
1:E:629:ASN:HD22	1:E:630:ARG:N	2.16	0.43
1:E:635:ILE:N	1:E:635:ILE:CD1	2.79	0.43
1:F:161:ILE:HG21	1:F:168:GLU:HB2	2.00	0.43
1:F:173:ILE:HG23	1:F:174:GLY:N	2.33	0.43
1:F:311:HIS:O	1:F:312:ALA:C	2.61	0.43
1:F:486:LYS:HE3	1:F:570:THR:O	2.17	0.43
1:F:764:LEU:C	1:F:766:HIS:H	2.25	0.43
1:F:765:THR:HG22	1:F:769:SER:HB2	2.00	0.43
2:O:109:MET:HG3	2:O:116:LEU:HD11	1.99	0.43
2:O:138:TYR:O	2:O:142:VAL:HG23	2.18	0.43
2:Q:92:PHE:C	2:Q:94:LYS:N	2.76	0.43
2:Q:94:LYS:NZ	2:Q:94:LYS:HB3	2.32	0.43
1:A:90:PRO:HG2	1:A:93:VAL:HB	2.00	0.43
1:A:252:ASP:OD2	1:A:253:HIS:CD2	2.72	0.43
1:A:295:VAL:HG21	1:A:603:ILE:CG2	2.47	0.43
1:A:323:ASN:ND2	1:A:598:PRO:CB	2.81	0.43
1:A:443:GLU:CG	1:A:458:LYS:HE3	2.48	0.43
1:A:480:ASN:C	1:A:480:ASN:ND2	2.76	0.43
1:A:595:ILE:CG2	1:A:596:ILE:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:PHE:HD1	1:B:108:ASP:OD1	2.00	0.43
1:B:88:LYS:HE3	1:B:88:LYS:HB3	1.88	0.43
1:B:107:THR:HG21	1:B:115:LYS:CD	2.38	0.43
1:B:364:ILE:O	1:B:365:PRO:C	2.60	0.43
1:B:411:GLU:O	1:B:414:LYS:HB3	2.18	0.43
1:B:439:ASN:OD1	1:B:440:GLN:N	2.51	0.43
1:B:450:ASN:O	1:B:452:GLU:N	2.49	0.43
1:B:595:ILE:CG2	1:B:596:ILE:N	2.81	0.43
1:B:614:PHE:O	1:B:614:PHE:CD2	2.71	0.43
1:C:71:PHE:CG	1:C:73:ASN:HB2	2.53	0.43
1:C:77:ASP:O	1:C:81:GLN:HB2	2.19	0.43
1:C:115:LYS:C	1:C:117:LEU:N	2.77	0.43
1:C:443:GLU:CG	1:C:458:LYS:HE3	2.48	0.43
1:C:505:LYS:HE3	1:C:513:TRP:CD2	2.53	0.43
1:C:738:SER:OG	1:C:739:LYS:N	2.38	0.43
1:C:743:PRO:HA	1:C:746:LYS:CB	2.46	0.43
1:D:307:LEU:HD12	1:D:307:LEU:N	2.34	0.43
1:D:523:LEU:HD22	2:R:127:GLU:HG2	2.01	0.43
1:D:690:LYS:CD	1:D:741:ILE:HG23	2.48	0.43
1:E:186:LYS:HB2	1:E:186:LYS:HE2	1.85	0.43
1:F:71:PHE:HD1	1:F:108:ASP:OD1	2.00	0.43
1:F:104:ILE:HG23	1:F:152:LEU:HD22	1.99	0.43
1:F:234:LEU:H	1:F:234:LEU:CD2	2.31	0.43
1:F:439:ASN:OD1	1:F:440:GLN:N	2.51	0.43
2:O:94:LYS:NZ	2:O:94:LYS:HB3	2.33	0.43
2:O:104:GLU:O	2:O:105:LEU:C	2.60	0.43
2:Q:102:ALA:CB	2:Q:125:ILE:HG13	2.48	0.43
2:R:58:ASP:HB3	2:R:62:THR:CG2	2.44	0.43
1:A:89:ILE:HG22	1:A:90:PRO:HD2	1.99	0.43
1:A:140:ARG:NH1	1:A:141:PHE:HE1	2.16	0.43
1:A:271:LEU:HD13	1:A:276:PHE:CE2	2.54	0.43
1:A:325:TYR:HB2	1:A:498:ALA:HB3	1.99	0.43
1:A:437:SER:O	1:A:439:ASN:N	2.43	0.43
1:A:708:ALA:C	1:A:710:HIS:H	2.26	0.43
1:B:252:ASP:OD2	1:B:253:HIS:CD2	2.72	0.43
1:B:349:ASN:HD22	1:B:350:VAL:N	2.16	0.43
1:B:794:GLN:HE21	1:B:794:GLN:HB3	1.66	0.43
1:C:91:LYS:O	1:C:94:LEU:HB2	2.18	0.43
1:C:135:VAL:N	1:C:136:PRO:HD3	2.34	0.43
1:C:365:PRO:HB2	1:C:367:ASP:O	2.18	0.43
1:C:501:LEU:HD22	2:Q:112:LEU:CD2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:O	1:D:94:LEU:HB2	2.19	0.43
1:D:135:VAL:N	1:D:136:PRO:HD3	2.33	0.43
1:D:153:ILE:C	1:D:154:ILE:HD13	2.41	0.43
1:D:169:VAL:CG2	1:D:246:SER:HB2	2.48	0.43
1:D:192:PHE:HB3	1:D:196:ILE:CD1	2.47	0.43
1:D:325:TYR:HB2	1:D:498:ALA:HB3	2.00	0.43
1:D:391:ILE:O	1:D:393:GLU:N	2.51	0.43
1:E:90:PRO:HG2	1:E:93:VAL:HB	2.00	0.43
1:E:325:TYR:HB2	1:E:498:ALA:HB3	1.99	0.43
1:E:391:ILE:O	1:E:393:GLU:N	2.52	0.43
1:E:446:ILE:CG1	1:E:447:SER:N	2.81	0.43
1:E:529:VAL:O	1:E:532:LEU:N	2.51	0.43
1:E:775:LEU:O	1:E:776:LEU:C	2.62	0.43
1:F:90:PRO:O	1:F:93:VAL:N	2.51	0.43
1:F:225:ILE:HG23	1:F:229:PHE:CE2	2.52	0.43
2:O:24:ASP:CG	2:O:25:GLY:H	2.27	0.43
2:P:76:MET:HA	2:P:79:THR:HG22	2.00	0.43
2:Q:97:ASN:ND2	2:Q:99:TYR:H	2.16	0.43
2:Q:138:TYR:O	2:Q:142:VAL:HG23	2.18	0.43
2:T:44:THR:HG23	2:T:47:GLU:OE2	2.19	0.43
1:A:225:ILE:HG23	1:A:229:PHE:CD2	2.53	0.43
1:A:364:ILE:O	1:A:365:PRO:C	2.61	0.43
1:A:683:GLY:O	1:A:684:ASP:C	2.62	0.43
1:A:777:TYR:O	1:A:778:LYS:C	2.61	0.43
1:B:437:SER:C	1:B:439:ASN:H	2.27	0.43
1:B:722:ILE:HD13	1:B:764:LEU:HD23	2.01	0.43
1:C:279:ILE:HD13	1:C:279:ILE:H	1.82	0.43
1:C:405:LEU:CD1	1:C:405:LEU:H	2.30	0.43
1:C:609:GLU:O	1:C:613:ARG:N	2.48	0.43
1:C:665:LYS:HE2	2:Q:11:GLU:CD	2.43	0.43
1:C:677:GLY:HA2	1:C:745:TYR:OH	2.17	0.43
1:C:708:ALA:C	1:C:710:HIS:H	2.26	0.43
1:C:722:ILE:HD13	1:C:764:LEU:HD21	2.00	0.43
1:D:278:LYS:HB2	1:D:279:ILE:HD13	2.01	0.43
1:D:443:GLU:CG	1:D:458:LYS:HE3	2.48	0.43
1:E:523:LEU:HD22	2:S:127:GLU:HG2	2.01	0.43
1:E:660:SER:O	1:E:663:PHE:HB3	2.18	0.43
1:F:135:VAL:N	1:F:136:PRO:HD3	2.34	0.43
1:F:175:LYS:O	1:F:176:GLY:C	2.61	0.43
1:F:240:ALA:O	1:F:241:PHE:C	2.61	0.43
1:F:391:ILE:O	1:F:393:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:GLU:O	1:F:484:VAL:HG23	2.18	0.43
1:F:566:TYR:CD2	1:F:566:TYR:N	2.84	0.43
2:P:73:ALA:O	2:P:75:LYS:N	2.51	0.43
2:P:97:ASN:HD22	2:P:98:GLY:N	2.16	0.43
2:Q:110:THR:O	2:Q:113:GLY:N	2.47	0.43
1:A:176:GLY:O	1:A:180:ASP:OD1	2.37	0.43
1:A:295:VAL:HG12	1:A:605:THR:HA	2.00	0.43
1:A:538:ILE:HG21	2:O:87:GLU:HB2	2.01	0.43
1:A:692:GLU:OE2	1:A:692:GLU:HA	2.19	0.43
1:A:723:PHE:O	1:A:724:ARG:C	2.61	0.43
1:B:179:LEU:O	1:B:183:SER:HB3	1.95	0.43
1:B:192:PHE:O	1:B:193:LEU:C	2.61	0.43
1:B:747:ASN:O	1:B:748:TYR:C	2.62	0.43
1:C:337:ASN:C	1:C:339:ILE:N	2.74	0.43
1:C:566:TYR:CD2	1:C:566:TYR:N	2.85	0.43
1:D:77:ASP:O	1:D:81:GLN:HB2	2.17	0.43
1:D:115:LYS:C	1:D:117:LEU:N	2.77	0.43
1:D:344:ALA:HB3	1:D:488:LEU:HD23	2.01	0.43
1:D:463:THR:O	1:D:466:GLY:N	2.50	0.43
1:D:482:GLU:O	1:D:484:VAL:HG23	2.18	0.43
1:D:538:ILE:HG21	2:R:87:GLU:HB2	2.01	0.43
1:E:270:LYS:O	1:E:273:LYS:HB2	2.18	0.43
1:E:678:VAL:HG13	1:E:745:TYR:CD2	2.52	0.43
1:E:777:TYR:O	1:E:778:LYS:C	2.61	0.43
1:F:391:ILE:O	1:F:392:THR:C	2.61	0.43
1:F:500:SER:OG	1:F:502:THR:OG1	2.34	0.43
1:F:517:VAL:HG23	1:F:518:ASN:ND2	2.33	0.43
2:O:92:PHE:C	2:O:94:LYS:N	2.76	0.43
2:Q:104:GLU:O	2:Q:105:LEU:C	2.60	0.43
2:R:104:GLU:O	2:R:105:LEU:C	2.61	0.43
2:S:5:THR:O	2:S:6:GLU:C	2.60	0.43
2:S:94:LYS:NZ	2:S:94:LYS:HB3	2.32	0.43
2:T:58:ASP:O	2:T:60:ASN:N	2.48	0.43
1:A:234:LEU:H	1:A:234:LEU:CD2	2.31	0.43
1:A:279:ILE:HD13	1:A:279:ILE:H	1.84	0.43
1:A:307:LEU:HD12	1:A:307:LEU:N	2.34	0.43
1:A:332:ASN:OD1	1:A:334:LEU:CD1	2.66	0.43
1:A:517:VAL:HG23	1:A:518:ASN:ND2	2.33	0.43
1:A:699:GLY:O	1:A:700:TYR:C	2.60	0.43
1:B:100:LEU:HD11	1:B:182:ILE:HG21	2.01	0.43
1:B:579:THR:O	1:B:581:GLN:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:LYS:O	1:B:720:ILE:C	2.60	0.43
1:C:522:SER:O	2:Q:124:MET:HE2	2.19	0.43
1:C:614:PHE:CD2	1:C:614:PHE:O	2.71	0.43
1:D:173:ILE:O	1:D:176:GLY:N	2.52	0.43
1:D:217:LYS:HZ1	1:D:236:GLU:HB2	1.83	0.43
1:D:332:ASN:OD1	1:D:334:LEU:N	2.46	0.43
1:D:517:VAL:HG23	1:D:518:ASN:ND2	2.33	0.43
1:E:690:LYS:CD	1:E:741:ILE:HG23	2.47	0.43
1:F:77:ASP:O	1:F:81:GLN:HB2	2.19	0.43
1:F:130:SER:O	1:F:132:GLY:O	2.36	0.43
1:F:243:LEU:O	1:F:247:TYR:HB2	2.18	0.43
1:F:288:VAL:CG2	1:F:289:GLU:N	2.75	0.43
1:F:443:GLU:CG	1:F:458:LYS:HE3	2.48	0.43
1:F:522:SER:O	2:T:124:MET:HE2	2.18	0.43
2:O:42:ASN:HA	2:O:43:PRO:HD2	1.90	0.43
2:P:26:THR:HB	2:P:62:THR:OG1	2.18	0.43
2:Q:43:PRO:HG3	2:Q:48:LEU:HD13	2.00	0.43
2:S:81:SER:O	2:S:82:GLU:C	2.60	0.43
2:T:92:PHE:C	2:T:94:LYS:N	2.76	0.43
1:A:368:GLN:HG3	1:A:384:ASN:N	2.33	0.43
1:A:432:TYR:CD2	1:A:447:SER:HA	2.54	0.43
1:A:439:ASN:OD1	1:A:440:GLN:N	2.52	0.43
1:A:614:PHE:CD2	1:A:614:PHE:O	2.72	0.43
1:B:71:PHE:CG	1:B:73:ASN:HB2	2.53	0.43
1:B:88:LYS:HZ2	1:B:172:GLU:CD	2.27	0.43
1:B:526:GLN:O	1:B:527:LYS:C	2.61	0.43
1:B:663:PHE:CE1	1:B:752:LEU:HD11	2.53	0.43
1:B:759:GLN:CA	1:B:759:GLN:NE2	2.80	0.43
1:C:123:GLU:CG	1:C:124:GLU:H	2.24	0.43
1:C:344:ALA:HB3	1:C:488:LEU:HD23	2.01	0.43
1:C:678:VAL:HG13	1:C:745:TYR:CD2	2.53	0.43
1:D:88:LYS:NZ	1:D:172:GLU:OE1	2.51	0.43
1:D:115:LYS:NZ	1:D:117:LEU:HB2	2.33	0.43
1:D:192:PHE:O	1:D:193:LEU:C	2.62	0.43
1:D:722:ILE:HD13	1:D:764:LEU:HD21	2.01	0.43
1:E:144:GLU:CG	1:E:177:ILE:HD11	2.47	0.43
1:E:364:ILE:O	1:E:365:PRO:C	2.61	0.43
1:E:446:ILE:HA	1:E:453:VAL:HA	2.01	0.43
1:E:482:GLU:O	1:E:484:VAL:HG23	2.18	0.43
1:E:716:LYS:O	1:E:720:ILE:HG22	2.19	0.43
1:F:257:LEU:CD1	1:F:261:ALA:HB3	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:551:ASN:HD22	1:F:551:ASN:HA	1.55	0.43
2:O:55:VAL:CG2	2:O:67:GLU:OE1	2.66	0.43
2:O:97:ASN:HD22	2:O:98:GLY:N	2.17	0.43
2:R:44:THR:HG23	2:R:47:GLU:OE2	2.18	0.43
2:R:73:ALA:C	2:R:75:LYS:N	2.77	0.43
1:A:192:PHE:O	1:A:193:LEU:C	2.62	0.43
1:A:411:GLU:O	1:A:414:LYS:HB3	2.19	0.43
1:A:435:LEU:HG	1:A:446:ILE:HG22	2.01	0.43
1:A:663:PHE:CE1	1:A:752:LEU:HD11	2.54	0.43
1:B:275:GLY:CA	1:B:278:LYS:HE2	2.49	0.43
1:B:692:GLU:HA	1:B:692:GLU:OE2	2.18	0.43
1:B:765:THR:HG22	1:B:769:SER:HB2	2.00	0.43
1:C:305:SER:C	1:C:307:LEU:H	2.27	0.43
1:C:338:LEU:O	1:C:343:VAL:CG2	2.67	0.43
1:C:529:VAL:O	1:C:532:LEU:N	2.52	0.43
1:C:690:LYS:CD	1:C:741:ILE:HG23	2.49	0.43
1:D:327:LEU:HD12	1:D:327:LEU:N	2.33	0.43
1:D:546:LYS:NZ	1:D:554:LYS:HE2	2.34	0.43
1:D:579:THR:O	1:D:581:GLN:N	2.52	0.43
1:D:708:ALA:C	1:D:710:HIS:H	2.27	0.43
1:E:115:LYS:NZ	1:E:117:LEU:HB2	2.33	0.43
1:E:665:LYS:HE2	2:S:11:GLU:CD	2.43	0.43
1:F:271:LEU:HD13	1:F:276:PHE:CE2	2.53	0.43
1:F:278:LYS:HB2	1:F:279:ILE:HD13	2.01	0.43
1:F:343:VAL:HG12	1:F:344:ALA:N	2.34	0.43
1:F:493:ASP:OD2	1:F:577:HIS:CE1	2.71	0.43
1:F:595:ILE:CG2	1:F:596:ILE:N	2.81	0.43
1:F:628:PHE:CE2	2:T:90:ARG:HD3	2.36	0.43
2:S:138:TYR:CZ	2:S:142:VAL:CG2	3.01	0.43
2:S:146:THR:O	2:S:148:LYS:N	2.51	0.43
2:T:21:LYS:C	2:T:23:GLY:H	2.27	0.43
1:A:169:VAL:HG23	1:A:246:SER:HB2	2.01	0.43
1:A:327:LEU:HD12	1:A:327:LEU:N	2.34	0.43
1:A:405:LEU:CD1	1:A:405:LEU:H	2.30	0.43
1:A:581:GLN:HE22	1:A:632:TYR:HE1	1.67	0.43
1:B:236:GLU:HA	1:B:239:HIS:HD2	1.75	0.43
1:B:305:SER:C	1:B:307:LEU:H	2.27	0.43
1:B:413:LEU:N	1:B:413:LEU:HD23	2.34	0.43
1:B:462:ILE:CD1	1:B:466:GLY:HA2	2.44	0.43
1:B:630:ARG:CD	2:P:83:GLU:HG2	2.48	0.43
1:B:671:ARG:NH1	1:B:671:ARG:HG3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PHE:O	1:C:193:LEU:C	2.61	0.43
1:C:231:LYS:O	1:C:232:GLU:C	2.61	0.43
1:C:364:ILE:O	1:C:365:PRO:C	2.61	0.43
1:C:505:LYS:C	1:C:507:GLN:N	2.68	0.43
1:C:607:ASN:HB2	1:C:610:MET:H	1.84	0.43
1:D:107:THR:HG21	1:D:115:LYS:CD	2.46	0.43
1:D:184:LYS:HE2	1:D:193:LEU:HD12	2.01	0.43
1:D:243:LEU:O	1:D:247:TYR:HB2	2.19	0.43
1:D:678:VAL:HG13	1:D:745:TYR:CD2	2.54	0.43
1:D:692:GLU:OE2	1:D:692:GLU:HA	2.19	0.43
1:D:732:ILE:HG23	1:D:749:PHE:HD1	1.84	0.43
1:E:89:ILE:CG2	1:E:90:PRO:HD2	2.49	0.43
1:F:115:LYS:O	1:F:117:LEU:N	2.52	0.43
1:F:225:ILE:HG12	1:F:229:PHE:CE2	2.53	0.43
1:F:505:LYS:C	1:F:507:GLN:N	2.69	0.43
1:F:671:ARG:NH1	1:F:671:ARG:HG3	2.34	0.43
1:F:708:ALA:C	1:F:710:HIS:H	2.27	0.43
2:P:39:LEU:HD23	2:P:39:LEU:HA	1.86	0.43
2:Q:146:THR:O	2:Q:148:LYS:N	2.52	0.43
2:T:43:PRO:HG3	2:T:48:LEU:HD13	2.01	0.43
1:A:78:LYS:CD	1:A:156:ILE:HD13	2.49	0.42
1:A:97:TYR:HD2	1:A:102:GLY:HA3	1.83	0.42
1:A:100:LEU:HD11	1:A:182:ILE:HG21	2.01	0.42
1:A:179:LEU:O	1:A:183:SER:HB3	1.97	0.42
1:A:217:LYS:HZ2	1:A:236:GLU:HB2	1.81	0.42
1:A:278:LYS:HB2	1:A:279:ILE:HD13	2.01	0.42
1:A:292:ARG:NE	1:A:617:LYS:NZ	2.67	0.42
1:A:324:THR:CB	1:A:499:PRO:HA	2.41	0.42
1:A:478:ALA:HA	1:A:488:LEU:HG	2.01	0.42
1:B:549:LEU:HB2	1:B:553:GLN:HE21	1.84	0.42
1:B:716:LYS:O	1:B:720:ILE:HG22	2.18	0.42
1:C:192:PHE:H	1:C:192:PHE:HD1	1.67	0.42
1:C:411:GLU:O	1:C:414:LYS:HB3	2.19	0.42
1:C:526:GLN:O	1:C:527:LYS:C	2.62	0.42
1:C:660:SER:O	1:C:663:PHE:HB3	2.18	0.42
1:C:671:ARG:NH1	1:C:671:ARG:HG3	2.34	0.42
1:D:668:SER:OG	2:R:10:ALA:HB1	2.19	0.42
1:E:350:VAL:HG12	1:E:352:GLY:H	1.84	0.42
1:E:437:SER:C	1:E:439:ASN:H	2.27	0.42
1:E:439:ASN:OD1	1:E:440:GLN:N	2.51	0.42
1:E:458:LYS:C	1:E:460:GLY:H	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:ILE:CD1	1:E:466:GLY:HA2	2.45	0.42
1:E:478:ALA:HA	1:E:488:LEU:HG	2.01	0.42
1:E:480:ASN:C	1:E:480:ASN:ND2	2.76	0.42
1:E:595:ILE:CG2	1:E:596:ILE:N	2.81	0.42
1:E:722:ILE:HD13	1:E:764:LEU:HD23	2.01	0.42
1:F:295:VAL:HG12	1:F:605:THR:HA	2.00	0.42
1:F:690:LYS:CD	1:F:741:ILE:HG23	2.48	0.42
2:P:3:GLN:N	2:P:77:LYS:NZ	2.61	0.42
2:P:97:ASN:ND2	2:P:99:TYR:H	2.17	0.42
2:Q:21:LYS:C	2:Q:23:GLY:H	2.27	0.42
2:S:76:MET:HA	2:S:79:THR:HG22	2.00	0.42
2:S:89:PHE:O	2:S:91:VAL:N	2.52	0.42
2:T:117:THR:C	2:T:119:GLU:N	2.76	0.42
1:A:90:PRO:HD3	1:A:249:PHE:CE2	2.54	0.42
1:A:144:GLU:HG2	1:A:177:ILE:CD1	2.47	0.42
1:A:175:LYS:O	1:A:176:GLY:C	2.62	0.42
1:A:305:SER:C	1:A:307:LEU:H	2.27	0.42
1:B:175:LYS:O	1:B:176:GLY:C	2.62	0.42
1:B:343:VAL:HG12	1:B:344:ALA:N	2.35	0.42
1:B:365:PRO:HB2	1:B:367:ASP:O	2.19	0.42
1:B:715:GLU:OE1	1:B:767:GLN:NE2	2.51	0.42
1:C:122:GLU:HG3	1:C:147:ARG:H	1.84	0.42
1:C:134:LYS:O	1:C:135:VAL:HG12	2.19	0.42
1:C:462:ILE:CD1	1:C:466:GLY:HA2	2.45	0.42
1:D:279:ILE:HD13	1:D:279:ILE:H	1.84	0.42
1:D:439:ASN:OD1	1:D:440:GLN:N	2.52	0.42
1:D:462:ILE:CG1	1:D:463:THR:N	2.78	0.42
1:D:597:ASN:O	1:D:599:GLU:N	2.49	0.42
1:E:135:VAL:N	1:E:136:PRO:HD3	2.34	0.42
1:E:337:ASN:C	1:E:339:ILE:N	2.75	0.42
1:E:609:GLU:O	1:E:613:ARG:N	2.47	0.42
1:E:759:GLN:HA	1:E:759:GLN:NE2	2.20	0.42
1:F:197:LYS:HD3	1:F:263:ASP:CB	2.44	0.42
1:F:327:LEU:HD12	1:F:327:LEU:N	2.34	0.42
1:F:365:PRO:HB2	1:F:367:ASP:O	2.18	0.42
1:F:607:ASN:HB2	1:F:610:MET:H	1.84	0.42
1:F:671:ARG:HD2	2:T:14:GLU:HG2	2.01	0.42
2:S:21:LYS:C	2:S:23:GLY:H	2.27	0.42
2:T:69:LEU:HD12	2:T:69:LEU:C	2.44	0.42
1:A:115:LYS:C	1:A:117:LEU:N	2.77	0.42
1:A:123:GLU:OE2	1:A:123:GLU:N	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:HB2	1:A:170:TYR:HE2	1.80	0.42
1:A:161:ILE:HG21	1:A:168:GLU:HB2	2.00	0.42
1:A:413:LEU:N	1:A:413:LEU:HD23	2.34	0.42
1:A:607:ASN:HB2	1:A:610:MET:H	1.85	0.42
1:A:665:LYS:HE2	2:O:11:GLU:CD	2.43	0.42
1:B:480:ASN:C	1:B:480:ASN:ND2	2.77	0.42
1:B:722:ILE:HD13	1:B:764:LEU:HD21	2.01	0.42
1:B:777:TYR:O	1:B:778:LYS:C	2.61	0.42
1:C:173:ILE:O	1:C:176:GLY:N	2.52	0.42
1:C:234:LEU:H	1:C:234:LEU:CD2	2.31	0.42
1:C:323:ASN:C	1:C:324:THR:HG22	2.44	0.42
1:C:595:ILE:CG2	1:C:596:ILE:N	2.82	0.42
1:C:654:ILE:HG22	1:C:655:ASN:HD22	1.85	0.42
1:C:722:ILE:HD13	1:C:764:LEU:HD23	2.01	0.42
1:D:218:LEU:O	1:D:218:LEU:CG	2.67	0.42
1:D:462:ILE:CD1	1:D:466:GLY:HA2	2.45	0.42
1:D:499:PRO:HD2	1:D:625:LEU:O	2.19	0.42
1:D:635:ILE:N	1:D:635:ILE:CD1	2.78	0.42
1:E:81:GLN:NE2	1:E:156:ILE:HG21	2.34	0.42
1:E:169:VAL:CG2	1:E:246:SER:HB2	2.49	0.42
1:E:179:LEU:HB2	1:E:183:SER:HB2	1.99	0.42
1:E:231:LYS:O	1:E:232:GLU:C	2.62	0.42
1:E:311:HIS:O	1:E:312:ALA:C	2.62	0.42
1:F:279:ILE:HD13	1:F:279:ILE:H	1.84	0.42
1:F:370:LEU:HD23	1:F:370:LEU:HA	1.89	0.42
1:F:604:LEU:HG	1:F:605:THR:O	2.19	0.42
2:Q:117:THR:C	2:Q:119:GLU:N	2.76	0.42
2:R:102:ALA:HA	2:R:125:ILE:HG13	2.00	0.42
2:S:97:ASN:HD22	2:S:98:GLY:N	2.17	0.42
1:A:79:ILE:O	1:A:81:GLN:N	2.52	0.42
1:A:505:LYS:HE3	1:A:513:TRP:CD2	2.53	0.42
1:B:144:GLU:HB3	1:B:177:ILE:HD11	2.01	0.42
1:B:186:LYS:HB2	1:B:186:LYS:HE2	1.85	0.42
1:B:188:LEU:H	1:B:188:LEU:HD22	1.75	0.42
1:B:269:ASN:O	1:B:273:LYS:HG3	2.20	0.42
1:B:687:GLU:OE2	1:B:687:GLU:HA	2.20	0.42
1:C:94:LEU:O	1:C:97:TYR:N	2.51	0.42
1:C:225:ILE:HG12	1:C:229:PHE:CE2	2.54	0.42
1:C:252:ASP:OD2	1:C:253:HIS:CD2	2.72	0.42
1:C:335:ALA:O	1:C:339:ILE:HG13	2.20	0.42
1:C:380:VAL:C	1:C:383:GLY:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ILE:CG1	1:C:447:SER:N	2.81	0.42
1:C:493:ASP:OD2	1:C:577:HIS:CE1	2.72	0.42
1:D:175:LYS:O	1:D:176:GLY:C	2.62	0.42
1:D:457:THR:CG2	1:D:468:LYS:HA	2.42	0.42
1:D:764:LEU:O	1:D:766:HIS:N	2.52	0.42
1:E:115:LYS:O	1:E:117:LEU:N	2.52	0.42
1:E:161:ILE:O	1:E:165:GLN:HA	2.19	0.42
1:E:292:ARG:NE	1:E:617:LYS:NZ	2.67	0.42
1:E:307:LEU:N	1:E:307:LEU:HD12	2.34	0.42
1:E:343:VAL:HG12	1:E:344:ALA:N	2.35	0.42
1:E:435:LEU:HG	1:E:446:ILE:HG22	2.00	0.42
1:E:581:GLN:HE21	1:E:629:ASN:H	1.65	0.42
1:E:614:PHE:O	1:E:614:PHE:CD2	2.72	0.42
1:E:671:ARG:HG3	1:E:671:ARG:HH11	1.84	0.42
1:E:759:GLN:CA	1:E:759:GLN:NE2	2.81	0.42
1:F:231:LYS:O	1:F:232:GLU:C	2.62	0.42
1:F:301:ALA:O	1:F:302:LEU:C	2.63	0.42
1:F:335:ALA:O	1:F:339:ILE:HG13	2.20	0.42
2:O:24:ASP:OD1	2:O:25:GLY:N	2.52	0.42
2:P:21:LYS:C	2:P:23:GLY:H	2.27	0.42
2:P:92:PHE:C	2:P:94:LYS:N	2.77	0.42
2:S:92:PHE:C	2:S:94:LYS:N	2.77	0.42
2:T:104:GLU:O	2:T:105:LEU:C	2.61	0.42
2:T:146:THR:O	2:T:148:LYS:N	2.52	0.42
1:A:97:TYR:O	1:A:100:LEU:N	2.52	0.42
1:A:135:VAL:N	1:A:136:PRO:HD3	2.34	0.42
1:A:239:HIS:O	1:A:243:LEU:HD12	2.19	0.42
1:A:389:LYS:HD2	1:A:393:GLU:OE1	2.20	0.42
1:B:493:ASP:OD2	1:B:577:HIS:CE1	2.72	0.42
1:B:776:LEU:C	1:B:776:LEU:CD2	2.93	0.42
1:C:88:LYS:HE2	1:C:168:GLU:OE1	2.20	0.42
1:C:157:LYS:HA	1:C:157:LYS:HD2	1.85	0.42
1:D:130:SER:O	1:D:131:ARG:C	2.63	0.42
1:D:335:ALA:O	1:D:339:ILE:HG13	2.19	0.42
1:D:450:ASN:O	1:D:452:GLU:N	2.51	0.42
1:D:478:ALA:HA	1:D:488:LEU:HG	2.02	0.42
1:E:131:ARG:HB2	1:E:170:TYR:CE2	2.54	0.42
1:E:131:ARG:HB2	1:E:170:TYR:CZ	2.55	0.42
1:E:708:ALA:C	1:E:710:HIS:H	2.28	0.42
1:F:218:LEU:O	1:F:218:LEU:CG	2.67	0.42
1:F:323:ASN:C	1:F:324:THR:HG22	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:722:ILE:HD13	1:F:764:LEU:HD23	2.01	0.42
1:F:767:GLN:HG2	1:F:768:LYS:HG2	2.02	0.42
2:O:21:LYS:C	2:O:23:GLY:H	2.27	0.42
2:P:44:THR:HG23	2:P:47:GLU:OE2	2.18	0.42
2:R:5:THR:O	2:R:6:GLU:C	2.61	0.42
2:R:21:LYS:C	2:R:23:GLY:H	2.28	0.42
2:T:10:ALA:O	2:T:14:GLU:HB2	2.20	0.42
2:T:102:ALA:HA	2:T:125:ILE:HG13	2.01	0.42
1:A:104:ILE:HG23	1:A:152:LEU:HD22	2.01	0.42
1:A:161:ILE:O	1:A:165:GLN:HA	2.19	0.42
1:A:218:LEU:O	1:A:218:LEU:CG	2.67	0.42
1:A:596:ILE:O	1:A:596:ILE:HG22	2.19	0.42
1:A:656:THR:O	1:A:755:ARG:NH1	2.53	0.42
1:A:670:ILE:CG2	1:A:744:GLU:HB2	2.47	0.42
1:A:735:VAL:HA	1:A:738:SER:HB2	2.02	0.42
1:B:91:LYS:O	1:B:94:LEU:HB2	2.19	0.42
1:B:135:VAL:N	1:B:136:PRO:HD3	2.33	0.42
1:B:191:GLU:C	1:B:193:LEU:N	2.77	0.42
1:B:218:LEU:C	1:B:220:LEU:N	2.68	0.42
1:B:323:ASN:O	1:B:324:THR:HG22	2.19	0.42
1:B:457:THR:CG2	1:B:468:LYS:HA	2.42	0.42
1:B:670:ILE:CG2	1:B:744:GLU:HB2	2.47	0.42
1:C:104:ILE:HG23	1:C:152:LEU:HD22	2.01	0.42
1:C:225:ILE:HG23	1:C:229:PHE:CD2	2.55	0.42
1:C:254:ARG:HB3	1:C:254:ARG:NH1	2.34	0.42
1:C:395:GLU:OE1	1:C:395:GLU:N	2.53	0.42
1:C:748:TYR:O	1:C:751:TYR:HB3	2.20	0.42
1:C:777:TYR:O	1:C:778:LYS:C	2.62	0.42
1:D:90:PRO:HD3	1:D:249:PHE:CE2	2.54	0.42
1:D:217:LYS:HZ2	1:D:217:LYS:CB	2.27	0.42
1:D:526:GLN:O	1:D:527:LYS:C	2.63	0.42
1:E:100:LEU:CD1	1:E:182:ILE:HG21	2.49	0.42
1:E:301:ALA:O	1:E:302:LEU:C	2.62	0.42
1:E:692:GLU:HA	1:E:692:GLU:OE2	2.18	0.42
1:F:76:LEU:CD2	1:F:76:LEU:N	2.83	0.42
1:F:122:GLU:HG3	1:F:147:ARG:H	1.84	0.42
1:F:337:ASN:C	1:F:339:ILE:N	2.74	0.42
1:F:338:LEU:O	1:F:343:VAL:CG2	2.68	0.42
1:F:656:THR:O	1:F:755:ARG:NH1	2.52	0.42
1:F:775:LEU:O	1:F:776:LEU:C	2.63	0.42
2:O:18:LEU:HD23	2:O:18:LEU:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:117:THR:C	2:R:119:GLU:N	2.76	0.42
2:R:146:THR:O	2:R:148:LYS:N	2.52	0.42
2:S:117:THR:C	2:S:119:GLU:N	2.76	0.42
1:A:71:PHE:CG	1:A:73:ASN:HB2	2.53	0.42
1:A:90:PRO:O	1:A:93:VAL:N	2.51	0.42
1:A:115:LYS:O	1:A:117:LEU:N	2.53	0.42
1:A:529:VAL:O	1:A:532:LEU:N	2.53	0.42
1:A:565:LYS:C	1:A:567:THR:N	2.78	0.42
1:B:90:PRO:HG2	1:B:93:VAL:HB	2.02	0.42
1:B:141:PHE:CD1	1:B:141:PHE:N	2.87	0.42
1:B:218:LEU:O	1:B:218:LEU:CG	2.67	0.42
1:B:325:TYR:HB2	1:B:498:ALA:HB3	2.00	0.42
1:C:175:LYS:C	1:C:177:ILE:N	2.78	0.42
1:C:343:VAL:HG12	1:C:344:ALA:N	2.34	0.42
1:D:71:PHE:O	1:D:78:LYS:NZ	2.52	0.42
1:D:141:PHE:N	1:D:141:PHE:CD1	2.88	0.42
1:D:549:LEU:HB2	1:D:553:GLN:HE21	1.85	0.42
1:D:687:GLU:HA	1:D:687:GLU:OE2	2.18	0.42
1:D:723:PHE:O	1:D:724:ARG:C	2.62	0.42
1:D:776:LEU:C	1:D:776:LEU:CD2	2.93	0.42
1:E:76:LEU:N	1:E:76:LEU:CD2	2.83	0.42
1:E:144:GLU:HG2	1:E:177:ILE:CD1	2.49	0.42
1:E:173:ILE:O	1:E:176:GLY:N	2.53	0.42
1:E:188:LEU:H	1:E:188:LEU:HD22	1.75	0.42
1:E:323:ASN:C	1:E:324:THR:HG22	2.44	0.42
1:E:370:LEU:HD23	1:E:370:LEU:HA	1.90	0.42
1:E:391:ILE:O	1:E:392:THR:C	2.61	0.42
1:F:217:LYS:HB2	1:F:236:GLU:OE1	2.19	0.42
1:F:308:VAL:O	1:F:311:HIS:N	2.42	0.42
1:F:501:LEU:HD22	2:T:112:LEU:CD2	2.49	0.42
1:F:660:SER:O	1:F:663:PHE:HB3	2.19	0.42
1:F:719:LYS:O	1:F:720:ILE:C	2.61	0.42
2:P:100:ILE:O	2:P:136:VAL:HG22	2.20	0.42
2:S:10:ALA:O	2:S:14:GLU:HB2	2.20	0.42
2:T:97:ASN:ND2	2:T:99:TYR:H	2.17	0.42
1:A:81:GLN:NE2	1:A:156:ILE:HG21	2.35	0.42
1:A:107:THR:HG21	1:A:115:LYS:CD	2.41	0.42
1:A:185:ASP:O	1:A:190:PRO:CD	2.67	0.42
1:A:350:VAL:HG12	1:A:352:GLY:H	1.84	0.42
1:A:461:LYS:HD2	1:A:461:LYS:HA	1.79	0.42
1:A:671:ARG:HG3	1:A:671:ARG:HH11	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ALA:C	1:A:730:ASN:N	2.77	0.42
1:B:76:LEU:N	1:B:76:LEU:CD2	2.83	0.42
1:B:104:ILE:HG23	1:B:152:LEU:HD22	2.01	0.42
1:B:115:LYS:C	1:B:117:LEU:N	2.78	0.42
1:B:278:LYS:HB2	1:B:279:ILE:HD13	2.02	0.42
1:B:350:VAL:HG12	1:B:352:GLY:H	1.84	0.42
1:B:446:ILE:HA	1:B:453:VAL:HA	2.00	0.42
1:B:529:VAL:O	1:B:532:LEU:N	2.53	0.42
1:B:660:SER:O	1:B:663:PHE:HB3	2.20	0.42
1:C:71:PHE:O	1:C:78:LYS:NZ	2.53	0.42
1:C:107:THR:HG21	1:C:115:LYS:CD	2.44	0.42
1:C:271:LEU:HD13	1:C:276:PHE:CE2	2.54	0.42
1:C:295:VAL:CG2	1:C:603:ILE:CG2	2.97	0.42
1:C:322:LEU:O	1:C:323:ASN:HB3	2.20	0.42
1:C:480:ASN:HD21	1:C:483:GLY:CA	2.31	0.42
1:C:639:ASN:HD22	1:C:640:LYS:N	2.18	0.42
1:C:663:PHE:CE1	1:C:752:LEU:HD11	2.55	0.42
1:D:115:LYS:O	1:D:117:LEU:N	2.53	0.42
1:D:413:LEU:HD23	1:D:413:LEU:N	2.35	0.42
1:E:243:LEU:O	1:E:247:TYR:HB2	2.19	0.42
1:E:767:GLN:HG2	1:E:768:LYS:HG2	2.02	0.42
1:F:141:PHE:N	1:F:141:PHE:CD1	2.88	0.42
1:F:186:LYS:HB2	1:F:186:LYS:HE2	1.85	0.42
1:F:192:PHE:O	1:F:193:LEU:C	2.62	0.42
1:F:380:VAL:C	1:F:383:GLY:H	2.28	0.42
1:F:526:GLN:O	1:F:527:LYS:C	2.61	0.42
1:F:538:ILE:HG21	2:T:87:GLU:HB2	2.01	0.42
1:F:654:ILE:HG22	1:F:655:ASN:HD22	1.85	0.42
1:F:668:SER:OG	2:T:10:ALA:HB1	2.20	0.42
2:P:102:ALA:HA	2:P:125:ILE:HG13	2.01	0.42
2:S:43:PRO:HG3	2:S:48:LEU:HD13	2.01	0.42
1:A:76:LEU:CD2	1:A:76:LEU:N	2.83	0.42
1:A:243:LEU:O	1:A:247:TYR:HB2	2.19	0.42
1:A:526:GLN:O	1:A:527:LYS:C	2.62	0.42
1:B:173:ILE:O	1:B:176:GLY:N	2.53	0.42
1:B:732:ILE:HG23	1:B:749:PHE:HD1	1.85	0.42
1:C:141:PHE:N	1:C:141:PHE:CD1	2.88	0.42
1:C:546:LYS:NZ	1:C:554:LYS:HE2	2.35	0.42
1:D:271:LEU:HD13	1:D:276:PHE:CE2	2.55	0.42
1:D:480:ASN:HD21	1:D:483:GLY:CA	2.32	0.42
1:D:561:ASN:OD1	1:D:574:VAL:N	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:PRO:O	1:D:649:ILE:C	2.63	0.42
1:D:654:ILE:HG22	1:D:655:ASN:HD22	1.85	0.42
1:D:722:ILE:HD13	1:D:764:LEU:HD23	2.02	0.42
1:E:192:PHE:O	1:E:193:LEU:C	2.62	0.42
1:F:218:LEU:HD21	1:F:225:ILE:CD1	2.50	0.42
1:F:225:ILE:HG23	1:F:229:PHE:CD2	2.55	0.42
1:F:344:ALA:HB3	1:F:488:LEU:HD23	2.01	0.42
2:O:19:PHE:N	2:O:19:PHE:CD1	2.88	0.42
2:O:43:PRO:CG	2:O:48:LEU:HD13	2.50	0.42
2:O:102:ALA:HA	2:O:125:ILE:HG13	2.01	0.42
2:P:5:THR:O	2:P:6:GLU:C	2.59	0.42
2:P:28:THR:HB	2:P:30:LYS:HZ3	1.83	0.42
2:P:104:GLU:O	2:P:105:LEU:C	2.62	0.42
2:R:43:PRO:HG3	2:R:48:LEU:HD13	2.01	0.42
2:S:24:ASP:OD1	2:S:25:GLY:N	2.53	0.42
2:T:18:LEU:HD23	2:T:18:LEU:HA	1.83	0.42
1:A:192:PHE:HD1	1:A:192:PHE:H	1.68	0.42
1:A:380:VAL:C	1:A:383:GLY:H	2.28	0.42
1:A:395:GLU:O	1:A:395:GLU:CD	2.63	0.42
1:A:629:ASN:ND2	1:A:630:ARG:N	2.68	0.42
1:A:636:ALA:O	1:A:640:LYS:CA	2.68	0.42
1:A:687:GLU:OE2	1:A:687:GLU:HA	2.20	0.42
1:B:78:LYS:CD	1:B:156:ILE:HD13	2.50	0.42
1:B:81:GLN:NE2	1:B:156:ILE:HG21	2.34	0.42
1:B:157:LYS:HA	1:B:157:LYS:HD2	1.86	0.42
1:B:243:LEU:O	1:B:247:TYR:HB2	2.19	0.42
1:B:271:LEU:HD13	1:B:276:PHE:CE2	2.55	0.42
1:B:581:GLN:HE22	1:B:632:TYR:HE1	1.68	0.42
1:C:175:LYS:O	1:C:176:GLY:C	2.62	0.42
1:C:197:LYS:HD3	1:C:263:ASP:CB	2.44	0.42
1:C:639:ASN:C	1:C:639:ASN:ND2	2.73	0.42
1:D:236:GLU:HA	1:D:239:HIS:HD2	1.76	0.42
1:D:323:ASN:C	1:D:324:THR:HG22	2.45	0.42
1:D:350:VAL:HG12	1:D:352:GLY:H	1.84	0.42
1:D:380:VAL:C	1:D:383:GLY:H	2.28	0.42
1:D:411:GLU:O	1:D:414:LYS:HB3	2.19	0.42
1:D:614:PHE:CD2	1:D:614:PHE:O	2.72	0.42
1:D:660:SER:O	1:D:663:PHE:HB3	2.20	0.42
1:E:71:PHE:O	1:E:78:LYS:NZ	2.53	0.42
1:E:175:LYS:O	1:E:176:GLY:C	2.62	0.42
1:E:338:LEU:O	1:E:343:VAL:CG2	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:GLU:OE1	1:E:395:GLU:N	2.53	0.42
1:E:604:LEU:HG	1:E:605:THR:O	2.19	0.42
1:E:630:ARG:HD2	2:S:83:GLU:HG2	2.02	0.42
1:E:636:ALA:O	1:E:640:LYS:CA	2.67	0.42
1:E:656:THR:O	1:E:755:ARG:NH1	2.52	0.42
1:E:730:ASN:C	1:E:732:ILE:H	2.28	0.42
1:F:123:GLU:OE2	1:F:123:GLU:N	2.44	0.42
1:F:307:LEU:N	1:F:307:LEU:HD12	2.35	0.42
1:F:332:ASN:OD1	1:F:334:LEU:CD1	2.66	0.42
1:F:446:ILE:CG1	1:F:447:SER:N	2.81	0.42
1:F:654:ILE:HG22	1:F:655:ASN:ND2	2.35	0.42
1:F:661:ALA:O	1:F:665:LYS:HB2	2.20	0.42
1:F:723:PHE:O	1:F:724:ARG:C	2.62	0.42
1:F:760:VAL:O	1:F:764:LEU:HG	2.20	0.42
2:P:24:ASP:CG	2:P:25:GLY:H	2.28	0.42
2:P:109:MET:HE3	2:P:114:GLU:HB3	2.02	0.42
2:T:24:ASP:CG	2:T:25:GLY:H	2.27	0.42
2:T:43:PRO:CG	2:T:48:LEU:HD13	2.50	0.42
1:A:760:VAL:O	1:A:764:LEU:HG	2.20	0.41
1:B:136:PRO:O	1:B:138:ALA:N	2.53	0.41
1:B:231:LYS:O	1:B:232:GLU:C	2.63	0.41
1:B:285:LYS:C	1:B:287:GLY:N	2.78	0.41
1:B:301:ALA:O	1:B:302:LEU:C	2.63	0.41
1:B:395:GLU:OE1	1:B:395:GLU:N	2.53	0.41
1:B:723:PHE:O	1:B:724:ARG:C	2.61	0.41
1:B:775:LEU:O	1:B:776:LEU:C	2.63	0.41
1:C:97:TYR:O	1:C:100:LEU:N	2.52	0.41
1:C:115:LYS:O	1:C:117:LEU:N	2.53	0.41
1:C:269:ASN:O	1:C:273:LYS:HG3	2.20	0.41
1:C:288:VAL:O	1:C:290:LYS:N	2.53	0.41
1:C:688:PHE:CD2	1:C:688:PHE:C	2.98	0.41
1:C:711:ILE:H	1:C:711:ILE:HG12	1.68	0.41
1:D:169:VAL:HG23	1:D:246:SER:HB2	2.02	0.41
1:D:522:SER:O	2:R:124:MET:HE2	2.20	0.41
1:E:157:LYS:HD2	1:E:157:LYS:HA	1.84	0.41
1:E:179:LEU:O	1:E:183:SER:HB3	1.98	0.41
1:E:252:ASP:OD2	1:E:253:HIS:CD2	2.72	0.41
1:E:688:PHE:C	1:E:688:PHE:CD2	2.98	0.41
1:F:292:ARG:NE	1:F:617:LYS:NZ	2.68	0.41
1:F:550:SER:OG	1:F:551:ASN:N	2.53	0.41
2:O:58:ASP:CB	2:O:62:THR:HG23	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:97:ASN:ND2	2:O:99:TYR:H	2.18	0.41
2:Q:24:ASP:CG	2:Q:25:GLY:H	2.28	0.41
2:Q:73:ALA:C	2:Q:75:LYS:N	2.77	0.41
2:R:19:PHE:N	2:R:19:PHE:CD1	2.88	0.41
2:R:24:ASP:CG	2:R:25:GLY:H	2.28	0.41
2:T:24:ASP:OD1	2:T:25:GLY:N	2.52	0.41
1:A:88:LYS:HZ2	1:A:172:GLU:CD	2.27	0.41
1:A:141:PHE:N	1:A:141:PHE:CD1	2.88	0.41
1:A:482:GLU:O	1:A:484:VAL:HG23	2.20	0.41
1:A:654:ILE:HG22	1:A:655:ASN:HD22	1.86	0.41
1:B:295:VAL:HG12	1:B:605:THR:HA	2.03	0.41
1:C:97:TYR:HD2	1:C:102:GLY:HA3	1.84	0.41
1:C:301:ALA:O	1:C:302:LEU:C	2.63	0.41
1:C:323:ASN:O	1:C:324:THR:HG22	2.20	0.41
1:C:550:SER:OG	1:C:551:ASN:N	2.53	0.41
1:C:630:ARG:HH11	1:C:630:ARG:HG3	1.85	0.41
1:C:719:LYS:HD2	1:C:797:ILE:HD11	2.02	0.41
1:C:756:ILE:O	1:C:757:THR:C	2.64	0.41
1:C:776:LEU:C	1:C:776:LEU:CD2	2.93	0.41
1:D:85:LEU:HD12	1:D:168:GLU:OE1	2.21	0.41
1:D:89:ILE:HG22	1:D:90:PRO:HD2	2.00	0.41
1:D:305:SER:O	1:D:307:LEU:HD12	2.20	0.41
1:D:671:ARG:NH1	1:D:671:ARG:HG3	2.35	0.41
1:E:123:GLU:HG2	1:E:124:GLU:H	1.80	0.41
1:E:141:PHE:N	1:E:141:PHE:CD1	2.88	0.41
1:E:335:ALA:O	1:E:339:ILE:HG13	2.20	0.41
1:E:344:ALA:HB3	1:E:488:LEU:HD23	2.01	0.41
1:E:365:PRO:HB2	1:E:367:ASP:O	2.20	0.41
1:E:628:PHE:CE2	2:S:90:ARG:HD3	2.35	0.41
1:E:687:GLU:OE2	1:E:687:GLU:HA	2.20	0.41
1:E:735:VAL:O	1:E:738:SER:HB3	2.20	0.41
1:E:747:ASN:O	1:E:748:TYR:C	2.63	0.41
1:F:174:GLY:O	1:F:177:ILE:HG12	2.20	0.41
1:F:181:ILE:HG12	1:F:181:ILE:O	2.20	0.41
1:F:395:GLU:OE1	1:F:395:GLU:N	2.53	0.41
1:F:478:ALA:HA	1:F:488:LEU:HG	2.02	0.41
1:F:694:VAL:CG2	2:T:18:LEU:HD21	2.50	0.41
2:O:110:THR:O	2:O:113:GLY:N	2.47	0.41
2:R:43:PRO:CG	2:R:48:LEU:HD13	2.50	0.41
2:R:97:ASN:ND2	2:R:99:TYR:H	2.17	0.41
2:S:104:GLU:O	2:S:105:LEU:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:O	1:A:311:HIS:N	2.42	0.41
1:A:323:ASN:C	1:A:324:THR:HG22	2.44	0.41
1:A:323:ASN:O	1:A:324:THR:HG22	2.20	0.41
1:A:499:PRO:HD2	1:A:625:LEU:O	2.20	0.41
1:A:614:PHE:CD2	1:A:614:PHE:C	2.99	0.41
1:B:175:LYS:C	1:B:177:ILE:N	2.78	0.41
1:C:90:PRO:O	1:C:93:VAL:N	2.53	0.41
1:C:478:ALA:HA	1:C:488:LEU:HG	2.01	0.41
1:D:288:VAL:O	1:D:290:LYS:N	2.53	0.41
1:D:338:LEU:O	1:D:343:VAL:CG2	2.68	0.41
1:D:405:LEU:CD1	1:D:405:LEU:H	2.31	0.41
1:D:688:PHE:CD2	1:D:688:PHE:C	2.99	0.41
1:E:218:LEU:O	1:E:218:LEU:CG	2.67	0.41
1:E:380:VAL:C	1:E:383:GLY:H	2.28	0.41
1:E:389:LYS:HD2	1:E:393:GLU:OE1	2.20	0.41
1:E:413:LEU:N	1:E:413:LEU:HD23	2.35	0.41
1:E:526:GLN:O	1:E:527:LYS:C	2.62	0.41
1:E:538:ILE:HG21	2:S:87:GLU:HB2	2.01	0.41
1:E:565:LYS:C	1:E:567:THR:N	2.78	0.41
1:E:722:ILE:HD13	1:E:764:LEU:HD21	2.01	0.41
1:F:185:ASP:O	1:F:190:PRO:CA	2.67	0.41
1:F:796:ILE:O	1:F:796:ILE:HG22	2.21	0.41
2:Q:3:GLN:N	2:Q:77:LYS:NZ	2.60	0.41
2:Q:43:PRO:CG	2:Q:48:LEU:HD13	2.50	0.41
2:S:28:THR:HB	2:S:30:LYS:HZ3	1.84	0.41
2:S:69:LEU:HD12	2:S:69:LEU:C	2.45	0.41
2:S:97:ASN:ND2	2:S:99:TYR:H	2.18	0.41
2:S:109:MET:HE3	2:S:114:GLU:HB3	2.02	0.41
2:T:3:GLN:N	2:T:77:LYS:NZ	2.62	0.41
1:A:136:PRO:O	1:A:138:ALA:N	2.53	0.41
1:A:184:LYS:HZ1	1:A:191:GLU:CB	2.31	0.41
1:A:218:LEU:HD21	1:A:225:ILE:CD1	2.51	0.41
1:A:549:LEU:HB2	1:A:553:GLN:HE21	1.86	0.41
1:A:725:GLY:O	1:A:728:ALA:HB3	2.20	0.41
1:B:71:PHE:O	1:B:78:LYS:NZ	2.53	0.41
1:B:99:GLU:HG2	1:B:283:LEU:HB3	2.02	0.41
1:B:149:THR:HA	1:B:150:PRO:HD2	1.95	0.41
1:B:292:ARG:NE	1:B:617:LYS:NZ	2.68	0.41
1:B:307:LEU:HD12	1:B:307:LEU:N	2.35	0.41
1:B:628:PHE:CE2	2:P:90:ARG:HD3	2.36	0.41
1:B:630:ARG:CZ	2:P:83:GLU:CG	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:HIS:O	1:C:314:ALA:HB3	2.19	0.41
1:C:444:PHE:CD1	1:C:444:PHE:N	2.88	0.41
1:C:551:ASN:HD22	1:C:551:ASN:HA	1.56	0.41
1:C:767:GLN:HG2	1:C:768:LYS:HG2	2.02	0.41
1:D:231:LYS:O	1:D:232:GLU:C	2.63	0.41
1:D:311:HIS:O	1:D:312:ALA:C	2.63	0.41
1:D:337:ASN:C	1:D:339:ILE:N	2.75	0.41
1:D:550:SER:OG	1:D:551:ASN:N	2.53	0.41
1:D:636:ALA:O	1:D:640:LYS:CA	2.68	0.41
1:D:794:GLN:HE21	1:D:794:GLN:HB3	1.67	0.41
1:E:192:PHE:HD1	1:E:192:PHE:H	1.69	0.41
1:E:225:ILE:HG23	1:E:229:PHE:CD2	2.55	0.41
1:E:240:ALA:C	1:E:242:SER:N	2.79	0.41
1:E:278:LYS:HB2	1:E:279:ILE:HD13	2.02	0.41
1:E:279:ILE:HD13	1:E:279:ILE:H	1.84	0.41
1:E:323:ASN:O	1:E:324:THR:HG22	2.20	0.41
1:E:502:THR:H	1:E:502:THR:HG1	1.64	0.41
1:E:732:ILE:HG23	1:E:749:PHE:HD1	1.85	0.41
1:F:97:TYR:HD2	1:F:102:GLY:HA3	1.86	0.41
1:F:189:ASP:O	1:F:190:PRO:C	2.60	0.41
1:F:305:SER:C	1:F:307:LEU:H	2.28	0.41
1:F:687:GLU:OE2	1:F:687:GLU:HA	2.20	0.41
1:F:688:PHE:CD2	1:F:688:PHE:C	2.98	0.41
1:F:722:ILE:HD13	1:F:764:LEU:HD21	2.01	0.41
1:F:764:LEU:O	1:F:766:HIS:N	2.53	0.41
2:P:42:ASN:HA	2:P:43:PRO:HD2	1.89	0.41
2:R:58:ASP:CB	2:R:62:THR:HG23	2.47	0.41
2:R:100:ILE:O	2:R:136:VAL:HG22	2.20	0.41
2:S:43:PRO:CG	2:S:48:LEU:HD13	2.51	0.41
2:S:104:GLU:HG2	2:S:104:GLU:H	1.65	0.41
1:A:301:ALA:O	1:A:302:LEU:C	2.63	0.41
1:A:395:GLU:N	1:A:395:GLU:OE1	2.53	0.41
1:A:457:THR:CG2	1:A:468:LYS:HA	2.42	0.41
1:A:775:LEU:O	1:A:776:LEU:C	2.62	0.41
1:B:327:LEU:N	1:B:327:LEU:HD12	2.35	0.41
1:B:370:LEU:HD23	1:B:370:LEU:HA	1.90	0.41
1:B:607:ASN:HB2	1:B:610:MET:H	1.86	0.41
1:C:285:LYS:C	1:C:287:GLY:N	2.79	0.41
1:C:307:LEU:N	1:C:307:LEU:HD12	2.35	0.41
1:C:661:ALA:O	1:C:665:LYS:HB2	2.21	0.41
1:D:76:LEU:CD2	1:D:76:LEU:N	2.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PRO:O	1:D:93:VAL:N	2.52	0.41
1:D:92:ASP:C	1:D:94:LEU:N	2.77	0.41
1:D:105:TYR:N	1:D:152:LEU:O	2.40	0.41
1:D:500:SER:OG	1:D:502:THR:OG1	2.34	0.41
1:D:565:LYS:C	1:D:567:THR:N	2.78	0.41
1:D:654:ILE:HG22	1:D:655:ASN:ND2	2.35	0.41
1:D:710:HIS:C	1:D:712:PHE:H	2.29	0.41
1:D:777:TYR:HA	1:D:780:LEU:HD23	2.02	0.41
1:E:322:LEU:O	1:E:323:ASN:HB3	2.21	0.41
1:E:513:TRP:CD1	1:E:532:LEU:HD13	2.56	0.41
1:E:607:ASN:HB2	1:E:610:MET:H	1.86	0.41
1:E:719:LYS:O	1:E:720:ILE:C	2.62	0.41
1:E:765:THR:HG22	1:E:769:SER:HB2	2.02	0.41
1:F:90:PRO:HG2	1:F:93:VAL:HB	2.01	0.41
1:F:123:GLU:CG	1:F:124:GLU:H	2.32	0.41
1:F:254:ARG:H	1:F:254:ARG:CD	2.32	0.41
1:F:437:SER:C	1:F:439:ASN:H	2.27	0.41
1:F:513:TRP:CD1	1:F:532:LEU:HD13	2.56	0.41
2:O:109:MET:HE3	2:O:114:GLU:HB3	2.01	0.41
2:Q:100:ILE:O	2:Q:136:VAL:HG22	2.20	0.41
2:R:28:THR:HB	2:R:30:LYS:HZ3	1.85	0.41
2:R:83:GLU:O	2:R:87:GLU:HG3	2.21	0.41
2:S:102:ALA:HA	2:S:125:ILE:HG13	2.01	0.41
2:T:104:GLU:HG2	2:T:104:GLU:H	1.65	0.41
2:T:110:THR:O	2:T:113:GLY:N	2.47	0.41
1:A:688:PHE:C	1:A:688:PHE:CD2	2.98	0.41
1:B:97:TYR:O	1:B:100:LEU:N	2.54	0.41
1:B:199:LEU:O	1:B:201:ASP:N	2.54	0.41
1:B:218:LEU:HD21	1:B:225:ILE:CD1	2.51	0.41
1:B:295:VAL:HG21	1:B:603:ILE:CG2	2.50	0.41
1:B:368:GLN:C	1:B:370:LEU:N	2.79	0.41
1:B:636:ALA:O	1:B:640:LYS:CA	2.68	0.41
1:B:730:ASN:C	1:B:732:ILE:H	2.28	0.41
1:C:123:GLU:OE2	1:C:123:GLU:N	2.44	0.41
1:C:295:VAL:CG2	1:C:603:ILE:HG23	2.50	0.41
1:C:454:GLN:CB	1:C:472:ARG:O	2.69	0.41
1:C:561:ASN:OD1	1:C:574:VAL:N	2.42	0.41
1:C:694:VAL:CG2	2:Q:18:LEU:HD21	2.50	0.41
1:C:760:VAL:O	1:C:764:LEU:HG	2.20	0.41
1:C:775:LEU:O	1:C:776:LEU:C	2.63	0.41
1:D:493:ASP:OD2	1:D:577:HIS:CE1	2.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:GLU:HG3	1:E:147:ARG:H	1.85	0.41
1:E:305:SER:O	1:E:307:LEU:HD12	2.21	0.41
1:E:546:LYS:NZ	1:E:554:LYS:HE2	2.34	0.41
1:F:85:LEU:HD12	1:F:168:GLU:OE1	2.21	0.41
1:F:169:VAL:HG23	1:F:246:SER:HB2	2.01	0.41
1:F:173:ILE:O	1:F:176:GLY:N	2.54	0.41
1:F:692:GLU:OE2	1:F:692:GLU:HA	2.19	0.41
2:O:143:GLN:O	2:O:147:ALA:CB	2.69	0.41
2:P:117:THR:HG23	2:P:120:GLU:CB	2.46	0.41
2:S:89:PHE:C	2:S:91:VAL:N	2.77	0.41
1:A:217:LYS:HB2	1:A:236:GLU:OE1	2.21	0.41
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.34	0.41
1:A:263:ASP:C	1:A:265:PHE:N	2.77	0.41
1:A:516:VAL:O	1:A:519:THR:HG22	2.21	0.41
1:A:732:ILE:HG23	1:A:749:PHE:HD1	1.85	0.41
1:A:745:TYR:O	1:A:749:PHE:HD2	2.03	0.41
1:A:776:LEU:C	1:A:776:LEU:CD2	2.94	0.41
1:B:254:ARG:H	1:B:254:ARG:CD	2.32	0.41
1:B:311:HIS:O	1:B:312:ALA:C	2.63	0.41
1:B:373:LYS:O	1:B:380:VAL:CG2	2.69	0.41
1:B:515:LYS:HB3	1:B:515:LYS:HZ3	1.84	0.41
1:B:546:LYS:NZ	1:B:554:LYS:HE2	2.35	0.41
1:B:796:ILE:O	1:B:796:ILE:HG22	2.21	0.41
1:C:350:VAL:HG12	1:C:352:GLY:H	1.85	0.41
1:C:565:LYS:C	1:C:567:THR:N	2.78	0.41
1:C:630:ARG:NH1	1:C:630:ARG:HG3	2.34	0.41
1:C:671:ARG:HG3	1:C:671:ARG:HH11	1.85	0.41
1:C:732:ILE:HG23	1:C:749:PHE:HD1	1.86	0.41
1:D:252:ASP:OD2	1:D:253:HIS:CD2	2.73	0.41
1:D:454:GLN:CB	1:D:472:ARG:O	2.69	0.41
1:D:639:ASN:HD22	1:D:640:LYS:N	2.19	0.41
1:D:728:ALA:C	1:D:730:ASN:N	2.78	0.41
1:D:775:LEU:O	1:D:776:LEU:C	2.62	0.41
1:E:88:LYS:HZ2	1:E:172:GLU:CD	2.29	0.41
1:E:444:PHE:CD1	1:E:444:PHE:N	2.88	0.41
1:E:723:PHE:O	1:E:724:ARG:C	2.64	0.41
1:E:776:LEU:C	1:E:776:LEU:CD2	2.94	0.41
1:E:777:TYR:HA	1:E:780:LEU:HD23	2.02	0.41
1:F:131:ARG:HB2	1:F:170:TYR:CZ	2.56	0.41
1:F:322:LEU:O	1:F:323:ASN:HB3	2.21	0.41
1:F:549:LEU:HB2	1:F:553:GLN:HE21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:581:GLN:HE22	1:F:632:TYR:HE1	1.69	0.41
1:F:776:LEU:C	1:F:776:LEU:CD2	2.93	0.41
2:S:32:LEU:O	2:S:33:GLY:C	2.64	0.41
2:S:73:ALA:O	2:S:75:LYS:N	2.52	0.41
1:A:144:GLU:HB3	1:A:177:ILE:HD11	2.03	0.41
1:A:338:LEU:O	1:A:343:VAL:CG2	2.68	0.41
1:A:472:ARG:HH11	1:A:472:ARG:CB	2.34	0.41
1:A:551:ASN:HD22	1:A:551:ASN:HA	1.56	0.41
1:B:169:VAL:HG23	1:B:246:SER:HB2	2.03	0.41
1:B:178:SER:OG	1:B:179:LEU:N	2.53	0.41
1:B:296:LEU:CD2	1:B:296:LEU:N	2.38	0.41
1:B:338:LEU:O	1:B:343:VAL:CG2	2.68	0.41
1:B:454:GLN:CB	1:B:472:ARG:O	2.69	0.41
1:B:478:ALA:HA	1:B:488:LEU:HG	2.02	0.41
1:B:550:SER:OG	1:B:551:ASN:N	2.54	0.41
1:B:614:PHE:CD2	1:B:614:PHE:C	2.98	0.41
1:B:654:ILE:HG22	1:B:655:ASN:HD22	1.86	0.41
1:C:257:LEU:CD1	1:C:261:ALA:HB3	2.46	0.41
1:C:332:ASN:OD1	1:C:334:LEU:CD1	2.67	0.41
1:C:668:SER:OG	2:Q:10:ALA:HB1	2.20	0.41
1:D:81:GLN:NE2	1:D:156:ILE:HG21	2.35	0.41
1:D:343:VAL:HG12	1:D:344:ALA:N	2.35	0.41
1:D:581:GLN:HE22	1:D:632:TYR:HE1	1.67	0.41
1:D:715:GLU:OE1	1:D:767:GLN:NE2	2.54	0.41
1:D:760:VAL:O	1:D:764:LEU:HG	2.20	0.41
1:E:648:PRO:O	1:E:651:LYS:CB	2.69	0.41
1:E:760:VAL:O	1:E:764:LEU:HG	2.21	0.41
1:F:81:GLN:NE2	1:F:156:ILE:HG21	2.35	0.41
1:F:323:ASN:O	1:F:324:THR:HG22	2.21	0.41
1:F:389:LYS:HD2	1:F:393:GLU:OE1	2.20	0.41
1:F:435:LEU:HG	1:F:446:ILE:HG22	2.02	0.41
1:F:444:PHE:N	1:F:444:PHE:CD1	2.89	0.41
1:F:461:LYS:HA	1:F:461:LYS:HD2	1.79	0.41
1:F:472:ARG:HH11	1:F:472:ARG:CB	2.34	0.41
1:F:614:PHE:CD2	1:F:614:PHE:C	2.98	0.41
1:F:777:TYR:HA	1:F:780:LEU:HD23	2.02	0.41
2:P:13:LYS:NZ	2:P:65:PHE:CB	2.75	0.41
2:P:24:ASP:OD1	2:P:25:GLY:N	2.54	0.41
2:Q:102:ALA:HA	2:Q:125:ILE:HG13	2.01	0.41
2:R:24:ASP:OD1	2:R:25:GLY:N	2.53	0.41
2:R:69:LEU:HD12	2:R:69:LEU:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:110:THR:O	2:S:113:GLY:N	2.48	0.41
1:A:173:ILE:O	1:A:176:GLY:N	2.54	0.41
1:A:174:GLY:O	1:A:177:ILE:HG12	2.20	0.41
1:A:311:HIS:O	1:A:312:ALA:C	2.62	0.41
1:A:463:THR:O	1:A:466:GLY:N	2.50	0.41
1:A:660:SER:O	1:A:663:PHE:HB3	2.21	0.41
1:A:710:HIS:C	1:A:712:PHE:H	2.29	0.41
1:A:719:LYS:HD2	1:A:797:ILE:HD11	2.03	0.41
1:A:753:LYS:O	1:A:754:GLU:C	2.64	0.41
1:B:175:LYS:CB	1:B:175:LYS:HZ3	2.28	0.41
1:B:176:GLY:C	1:B:178:SER:H	2.28	0.41
1:B:380:VAL:C	1:B:383:GLY:H	2.29	0.41
1:B:389:LYS:HD2	1:B:393:GLU:OE1	2.20	0.41
1:B:671:ARG:HD2	2:P:14:GLU:HG2	2.02	0.41
1:C:81:GLN:NE2	1:C:156:ILE:HG21	2.35	0.41
1:C:153:ILE:C	1:C:154:ILE:HD13	2.43	0.41
1:C:169:VAL:HG23	1:C:246:SER:HB2	2.02	0.41
1:C:395:GLU:O	1:C:395:GLU:CD	2.64	0.41
1:C:413:LEU:N	1:C:413:LEU:HD23	2.35	0.41
1:C:549:LEU:HB2	1:C:553:GLN:HE21	1.86	0.41
1:C:654:ILE:HG22	1:C:655:ASN:ND2	2.35	0.41
1:D:90:PRO:HG2	1:D:93:VAL:HB	2.02	0.41
1:D:131:ARG:CB	1:D:170:TYR:OH	2.69	0.41
1:D:136:PRO:O	1:D:138:ALA:N	2.54	0.41
1:D:148:GLU:HG3	1:D:149:THR:H	1.83	0.41
1:D:161:ILE:CG2	1:D:161:ILE:O	2.69	0.41
1:D:218:LEU:HD21	1:D:225:ILE:CD1	2.50	0.41
1:D:239:HIS:O	1:D:243:LEU:HD12	2.21	0.41
1:D:322:LEU:O	1:D:323:ASN:HB3	2.21	0.41
1:D:326:ILE:C	1:D:327:LEU:HD12	2.45	0.41
1:D:368:GLN:C	1:D:370:LEU:N	2.78	0.41
1:D:389:LYS:HD2	1:D:393:GLU:OE1	2.21	0.41
1:D:395:GLU:OE1	1:D:395:GLU:N	2.54	0.41
1:D:614:PHE:CD2	1:D:614:PHE:C	2.99	0.41
1:D:622:LYS:HA	1:D:622:LYS:HD3	1.30	0.41
1:D:648:PRO:O	1:D:651:LYS:CB	2.69	0.41
1:D:668:SER:OG	2:R:10:ALA:CB	2.69	0.41
1:D:759:GLN:HA	1:D:759:GLN:NE2	2.21	0.41
1:E:90:PRO:O	1:E:93:VAL:N	2.53	0.41
1:E:97:TYR:O	1:E:100:LEU:N	2.54	0.41
1:E:175:LYS:C	1:E:177:ILE:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:HD21	1:E:225:ILE:CD1	2.51	0.41
1:E:279:ILE:CD1	1:E:279:ILE:H	2.29	0.41
1:E:305:SER:C	1:E:307:LEU:H	2.27	0.41
1:E:368:GLN:C	1:E:370:LEU:N	2.78	0.41
1:E:551:ASN:HD22	1:E:551:ASN:HA	1.56	0.41
1:E:614:PHE:CD2	1:E:614:PHE:C	2.99	0.41
1:E:639:ASN:HD22	1:E:640:LYS:N	2.19	0.41
1:E:668:SER:OG	2:S:10:ALA:HB1	2.21	0.41
1:F:136:PRO:O	1:F:138:ALA:N	2.54	0.41
1:F:149:THR:HA	1:F:150:PRO:HD2	1.94	0.41
1:F:184:LYS:HZ1	1:F:191:GLU:CB	2.32	0.41
1:F:240:ALA:C	1:F:242:SER:N	2.78	0.41
1:F:252:ASP:OD2	1:F:253:HIS:CD2	2.73	0.41
1:F:269:ASN:O	1:F:273:LYS:HG3	2.21	0.41
1:F:305:SER:O	1:F:307:LEU:HD12	2.21	0.41
1:F:350:VAL:HG12	1:F:352:GLY:H	1.85	0.41
1:F:454:GLN:CB	1:F:472:ARG:O	2.69	0.41
1:F:561:ASN:OD1	1:F:574:VAL:N	2.41	0.41
1:F:621:GLY:HA2	2:T:94:LYS:NZ	2.36	0.41
1:F:635:ILE:N	1:F:635:ILE:CD1	2.79	0.41
1:F:747:ASN:O	1:F:748:TYR:C	2.64	0.41
1:F:759:GLN:CA	1:F:759:GLN:NE2	2.82	0.41
2:O:43:PRO:HG3	2:O:48:LEU:HD13	2.01	0.41
2:P:43:PRO:HG3	2:P:48:LEU:HD13	2.01	0.41
2:P:43:PRO:CG	2:P:48:LEU:HD13	2.50	0.41
2:Q:19:PHE:CD1	2:Q:19:PHE:N	2.88	0.41
2:Q:24:ASP:OD1	2:Q:25:GLY:N	2.54	0.41
2:Q:42:ASN:HA	2:Q:43:PRO:HD2	1.93	0.41
2:Q:58:ASP:CB	2:Q:62:THR:HG23	2.46	0.41
2:S:3:GLN:N	2:S:77:LYS:NZ	2.61	0.41
2:S:18:LEU:HD23	2:S:18:LEU:HA	1.83	0.41
2:S:24:ASP:CG	2:S:25:GLY:H	2.28	0.41
2:T:32:LEU:O	2:T:33:GLY:C	2.64	0.41
2:T:89:PHE:O	2:T:91:VAL:N	2.54	0.41
1:A:322:LEU:O	1:A:323:ASN:HB3	2.21	0.41
1:A:639:ASN:HD22	1:A:640:LYS:N	2.19	0.41
1:B:184:LYS:HE2	1:B:193:LEU:CD1	2.51	0.41
1:B:444:PHE:CD1	1:B:444:PHE:N	2.88	0.41
1:B:499:PRO:HD2	1:B:625:LEU:O	2.21	0.41
1:B:565:LYS:C	1:B:567:THR:N	2.78	0.41
1:B:741:ILE:O	1:B:742:ALA:O	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LYS:O	1:B:754:GLU:C	2.64	0.41
1:C:131:ARG:HB2	1:C:170:TYR:OH	2.21	0.41
1:C:184:LYS:HE2	1:C:193:LEU:HD12	2.03	0.41
1:C:218:LEU:O	1:C:218:LEU:CG	2.67	0.41
1:C:444:PHE:HA	1:C:454:GLN:O	2.21	0.41
1:C:581:GLN:HE22	1:C:632:TYR:HE1	1.68	0.41
1:C:656:THR:O	1:C:755:ARG:NH1	2.54	0.41
1:C:710:HIS:C	1:C:712:PHE:H	2.28	0.41
1:D:373:LYS:O	1:D:380:VAL:CG2	2.69	0.41
1:E:104:ILE:HG23	1:E:152:LEU:HD22	2.01	0.41
1:E:136:PRO:O	1:E:138:ALA:N	2.54	0.41
1:E:254:ARG:H	1:E:254:ARG:CD	2.32	0.41
1:E:735:VAL:O	1:E:738:SER:CB	2.69	0.41
1:F:413:LEU:N	1:F:413:LEU:HD23	2.35	0.41
1:F:565:LYS:C	1:F:567:THR:N	2.79	0.41
1:F:639:ASN:HD22	1:F:640:LYS:N	2.19	0.41
2:P:55:VAL:CG2	2:P:67:GLU:OE1	2.67	0.41
2:P:69:LEU:HD12	2:P:69:LEU:C	2.45	0.41
2:R:13:LYS:NZ	2:R:65:PHE:CB	2.73	0.41
2:S:48:LEU:HA	2:S:51:MET:CE	2.51	0.41
1:A:89:ILE:CG2	1:A:93:VAL:HG11	2.40	0.40
1:A:777:TYR:HA	1:A:780:LEU:HD23	2.03	0.40
1:B:345:THR:CG2	1:B:491:ASP:HA	2.51	0.40
1:B:395:GLU:CD	1:B:395:GLU:O	2.65	0.40
1:B:665:LYS:O	1:B:668:SER:HB3	2.21	0.40
1:B:710:HIS:C	1:B:712:PHE:H	2.28	0.40
1:C:461:LYS:HA	1:C:461:LYS:HD2	1.79	0.40
1:C:501:LEU:CD1	2:Q:108:VAL:HG13	2.50	0.40
1:C:777:TYR:HA	1:C:780:LEU:HD23	2.01	0.40
1:D:122:GLU:HG3	1:D:147:ARG:H	1.85	0.40
1:D:296:LEU:N	1:D:296:LEU:CD2	2.38	0.40
1:D:323:ASN:O	1:D:324:THR:HG22	2.21	0.40
1:D:403:LEU:CG	1:D:405:LEU:CD1	2.99	0.40
1:E:90:PRO:HD3	1:E:249:PHE:CE2	2.56	0.40
1:E:128:MET:HE2	1:E:239:HIS:CE1	2.55	0.40
1:E:176:GLY:C	1:E:178:SER:H	2.29	0.40
1:E:596:ILE:O	1:E:596:ILE:HG22	2.20	0.40
1:E:630:ARG:NH1	1:E:630:ARG:HG3	2.37	0.40
1:F:499:PRO:HD2	1:F:625:LEU:O	2.21	0.40
1:F:636:ALA:O	1:F:640:LYS:CA	2.69	0.40
2:O:124:MET:O	2:O:125:ILE:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:117:THR:C	2:P:119:GLU:N	2.76	0.40
2:Q:10:ALA:O	2:Q:14:GLU:HB2	2.21	0.40
2:Q:18:LEU:HD23	2:Q:18:LEU:HA	1.83	0.40
2:Q:32:LEU:O	2:Q:33:GLY:C	2.64	0.40
2:Q:124:MET:O	2:Q:125:ILE:C	2.64	0.40
2:R:89:PHE:C	2:R:91:VAL:N	2.79	0.40
2:S:71:MET:HG2	2:S:71:MET:O	2.21	0.40
1:A:91:LYS:O	1:A:94:LEU:HB2	2.21	0.40
1:A:175:LYS:C	1:A:177:ILE:N	2.79	0.40
1:A:184:LYS:HE2	1:A:193:LEU:CD1	2.51	0.40
1:A:335:ALA:O	1:A:339:ILE:HG13	2.21	0.40
1:A:767:GLN:HG2	1:A:768:LYS:HG2	2.02	0.40
1:B:513:TRP:CD1	1:B:532:LEU:HD13	2.56	0.40
1:B:632:TYR:O	1:B:633:ASN:CB	2.69	0.40
1:B:688:PHE:C	1:B:688:PHE:CD2	2.99	0.40
1:B:760:VAL:O	1:B:764:LEU:HG	2.21	0.40
1:C:310:GLU:O	1:C:314:ALA:HB2	2.21	0.40
1:C:397:GLU:O	1:C:480:ASN:N	2.55	0.40
1:C:538:ILE:HG21	2:Q:87:GLU:HB2	2.03	0.40
1:C:636:ALA:O	1:C:640:LYS:CA	2.69	0.40
1:C:668:SER:OG	2:Q:10:ALA:CB	2.69	0.40
1:C:747:ASN:O	1:C:748:TYR:C	2.63	0.40
1:D:175:LYS:C	1:D:177:ILE:N	2.79	0.40
1:D:239:HIS:O	1:D:243:LEU:HG	2.22	0.40
1:D:301:ALA:O	1:D:302:LEU:C	2.63	0.40
1:D:444:PHE:CD1	1:D:444:PHE:N	2.88	0.40
1:D:513:TRP:CD1	1:D:532:LEU:HD13	2.57	0.40
1:D:661:ALA:O	1:D:665:LYS:HB2	2.22	0.40
1:E:144:GLU:HB3	1:E:177:ILE:HD11	2.04	0.40
1:E:269:ASN:O	1:E:273:LYS:HG3	2.21	0.40
1:E:285:LYS:C	1:E:287:GLY:N	2.79	0.40
1:E:454:GLN:CB	1:E:472:ARG:O	2.69	0.40
1:F:175:LYS:C	1:F:177:ILE:N	2.77	0.40
2:P:71:MET:HG2	2:P:71:MET:O	2.21	0.40
2:R:10:ALA:O	2:R:14:GLU:HB2	2.20	0.40
2:R:102:ALA:CA	2:R:125:ILE:HG13	2.52	0.40
2:T:29:THR:O	2:T:30:LYS:C	2.65	0.40
2:T:48:LEU:HA	2:T:51:MET:CE	2.51	0.40
2:T:73:ALA:C	2:T:75:LYS:N	2.79	0.40
2:T:100:ILE:O	2:T:136:VAL:HG22	2.21	0.40
1:A:176:GLY:C	1:A:178:SER:H	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:O	1:A:232:GLU:C	2.63	0.40
1:A:269:ASN:O	1:A:273:LYS:HG3	2.21	0.40
1:A:310:GLU:O	1:A:314:ALA:HB2	2.22	0.40
1:A:444:PHE:CD1	1:A:444:PHE:N	2.89	0.40
1:A:630:ARG:HG3	1:A:630:ARG:HH11	1.87	0.40
1:A:632:TYR:O	1:A:633:ASN:CB	2.70	0.40
1:A:665:LYS:O	1:A:668:SER:HB3	2.21	0.40
1:A:715:GLU:OE1	1:A:767:GLN:NE2	2.54	0.40
1:A:759:GLN:HA	1:A:759:GLN:NE2	2.22	0.40
1:B:115:LYS:O	1:B:117:LEU:N	2.54	0.40
1:B:288:VAL:O	1:B:290:LYS:N	2.54	0.40
1:B:308:VAL:O	1:B:311:HIS:N	2.42	0.40
1:B:472:ARG:HH11	1:B:472:ARG:CB	2.35	0.40
1:B:635:ILE:H	1:B:635:ILE:CD1	2.16	0.40
1:C:85:LEU:HD12	1:C:85:LEU:HA	1.81	0.40
1:C:136:PRO:O	1:C:138:ALA:N	2.55	0.40
1:C:311:HIS:O	1:C:312:ALA:C	2.63	0.40
1:C:326:ILE:C	1:C:327:LEU:HD12	2.46	0.40
1:C:373:LYS:O	1:C:380:VAL:CG2	2.69	0.40
1:C:472:ARG:HH11	1:C:472:ARG:CB	2.34	0.40
1:C:614:PHE:CD2	1:C:614:PHE:C	2.98	0.40
1:C:728:ALA:C	1:C:730:ASN:N	2.78	0.40
1:D:99:GLU:OE2	1:D:284:LYS:HE3	2.21	0.40
1:D:176:GLY:C	1:D:178:SER:H	2.28	0.40
1:D:472:ARG:HH11	1:D:472:ARG:CB	2.34	0.40
1:D:609:GLU:O	1:D:613:ARG:N	2.49	0.40
1:D:677:GLY:HA2	1:D:745:TYR:OH	2.20	0.40
1:D:756:ILE:O	1:D:757:THR:C	2.64	0.40
1:E:239:HIS:O	1:E:243:LEU:HG	2.22	0.40
1:E:332:ASN:OD1	1:E:334:LEU:N	2.47	0.40
1:F:71:PHE:O	1:F:78:LYS:NZ	2.54	0.40
1:F:176:GLY:C	1:F:178:SER:H	2.30	0.40
1:F:373:LYS:O	1:F:380:VAL:CG2	2.69	0.40
1:F:719:LYS:HD2	1:F:797:ILE:HD11	2.03	0.40
1:F:732:ILE:HG23	1:F:749:PHE:HD1	1.86	0.40
2:O:66:PRO:O	2:O:67:GLU:C	2.64	0.40
2:P:19:PHE:CD1	2:P:19:PHE:N	2.89	0.40
2:P:48:LEU:HA	2:P:51:MET:CE	2.50	0.40
2:S:29:THR:O	2:S:30:LYS:C	2.65	0.40
2:T:124:MET:O	2:T:125:ILE:C	2.63	0.40
1:A:153:ILE:C	1:A:154:ILE:HD13	2.43	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LYS:C	1:A:287:GLY:N	2.79	0.40
1:A:305:SER:O	1:A:307:LEU:HD12	2.21	0.40
1:A:500:SER:OG	1:A:502:THR:OG1	2.36	0.40
1:B:239:HIS:O	1:B:243:LEU:HD12	2.21	0.40
1:B:305:SER:O	1:B:307:LEU:HD12	2.21	0.40
1:B:728:ALA:C	1:B:730:ASN:N	2.78	0.40
1:C:239:HIS:O	1:C:243:LEU:HG	2.22	0.40
1:C:513:TRP:CD1	1:C:532:LEU:HD13	2.57	0.40
1:C:622:LYS:HD3	1:C:622:LYS:HA	1.93	0.40
1:C:661:ALA:HB2	2:Q:39:LEU:C	2.47	0.40
1:C:671:ARG:HD2	2:Q:14:GLU:HG2	2.04	0.40
1:D:199:LEU:C	1:D:201:ASP:N	2.70	0.40
1:D:254:ARG:HB3	1:D:254:ARG:NH1	2.34	0.40
1:D:332:ASN:OD1	1:D:334:LEU:CD1	2.67	0.40
1:D:753:LYS:O	1:D:754:GLU:C	2.65	0.40
1:D:767:GLN:HG2	1:D:768:LYS:HG2	2.02	0.40
1:D:796:ILE:O	1:D:796:ILE:HG22	2.21	0.40
1:E:263:ASP:C	1:E:265:PHE:N	2.77	0.40
1:E:378:LEU:HA	1:E:381:GLU:HB3	2.03	0.40
1:E:395:GLU:CD	1:E:395:GLU:O	2.65	0.40
1:F:88:LYS:HB3	1:F:88:LYS:HE3	1.89	0.40
1:F:91:LYS:O	1:F:94:LEU:HB2	2.21	0.40
1:F:663:PHE:CE1	1:F:752:LEU:HD11	2.56	0.40
1:F:671:ARG:HG3	1:F:671:ARG:HH11	1.85	0.40
1:F:690:LYS:O	1:F:693:SER:HB3	2.21	0.40
1:F:730:ASN:C	1:F:732:ILE:H	2.30	0.40
1:F:748:TYR:O	1:F:751:TYR:HB3	2.22	0.40
2:O:108:VAL:HG12	2:O:112:LEU:HD12	2.04	0.40
2:P:18:LEU:HA	2:P:18:LEU:HD23	1.83	0.40
2:P:30:LYS:H	2:P:30:LYS:CD	2.13	0.40
2:Q:69:LEU:HD12	2:Q:69:LEU:C	2.47	0.40
2:R:109:MET:HE3	2:R:114:GLU:HB3	2.02	0.40
2:R:143:GLN:O	2:R:147:ALA:CB	2.70	0.40
2:T:30:LYS:HE2	2:T:30:LYS:HB2	1.95	0.40
2:T:39:LEU:HD23	2:T:39:LEU:HA	1.84	0.40
1:A:71:PHE:O	1:A:78:LYS:NZ	2.54	0.40
1:A:426:ILE:HD13	1:A:426:ILE:HA	1.92	0.40
1:A:654:ILE:HG22	1:A:655:ASN:ND2	2.36	0.40
1:A:796:ILE:O	1:A:796:ILE:HG22	2.22	0.40
1:B:311:HIS:O	1:B:314:ALA:HB3	2.22	0.40
1:B:516:VAL:O	1:B:519:THR:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ILE:O	1:B:596:ILE:HG22	2.20	0.40
1:B:671:ARG:HG3	1:B:671:ARG:HH11	1.86	0.40
1:C:240:ALA:C	1:C:242:SER:N	2.79	0.40
1:C:389:LYS:HD2	1:C:393:GLU:OE1	2.21	0.40
1:C:597:ASN:C	1:C:599:GLU:N	2.79	0.40
1:C:687:GLU:OE2	1:C:687:GLU:HA	2.21	0.40
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.82	0.40
1:D:161:ILE:HG21	1:D:168:GLU:HB2	2.03	0.40
1:D:240:ALA:C	1:D:242:SER:N	2.79	0.40
1:D:789:ASN:O	1:D:792:VAL:HB	2.22	0.40
1:E:311:HIS:O	1:E:314:ALA:HB3	2.21	0.40
1:E:326:ILE:C	1:E:327:LEU:HD12	2.47	0.40
1:E:479:LYS:CG	1:E:488:LEU:HD21	2.41	0.40
1:E:499:PRO:HD2	1:E:625:LEU:O	2.22	0.40
1:E:525:LYS:HE2	2:S:114:GLU:CG	2.50	0.40
1:E:685:LYS:HD3	1:E:685:LYS:HA	1.91	0.40
1:F:188:LEU:H	1:F:188:LEU:HD22	1.75	0.40
1:F:288:VAL:O	1:F:290:LYS:N	2.54	0.40
1:F:397:GLU:HA	1:F:480:ASN:HB2	2.04	0.40
1:F:629:ASN:ND2	1:F:630:ARG:N	2.69	0.40
2:O:9:ILE:HD12	2:O:69:LEU:HD22	2.04	0.40
2:O:32:LEU:O	2:O:33:GLY:C	2.64	0.40
2:O:48:LEU:HA	2:O:51:MET:CE	2.51	0.40
2:P:10:ALA:O	2:P:14:GLU:HB2	2.20	0.40
2:R:48:LEU:HA	2:R:51:MET:CE	2.52	0.40
2:S:48:LEU:HA	2:S:51:MET:HE2	2.04	0.40
2:T:124:MET:O	2:T:126:ARG:N	2.54	0.40

There are no symmetry-related clashes.

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	733/777 (94%)	512 (70%)	172 (24%)	49 (7%)	1	6
1	B	733/777 (94%)	512 (70%)	172 (24%)	49 (7%)	1	6
1	C	733/777 (94%)	510 (70%)	172 (24%)	51 (7%)	1	6
1	D	733/777 (94%)	516 (70%)	168 (23%)	49 (7%)	1	6
1	E	733/777 (94%)	512 (70%)	171 (23%)	50 (7%)	1	6
1	F	733/777 (94%)	513 (70%)	169 (23%)	51 (7%)	1	6
2	O	144/149 (97%)	100 (69%)	35 (24%)	9 (6%)	1	7
2	P	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	7
2	Q	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	7
2	R	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	7
2	S	144/149 (97%)	102 (71%)	33 (23%)	9 (6%)	1	7
2	T	144/149 (97%)	100 (69%)	35 (24%)	9 (6%)	1	7
All	All	5262/5556 (95%)	3683 (70%)	1226 (23%)	353 (7%)	1	6

All (353) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PHE
1	A	183	SER
1	A	377	GLN
1	A	510	GLN
1	A	787	THR
1	B	137	PHE
1	B	183	SER
1	B	192	PHE
1	B	377	GLN
1	B	510	GLN
1	B	787	THR
1	C	137	PHE
1	C	181	ILE
1	C	183	SER
1	C	192	PHE
1	C	377	GLN
1	C	510	GLN
1	C	787	THR
1	D	137	PHE
1	D	183	SER
1	D	377	GLN
1	D	510	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	787	THR
1	E	137	PHE
1	E	183	SER
1	E	192	PHE
1	E	377	GLN
1	E	510	GLN
1	E	787	THR
1	F	137	PHE
1	F	181	ILE
1	F	192	PHE
1	F	377	GLN
1	F	510	GLN
1	F	787	THR
1	A	80	GLN
1	A	113	GLU
1	A	116	GLU
1	A	138	ALA
1	A	165	GLN
1	A	176	GLY
1	A	181	ILE
1	A	187	SER
1	A	192	PHE
1	A	302	LEU
1	A	376	GLN
1	A	385	LEU
1	A	438	ASN
1	A	580	GLU
1	A	756	ILE
1	A	765	THR
1	B	80	GLN
1	B	113	GLU
1	B	116	GLU
1	B	138	ALA
1	B	165	GLN
1	B	176	GLY
1	B	181	ILE
1	B	187	SER
1	B	302	LEU
1	B	376	GLN
1	B	385	LEU
1	B	438	ASN
1	B	580	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	620	THR
1	B	756	ILE
1	B	765	THR
1	C	80	GLN
1	C	113	GLU
1	C	116	GLU
1	C	138	ALA
1	C	165	GLN
1	C	176	GLY
1	C	187	SER
1	C	302	LEU
1	C	376	GLN
1	C	385	LEU
1	C	438	ASN
1	C	580	GLU
1	C	620	THR
1	C	765	THR
1	D	80	GLN
1	D	113	GLU
1	D	116	GLU
1	D	138	ALA
1	D	165	GLN
1	D	176	GLY
1	D	181	ILE
1	D	187	SER
1	D	192	PHE
1	D	302	LEU
1	D	376	GLN
1	D	385	LEU
1	D	438	ASN
1	D	580	GLU
1	D	756	ILE
1	D	765	THR
1	E	80	GLN
1	E	113	GLU
1	E	116	GLU
1	E	138	ALA
1	E	165	GLN
1	E	176	GLY
1	E	181	ILE
1	E	187	SER
1	E	302	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	376	GLN
1	E	385	LEU
1	E	438	ASN
1	E	580	GLU
1	E	765	THR
1	F	80	GLN
1	F	113	GLU
1	F	116	GLU
1	F	138	ALA
1	F	165	GLN
1	F	176	GLY
1	F	187	SER
1	F	302	LEU
1	F	376	GLN
1	F	385	LEU
1	F	438	ASN
1	F	580	GLU
1	F	756	ILE
1	F	765	THR
2	O	12	PHE
2	O	22	ASP
2	O	23	GLY
2	P	12	PHE
2	P	22	ASP
2	P	23	GLY
2	Q	12	PHE
2	Q	22	ASP
2	Q	23	GLY
2	R	12	PHE
2	R	22	ASP
2	R	23	GLY
2	S	12	PHE
2	S	22	ASP
2	S	23	GLY
2	T	12	PHE
2	T	22	ASP
2	T	23	GLY
1	A	84	ASP
1	A	180	ASP
1	A	290	LYS
1	A	392	THR
1	A	413	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	ASN
1	A	620	THR
1	A	646	THR
1	B	84	ASP
1	B	180	ASP
1	B	290	LYS
1	B	392	THR
1	B	413	LEU
1	B	451	ASN
1	B	646	THR
1	C	84	ASP
1	C	180	ASP
1	C	290	LYS
1	C	392	THR
1	C	413	LEU
1	C	451	ASN
1	C	646	THR
1	C	756	ILE
1	D	84	ASP
1	D	180	ASP
1	D	290	LYS
1	D	392	THR
1	D	413	LEU
1	D	451	ASN
1	D	620	THR
1	D	646	THR
1	E	84	ASP
1	E	180	ASP
1	E	290	LYS
1	E	392	THR
1	E	413	LEU
1	E	451	ASN
1	E	620	THR
1	E	646	THR
1	E	756	ILE
1	F	84	ASP
1	F	180	ASP
1	F	183	SER
1	F	290	LYS
1	F	392	THR
1	F	413	LEU
1	F	451	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	620	THR
1	F	646	THR
2	O	74	ARG
2	Q	74	ARG
2	R	74	ARG
2	T	74	ARG
1	A	91	LYS
1	A	274	GLY
1	A	515	LYS
1	A	598	PRO
1	A	675	ASN
1	A	731	GLU
1	A	755	ARG
1	B	91	LYS
1	B	112	VAL
1	B	274	GLY
1	B	515	LYS
1	B	598	PRO
1	B	675	ASN
1	B	731	GLU
1	B	755	ARG
1	C	131	ARG
1	C	274	GLY
1	C	515	LYS
1	C	598	PRO
1	C	675	ASN
1	C	755	ARG
1	D	274	GLY
1	D	515	LYS
1	D	598	PRO
1	D	675	ASN
1	D	755	ARG
1	E	190	PRO
1	E	274	GLY
1	E	515	LYS
1	E	598	PRO
1	E	675	ASN
1	E	755	ARG
1	F	91	LYS
1	F	274	GLY
1	F	334	LEU
1	F	515	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	598	PRO
1	F	675	ASN
1	F	755	ARG
2	O	147	ALA
2	P	74	ARG
2	S	74	ARG
1	A	100	LEU
1	A	232	GLU
1	A	278	LYS
1	A	334	LEU
1	A	449	GLU
1	A	506	LYS
1	A	520	PRO
1	B	100	LEU
1	B	232	GLU
1	B	278	LYS
1	B	334	LEU
1	B	449	GLU
1	B	520	PRO
1	B	779	GLN
1	C	91	LYS
1	C	100	LEU
1	C	232	GLU
1	C	278	LYS
1	C	334	LEU
1	C	506	LYS
1	C	520	PRO
1	C	779	GLN
1	D	91	LYS
1	D	100	LEU
1	D	232	GLU
1	D	334	LEU
1	D	520	PRO
1	D	731	GLU
1	D	779	GLN
1	E	91	LYS
1	E	100	LEU
1	E	112	VAL
1	E	232	GLU
1	E	278	LYS
1	E	334	LEU
1	E	449	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	506	LYS
1	E	520	PRO
1	E	731	GLU
1	E	779	GLN
1	F	100	LEU
1	F	190	PRO
1	F	232	GLU
1	F	449	GLU
1	F	506	LYS
1	F	520	PRO
1	F	731	GLU
1	F	779	GLN
2	O	24	ASP
2	P	24	ASP
2	P	147	ALA
2	Q	24	ASP
2	Q	147	ALA
2	R	24	ASP
2	R	147	ALA
2	S	24	ASP
2	S	147	ALA
2	T	24	ASP
2	T	147	ALA
1	A	779	GLN
1	B	506	LYS
1	B	742	ALA
1	C	423	LYS
1	C	449	GLU
1	C	731	GLU
1	D	278	LYS
1	D	369	ASP
1	D	449	GLU
1	F	278	LYS
1	F	423	LYS
1	F	742	ALA
2	P	61	GLY
2	Q	61	GLY
2	R	61	GLY
2	S	61	GLY
2	T	61	GLY
1	A	112	VAL
1	A	742	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	742	ALA
1	D	742	ALA
1	E	742	ALA
2	O	61	GLY
1	A	309	PRO
1	B	309	PRO
1	C	190	PRO
1	D	309	PRO
1	E	309	PRO
2	O	25	GLY
2	P	25	GLY
2	Q	25	GLY
2	R	25	GLY
2	S	25	GLY
2	T	25	GLY
1	A	441	VAL
1	B	441	VAL
1	C	309	PRO
1	C	441	VAL
1	D	441	VAL
1	E	441	VAL
1	F	112	VAL
1	F	309	PRO
1	F	441	VAL
2	T	125	ILE
1	A	637	PRO
1	B	637	PRO
1	C	637	PRO
2	P	125	ILE
2	Q	125	ILE
2	S	125	ILE
1	D	112	VAL
1	D	637	PRO
1	E	637	PRO
1	F	637	PRO
2	O	125	ILE
2	R	125	ILE

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	664/705 (94%)	576 (87%)	88 (13%)	4	15
1	B	664/705 (94%)	574 (86%)	90 (14%)	3	15
1	C	664/705 (94%)	576 (87%)	88 (13%)	4	15
1	D	664/705 (94%)	574 (86%)	90 (14%)	3	15
1	E	664/705 (94%)	574 (86%)	90 (14%)	3	15
1	F	664/705 (94%)	574 (86%)	90 (14%)	3	15
2	O	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	P	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	Q	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	R	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	S	123/127 (97%)	104 (85%)	19 (15%)	2	10
2	T	123/127 (97%)	104 (85%)	19 (15%)	2	10
All	All	4722/4992 (95%)	4068 (86%)	654 (14%)	3	14

All (654) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	78	LYS
1	A	110	ASP
1	A	112	VAL
1	A	114	HIS
1	A	115	LYS
1	A	117	LEU
1	A	120	LEU
1	A	124	GLU
1	A	129	ASN
1	A	133	GLU
1	A	137	PHE
1	A	144	GLU
1	A	147	ARG
1	A	149	THR
1	A	156	ILE
1	A	158	ASP
1	A	172	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	173	ILE
1	A	175	LYS
1	A	179	LEU
1	A	180	ASP
1	A	182	ILE
1	A	186	LYS
1	A	188	LEU
1	A	190	PRO
1	A	197	LYS
1	A	202	ASP
1	A	209	LEU
1	A	213	LYS
1	A	217	LYS
1	A	229	PHE
1	A	236	GLU
1	A	254	ARG
1	A	279	ILE
1	A	284	LYS
1	A	296	LEU
1	A	309	PRO
1	A	324	THR
1	A	334	LEU
1	A	349	ASN
1	A	356	ASP
1	A	385	LEU
1	A	395	GLU
1	A	397	GLU
1	A	400	LYS
1	A	408	LEU
1	A	410	ILE
1	A	414	LYS
1	A	415	GLU
1	A	420	LEU
1	A	434	LEU
1	A	446	ILE
1	A	455	TYR
1	A	473	ASN
1	A	475	GLU
1	A	479	LYS
1	A	484	VAL
1	A	501	LEU
1	A	502	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	514	ASP
1	A	515	LYS
1	A	533	LEU
1	A	562	GLU
1	A	582	ASP
1	A	588	GLU
1	A	602	PHE
1	A	635	ILE
1	A	639	ASN
1	A	644	GLU
1	A	646	THR
1	A	655	ASN
1	A	665	LYS
1	A	672	ARG
1	A	678	VAL
1	A	702	SER
1	A	709	ASN
1	A	714	GLN
1	A	715	GLU
1	A	734	ASN
1	A	744	GLU
1	A	755	ARG
1	A	759	GLN
1	A	766	HIS
1	A	767	GLN
1	A	770	ASN
1	A	780	LEU
1	A	794	GLN
1	B	64	ASN
1	B	71	PHE
1	B	78	LYS
1	B	110	ASP
1	B	112	VAL
1	B	114	HIS
1	B	115	LYS
1	B	117	LEU
1	B	120	LEU
1	B	124	GLU
1	B	129	ASN
1	B	130	SER
1	B	133	GLU
1	B	137	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	144	GLU
1	B	147	ARG
1	B	149	THR
1	B	156	ILE
1	B	158	ASP
1	B	172	GLU
1	B	173	ILE
1	B	175	LYS
1	B	179	LEU
1	B	180	ASP
1	B	182	ILE
1	B	186	LYS
1	B	188	LEU
1	B	197	LYS
1	B	202	ASP
1	B	209	LEU
1	B	213	LYS
1	B	217	LYS
1	B	229	PHE
1	B	236	GLU
1	B	254	ARG
1	B	279	ILE
1	B	284	LYS
1	B	296	LEU
1	B	309	PRO
1	B	324	THR
1	B	334	LEU
1	B	349	ASN
1	B	356	ASP
1	B	385	LEU
1	B	395	GLU
1	B	397	GLU
1	B	400	LYS
1	B	408	LEU
1	B	410	ILE
1	B	414	LYS
1	B	415	GLU
1	B	420	LEU
1	B	434	LEU
1	B	446	ILE
1	B	455	TYR
1	B	473	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	475	GLU
1	B	479	LYS
1	B	484	VAL
1	B	501	LEU
1	B	502	THR
1	B	514	ASP
1	B	515	LYS
1	B	533	LEU
1	B	562	GLU
1	B	582	ASP
1	B	588	GLU
1	B	602	PHE
1	B	622	LYS
1	B	635	ILE
1	B	639	ASN
1	B	644	GLU
1	B	646	THR
1	B	655	ASN
1	B	665	LYS
1	B	672	ARG
1	B	678	VAL
1	B	702	SER
1	B	709	ASN
1	B	714	GLN
1	B	715	GLU
1	B	734	ASN
1	B	744	GLU
1	B	755	ARG
1	B	759	GLN
1	B	766	HIS
1	B	767	GLN
1	B	770	ASN
1	B	780	LEU
1	B	794	GLN
1	C	71	PHE
1	C	78	LYS
1	C	110	ASP
1	C	112	VAL
1	C	114	HIS
1	C	115	LYS
1	C	117	LEU
1	C	120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	124	GLU
1	C	129	ASN
1	C	133	GLU
1	C	137	PHE
1	C	144	GLU
1	C	147	ARG
1	C	149	THR
1	C	156	ILE
1	C	158	ASP
1	C	172	GLU
1	C	173	ILE
1	C	175	LYS
1	C	179	LEU
1	C	180	ASP
1	C	182	ILE
1	C	186	LYS
1	C	188	LEU
1	C	190	PRO
1	C	197	LYS
1	C	202	ASP
1	C	209	LEU
1	C	213	LYS
1	C	217	LYS
1	C	229	PHE
1	C	236	GLU
1	C	254	ARG
1	C	279	ILE
1	C	284	LYS
1	C	296	LEU
1	C	309	PRO
1	C	324	THR
1	C	334	LEU
1	C	349	ASN
1	C	356	ASP
1	C	385	LEU
1	C	395	GLU
1	C	397	GLU
1	C	400	LYS
1	C	408	LEU
1	C	410	ILE
1	C	414	LYS
1	C	415	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	420	LEU
1	C	434	LEU
1	C	446	ILE
1	C	455	TYR
1	C	473	ASN
1	C	475	GLU
1	C	479	LYS
1	C	484	VAL
1	C	501	LEU
1	C	502	THR
1	C	514	ASP
1	C	515	LYS
1	C	533	LEU
1	C	562	GLU
1	C	582	ASP
1	C	588	GLU
1	C	602	PHE
1	C	635	ILE
1	C	639	ASN
1	C	644	GLU
1	C	646	THR
1	C	655	ASN
1	C	665	LYS
1	C	672	ARG
1	C	678	VAL
1	C	702	SER
1	C	709	ASN
1	C	714	GLN
1	C	715	GLU
1	C	734	ASN
1	C	744	GLU
1	C	755	ARG
1	C	759	GLN
1	C	766	HIS
1	C	767	GLN
1	C	770	ASN
1	C	780	LEU
1	C	794	GLN
1	D	71	PHE
1	D	78	LYS
1	D	110	ASP
1	D	112	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	HIS
1	D	115	LYS
1	D	117	LEU
1	D	120	LEU
1	D	124	GLU
1	D	128	MET
1	D	129	ASN
1	D	130	SER
1	D	133	GLU
1	D	137	PHE
1	D	144	GLU
1	D	147	ARG
1	D	149	THR
1	D	156	ILE
1	D	158	ASP
1	D	172	GLU
1	D	173	ILE
1	D	175	LYS
1	D	179	LEU
1	D	180	ASP
1	D	182	ILE
1	D	186	LYS
1	D	188	LEU
1	D	190	PRO
1	D	197	LYS
1	D	202	ASP
1	D	209	LEU
1	D	213	LYS
1	D	217	LYS
1	D	229	PHE
1	D	236	GLU
1	D	254	ARG
1	D	279	ILE
1	D	284	LYS
1	D	296	LEU
1	D	309	PRO
1	D	324	THR
1	D	334	LEU
1	D	349	ASN
1	D	356	ASP
1	D	385	LEU
1	D	395	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	397	GLU
1	D	400	LYS
1	D	408	LEU
1	D	410	ILE
1	D	414	LYS
1	D	415	GLU
1	D	420	LEU
1	D	434	LEU
1	D	446	ILE
1	D	455	TYR
1	D	473	ASN
1	D	475	GLU
1	D	479	LYS
1	D	484	VAL
1	D	501	LEU
1	D	502	THR
1	D	514	ASP
1	D	515	LYS
1	D	533	LEU
1	D	562	GLU
1	D	582	ASP
1	D	588	GLU
1	D	622	LYS
1	D	635	ILE
1	D	639	ASN
1	D	644	GLU
1	D	646	THR
1	D	655	ASN
1	D	665	LYS
1	D	672	ARG
1	D	678	VAL
1	D	702	SER
1	D	709	ASN
1	D	714	GLN
1	D	715	GLU
1	D	734	ASN
1	D	744	GLU
1	D	755	ARG
1	D	759	GLN
1	D	766	HIS
1	D	767	GLN
1	D	770	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	780	LEU
1	D	794	GLN
1	E	71	PHE
1	E	78	LYS
1	E	110	ASP
1	E	112	VAL
1	E	114	HIS
1	E	115	LYS
1	E	117	LEU
1	E	120	LEU
1	E	124	GLU
1	E	128	MET
1	E	129	ASN
1	E	130	SER
1	E	133	GLU
1	E	137	PHE
1	E	144	GLU
1	E	147	ARG
1	E	149	THR
1	E	156	ILE
1	E	158	ASP
1	E	172	GLU
1	E	173	ILE
1	E	175	LYS
1	E	179	LEU
1	E	180	ASP
1	E	182	ILE
1	E	186	LYS
1	E	188	LEU
1	E	190	PRO
1	E	197	LYS
1	E	202	ASP
1	E	209	LEU
1	E	213	LYS
1	E	217	LYS
1	E	229	PHE
1	E	236	GLU
1	E	254	ARG
1	E	279	ILE
1	E	284	LYS
1	E	296	LEU
1	E	309	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	324	THR
1	E	334	LEU
1	E	349	ASN
1	E	356	ASP
1	E	385	LEU
1	E	395	GLU
1	E	397	GLU
1	E	400	LYS
1	E	408	LEU
1	E	410	ILE
1	E	414	LYS
1	E	415	GLU
1	E	420	LEU
1	E	434	LEU
1	E	446	ILE
1	E	455	TYR
1	E	473	ASN
1	E	475	GLU
1	E	479	LYS
1	E	484	VAL
1	E	501	LEU
1	E	502	THR
1	E	514	ASP
1	E	515	LYS
1	E	533	LEU
1	E	562	GLU
1	E	582	ASP
1	E	588	GLU
1	E	602	PHE
1	E	635	ILE
1	E	639	ASN
1	E	644	GLU
1	E	646	THR
1	E	655	ASN
1	E	665	LYS
1	E	672	ARG
1	E	678	VAL
1	E	702	SER
1	E	709	ASN
1	E	714	GLN
1	E	715	GLU
1	E	734	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	744	GLU
1	E	755	ARG
1	E	759	GLN
1	E	766	HIS
1	E	767	GLN
1	E	770	ASN
1	E	780	LEU
1	E	794	GLN
1	F	64	ASN
1	F	71	PHE
1	F	78	LYS
1	F	110	ASP
1	F	112	VAL
1	F	114	HIS
1	F	115	LYS
1	F	117	LEU
1	F	120	LEU
1	F	124	GLU
1	F	128	MET
1	F	133	GLU
1	F	137	PHE
1	F	144	GLU
1	F	147	ARG
1	F	149	THR
1	F	155	ASN
1	F	156	ILE
1	F	158	ASP
1	F	172	GLU
1	F	173	ILE
1	F	175	LYS
1	F	179	LEU
1	F	180	ASP
1	F	182	ILE
1	F	186	LYS
1	F	188	LEU
1	F	197	LYS
1	F	202	ASP
1	F	209	LEU
1	F	213	LYS
1	F	217	LYS
1	F	229	PHE
1	F	236	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	254	ARG
1	F	279	ILE
1	F	284	LYS
1	F	296	LEU
1	F	309	PRO
1	F	324	THR
1	F	334	LEU
1	F	349	ASN
1	F	356	ASP
1	F	385	LEU
1	F	395	GLU
1	F	397	GLU
1	F	400	LYS
1	F	408	LEU
1	F	410	ILE
1	F	414	LYS
1	F	415	GLU
1	F	420	LEU
1	F	434	LEU
1	F	446	ILE
1	F	455	TYR
1	F	473	ASN
1	F	475	GLU
1	F	479	LYS
1	F	484	VAL
1	F	501	LEU
1	F	502	THR
1	F	514	ASP
1	F	515	LYS
1	F	533	LEU
1	F	562	GLU
1	F	582	ASP
1	F	588	GLU
1	F	602	PHE
1	F	622	LYS
1	F	635	ILE
1	F	639	ASN
1	F	644	GLU
1	F	646	THR
1	F	655	ASN
1	F	665	LYS
1	F	672	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	678	VAL
1	F	702	SER
1	F	709	ASN
1	F	714	GLN
1	F	715	GLU
1	F	734	ASN
1	F	744	GLU
1	F	755	ARG
1	F	759	GLN
1	F	766	HIS
1	F	767	GLN
1	F	770	ASN
1	F	780	LEU
1	F	794	GLN
2	O	5	THR
2	O	13	LYS
2	O	14	GLU
2	O	18	LEU
2	O	30	LYS
2	O	49	GLN
2	O	54	GLU
2	O	55	VAL
2	O	62	THR
2	O	63	ILE
2	O	65	PHE
2	O	70	THR
2	O	83	GLU
2	O	84	GLU
2	O	94	LYS
2	O	97	ASN
2	O	104	GLU
2	O	117	THR
2	O	140	GLU
2	O	146	THR
2	P	5	THR
2	P	13	LYS
2	P	14	GLU
2	P	18	LEU
2	P	30	LYS
2	P	49	GLN
2	P	54	GLU
2	P	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	62	THR
2	P	63	ILE
2	P	65	PHE
2	P	70	THR
2	P	83	GLU
2	P	84	GLU
2	P	94	LYS
2	P	97	ASN
2	P	104	GLU
2	P	117	THR
2	P	140	GLU
2	P	146	THR
2	Q	5	THR
2	Q	13	LYS
2	Q	14	GLU
2	Q	18	LEU
2	Q	30	LYS
2	Q	49	GLN
2	Q	54	GLU
2	Q	55	VAL
2	Q	62	THR
2	Q	63	ILE
2	Q	65	PHE
2	Q	70	THR
2	Q	83	GLU
2	Q	84	GLU
2	Q	94	LYS
2	Q	97	ASN
2	Q	104	GLU
2	Q	117	THR
2	Q	140	GLU
2	Q	146	THR
2	R	5	THR
2	R	13	LYS
2	R	14	GLU
2	R	18	LEU
2	R	30	LYS
2	R	49	GLN
2	R	54	GLU
2	R	55	VAL
2	R	62	THR
2	R	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	65	PHE
2	R	70	THR
2	R	83	GLU
2	R	84	GLU
2	R	94	LYS
2	R	97	ASN
2	R	104	GLU
2	R	117	THR
2	R	140	GLU
2	R	146	THR
2	S	5	THR
2	S	13	LYS
2	S	14	GLU
2	S	18	LEU
2	S	30	LYS
2	S	49	GLN
2	S	54	GLU
2	S	55	VAL
2	S	63	ILE
2	S	65	PHE
2	S	70	THR
2	S	83	GLU
2	S	84	GLU
2	S	94	LYS
2	S	97	ASN
2	S	104	GLU
2	S	117	THR
2	S	140	GLU
2	S	146	THR
2	T	5	THR
2	T	13	LYS
2	T	14	GLU
2	T	18	LEU
2	T	30	LYS
2	T	49	GLN
2	T	54	GLU
2	T	55	VAL
2	T	63	ILE
2	T	65	PHE
2	T	70	THR
2	T	83	GLU
2	T	84	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	94	LYS
2	T	97	ASN
2	T	104	GLU
2	T	117	THR
2	T	140	GLU
2	T	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (249) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	81	GLN
1	A	83	GLN
1	A	126	ASN
1	A	129	ASN
1	A	165	GLN
1	A	212	GLN
1	A	238	GLN
1	A	323	ASN
1	A	337	ASN
1	A	349	ASN
1	A	377	GLN
1	A	387	ASN
1	A	416	ASN
1	A	438	ASN
1	A	454	GLN
1	A	480	ASN
1	A	507	GLN
1	A	510	GLN
1	A	518	ASN
1	A	551	ASN
1	A	553	GLN
1	A	576	ASN
1	A	581	GLN
1	A	629	ASN
1	A	639	ASN
1	A	655	ASN
1	A	666	ASN
1	A	730	ASN
1	A	747	ASN
1	A	750	GLN
1	A	767	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	770	ASN
1	A	779	GLN
1	A	781	ASN
1	A	785	ASN
1	A	789	ASN
1	A	794	GLN
1	B	65	ASN
1	B	80	GLN
1	B	81	GLN
1	B	126	ASN
1	B	129	ASN
1	B	165	GLN
1	B	212	GLN
1	B	238	GLN
1	B	323	ASN
1	B	337	ASN
1	B	349	ASN
1	B	377	GLN
1	B	387	ASN
1	B	416	ASN
1	B	438	ASN
1	B	454	GLN
1	B	480	ASN
1	B	507	GLN
1	B	510	GLN
1	B	518	ASN
1	B	551	ASN
1	B	553	GLN
1	B	576	ASN
1	B	581	GLN
1	B	618	ASN
1	B	629	ASN
1	B	639	ASN
1	B	655	ASN
1	B	666	ASN
1	B	730	ASN
1	B	747	ASN
1	B	750	GLN
1	B	767	GLN
1	B	770	ASN
1	B	779	GLN
1	B	781	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	789	ASN
1	B	794	GLN
1	C	80	GLN
1	C	81	GLN
1	C	83	GLN
1	C	126	ASN
1	C	129	ASN
1	C	165	GLN
1	C	212	GLN
1	C	238	GLN
1	C	323	ASN
1	C	337	ASN
1	C	349	ASN
1	C	377	GLN
1	C	387	ASN
1	C	416	ASN
1	C	438	ASN
1	C	454	GLN
1	C	480	ASN
1	C	507	GLN
1	C	510	GLN
1	C	518	ASN
1	C	551	ASN
1	C	553	GLN
1	C	576	ASN
1	C	581	GLN
1	C	618	ASN
1	C	629	ASN
1	C	639	ASN
1	C	655	ASN
1	C	666	ASN
1	C	730	ASN
1	C	747	ASN
1	C	750	GLN
1	C	767	GLN
1	C	770	ASN
1	C	781	ASN
1	C	789	ASN
1	C	794	GLN
1	D	64	ASN
1	D	65	ASN
1	D	80	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	81	GLN
1	D	83	GLN
1	D	126	ASN
1	D	165	GLN
1	D	212	GLN
1	D	238	GLN
1	D	323	ASN
1	D	337	ASN
1	D	349	ASN
1	D	377	GLN
1	D	387	ASN
1	D	416	ASN
1	D	438	ASN
1	D	480	ASN
1	D	507	GLN
1	D	510	GLN
1	D	518	ASN
1	D	551	ASN
1	D	553	GLN
1	D	555	GLN
1	D	576	ASN
1	D	581	GLN
1	D	618	ASN
1	D	629	ASN
1	D	639	ASN
1	D	655	ASN
1	D	666	ASN
1	D	730	ASN
1	D	747	ASN
1	D	750	GLN
1	D	767	GLN
1	D	770	ASN
1	D	781	ASN
1	D	785	ASN
1	D	789	ASN
1	D	794	GLN
1	E	64	ASN
1	E	80	GLN
1	E	81	GLN
1	E	83	GLN
1	E	126	ASN
1	E	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	212	GLN
1	E	238	GLN
1	E	323	ASN
1	E	337	ASN
1	E	349	ASN
1	E	377	GLN
1	E	387	ASN
1	E	416	ASN
1	E	438	ASN
1	E	480	ASN
1	E	507	GLN
1	E	510	GLN
1	E	518	ASN
1	E	551	ASN
1	E	553	GLN
1	E	576	ASN
1	E	581	GLN
1	E	583	ASN
1	E	618	ASN
1	E	629	ASN
1	E	639	ASN
1	E	655	ASN
1	E	666	ASN
1	E	730	ASN
1	E	747	ASN
1	E	750	GLN
1	E	767	GLN
1	E	770	ASN
1	E	781	ASN
1	E	789	ASN
1	E	794	GLN
1	F	80	GLN
1	F	81	GLN
1	F	83	GLN
1	F	126	ASN
1	F	129	ASN
1	F	165	GLN
1	F	212	GLN
1	F	238	GLN
1	F	323	ASN
1	F	337	ASN
1	F	349	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	377	GLN
1	F	387	ASN
1	F	416	ASN
1	F	438	ASN
1	F	480	ASN
1	F	507	GLN
1	F	510	GLN
1	F	518	ASN
1	F	551	ASN
1	F	553	GLN
1	F	555	GLN
1	F	581	GLN
1	F	629	ASN
1	F	639	ASN
1	F	655	ASN
1	F	666	ASN
1	F	730	ASN
1	F	747	ASN
1	F	750	GLN
1	F	767	GLN
1	F	770	ASN
1	F	779	GLN
1	F	781	ASN
1	F	789	ASN
1	F	794	GLN
2	O	41	GLN
2	O	49	GLN
2	O	111	ASN
2	O	143	GLN
2	P	41	GLN
2	P	49	GLN
2	P	111	ASN
2	P	143	GLN
2	Q	41	GLN
2	Q	49	GLN
2	Q	111	ASN
2	Q	143	GLN
2	R	41	GLN
2	R	49	GLN
2	R	111	ASN
2	R	143	GLN
2	S	41	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	49	GLN
2	S	111	ASN
2	S	143	GLN
2	T	41	GLN
2	T	49	GLN
2	T	111	ASN
2	T	143	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
4	CMP	F	906	3	25,25,25	2.78	5 (20%)	37,39,39	1.78	6 (16%)
4	CMP	E	905	3	25,25,25	2.84	5 (20%)	37,39,39	1.76	5 (13%)
4	CMP	A	901	-	25,25,25	2.78	5 (20%)	37,39,39	1.81	6 (16%)
4	CMP	B	902	3	25,25,25	2.81	7 (28%)	37,39,39	1.73	6 (16%)
4	CMP	C	903	3	25,25,25	2.81	4 (16%)	37,39,39	1.73	5 (13%)
4	CMP	D	904	3	25,25,25	2.83	6 (24%)	37,39,39	1.73	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CMP	F	906	3	-	2/4/31/31	0/4/4/4
4	CMP	E	905	3	-	2/4/31/31	0/4/4/4
4	CMP	A	901	-	-	2/4/31/31	0/4/4/4
4	CMP	B	902	3	-	2/4/31/31	0/4/4/4
4	CMP	C	903	3	-	2/4/31/31	0/4/4/4
4	CMP	D	904	3	-	2/4/31/31	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	905	CMP	P-O5'	11.97	1.71	1.57
4	D	904	CMP	P-O5'	11.95	1.71	1.57
4	C	903	CMP	P-O5'	11.89	1.71	1.57
4	B	902	CMP	P-O5'	11.82	1.71	1.57
4	A	901	CMP	P-O5'	11.63	1.70	1.57
4	F	906	CMP	P-O5'	11.54	1.70	1.57
4	C	903	CMP	C2'-C3'	-4.42	1.43	1.53
4	A	901	CMP	C2'-C3'	-4.32	1.43	1.53
4	D	904	CMP	C2'-C3'	-4.30	1.43	1.53
4	F	906	CMP	C2'-C3'	-4.20	1.43	1.53
4	E	905	CMP	C2'-C3'	-4.20	1.43	1.53
4	B	902	CMP	C2'-C3'	-4.07	1.44	1.53
4	E	905	CMP	C5'-C4'	2.93	1.56	1.51
4	F	906	CMP	C5'-C4'	2.80	1.56	1.51
4	C	903	CMP	C5'-C4'	2.79	1.56	1.51
4	D	904	CMP	C5'-C4'	2.74	1.56	1.51
4	A	901	CMP	C5'-C4'	2.67	1.55	1.51
4	B	902	CMP	C5'-C4'	2.67	1.55	1.51
4	F	906	CMP	P-O3'	2.64	1.62	1.57
4	B	902	CMP	P-O3'	2.48	1.61	1.57
4	E	905	CMP	P-O3'	2.29	1.61	1.57
4	A	901	CMP	P-O3'	2.15	1.61	1.57
4	D	904	CMP	P-O3'	2.15	1.61	1.57
4	E	905	CMP	O4'-C4'	-2.06	1.40	1.45
4	A	901	CMP	C2-N1	2.05	1.37	1.33
4	C	903	CMP	O4'-C4'	-2.03	1.40	1.45
4	D	904	CMP	O4'-C4'	-2.02	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	906	CMP	C2-N1	2.02	1.37	1.33
4	D	904	CMP	C2-N1	2.02	1.37	1.33
4	B	902	CMP	O4'-C4'	-2.02	1.40	1.45
4	B	902	CMP	C4-N3	2.02	1.38	1.34
4	B	902	CMP	C2-N1	2.01	1.37	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	CMP	O3'-C3'-C4'	5.59	114.93	110.71
4	F	906	CMP	O3'-C3'-C4'	5.48	114.84	110.71
4	E	905	CMP	O3'-C3'-C4'	5.40	114.78	110.71
4	C	903	CMP	O3'-C3'-C4'	5.27	114.69	110.71
4	D	904	CMP	O3'-C3'-C4'	5.24	114.67	110.71
4	B	902	CMP	O3'-C3'-C4'	5.09	114.55	110.71
4	A	901	CMP	C4'-O4'-C1'	-4.95	98.53	109.47
4	F	906	CMP	C4'-O4'-C1'	-4.87	98.70	109.47
4	F	906	CMP	O5'-C5'-C4'	4.83	116.97	105.71
4	A	901	CMP	O5'-C5'-C4'	4.79	116.88	105.71
4	B	902	CMP	O5'-C5'-C4'	4.76	116.81	105.71
4	C	903	CMP	C4'-O4'-C1'	-4.75	98.98	109.47
4	E	905	CMP	C4'-O4'-C1'	-4.75	98.98	109.47
4	E	905	CMP	O5'-C5'-C4'	4.73	116.74	105.71
4	D	904	CMP	C4'-O4'-C1'	-4.69	99.10	109.47
4	D	904	CMP	O5'-C5'-C4'	4.68	116.61	105.71
4	B	902	CMP	C4'-O4'-C1'	-4.67	99.15	109.47
4	C	903	CMP	O5'-C5'-C4'	4.67	116.59	105.71
4	E	905	CMP	O5'-P-O1P	-2.82	103.93	110.44
4	C	903	CMP	O2P-P-O1P	2.81	117.20	108.56
4	A	901	CMP	O2P-P-O1P	2.77	117.08	108.56
4	A	901	CMP	O5'-P-O1P	-2.76	104.07	110.44
4	D	904	CMP	O2P-P-O1P	2.75	117.00	108.56
4	E	905	CMP	O2P-P-O1P	2.74	116.97	108.56
4	F	906	CMP	O5'-P-O1P	-2.72	104.16	110.44
4	B	902	CMP	O2P-P-O1P	2.72	116.91	108.56
4	F	906	CMP	O2P-P-O1P	2.69	116.84	108.56
4	D	904	CMP	O5'-P-O1P	-2.63	104.38	110.44
4	B	902	CMP	O5'-P-O1P	-2.58	104.48	110.44
4	C	903	CMP	O5'-P-O1P	-2.56	104.54	110.44
4	B	902	CMP	O2P-P-O3'	2.03	111.77	107.04
4	A	901	CMP	O2P-P-O3'	2.02	111.74	107.04
4	F	906	CMP	O2P-P-O3'	2.01	111.72	107.04

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	CMP	O4'-C1'-N9-C8
4	A	901	CMP	O4'-C1'-N9-C4
4	B	902	CMP	O4'-C1'-N9-C8
4	B	902	CMP	O4'-C1'-N9-C4
4	C	903	CMP	O4'-C1'-N9-C8
4	C	903	CMP	O4'-C1'-N9-C4
4	D	904	CMP	O4'-C1'-N9-C8
4	D	904	CMP	O4'-C1'-N9-C4
4	E	905	CMP	O4'-C1'-N9-C8
4	E	905	CMP	O4'-C1'-N9-C4
4	F	906	CMP	O4'-C1'-N9-C8
4	F	906	CMP	O4'-C1'-N9-C4

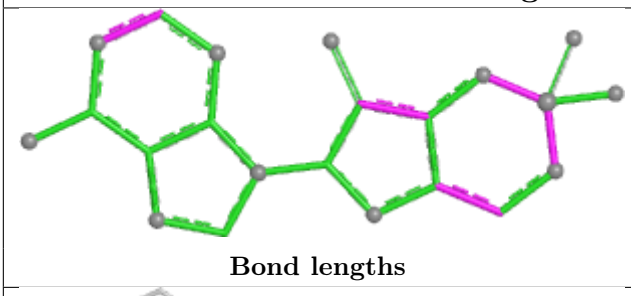
There are no ring outliers.

6 monomers are involved in 24 short contacts:

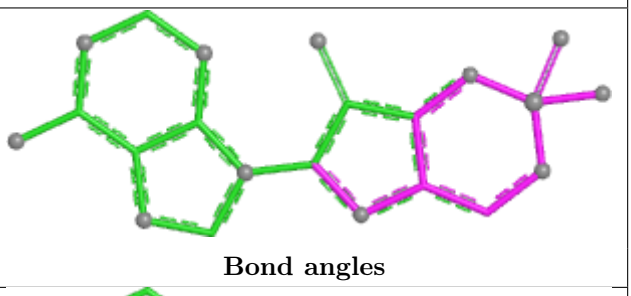
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	906	CMP	4	0
4	E	905	CMP	4	0
4	A	901	CMP	4	0
4	B	902	CMP	4	0
4	C	903	CMP	4	0
4	D	904	CMP	4	0

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

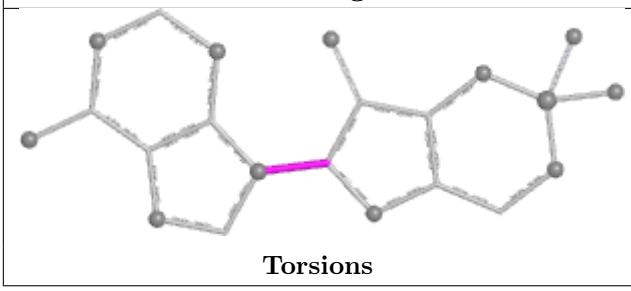
Ligand CMP F 906



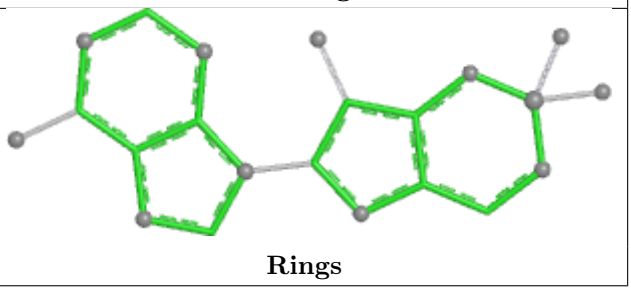
Bond lengths



Bond angles

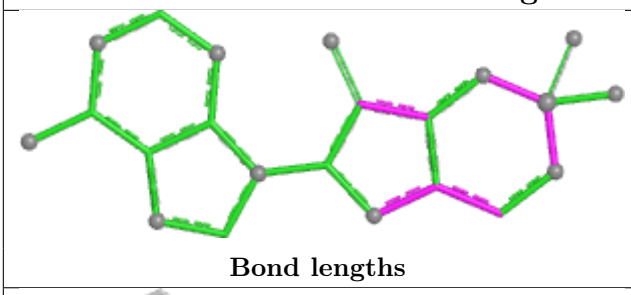


Torsions

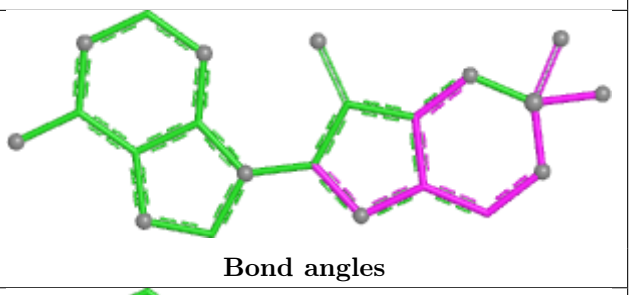


Rings

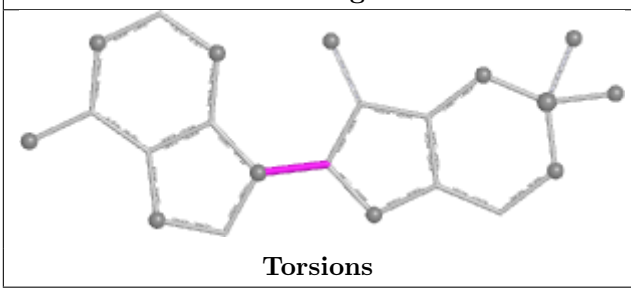
Ligand CMP E 905



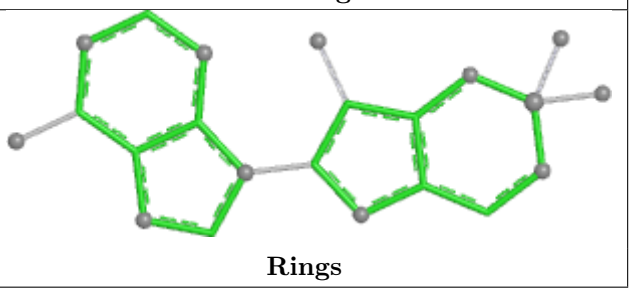
Bond lengths



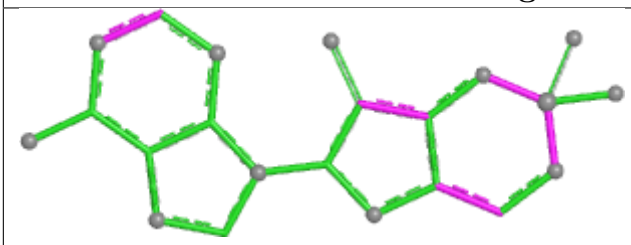
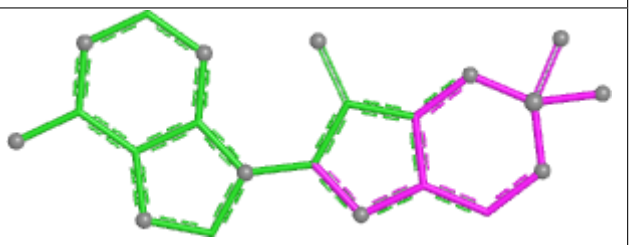
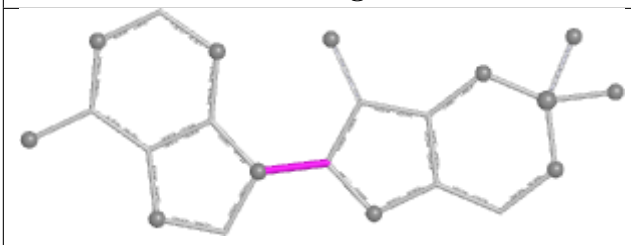
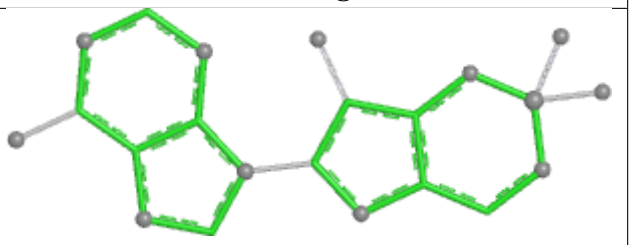
Bond angles

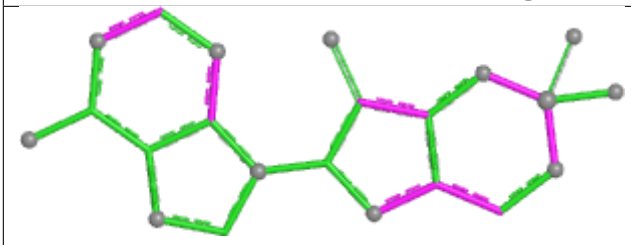
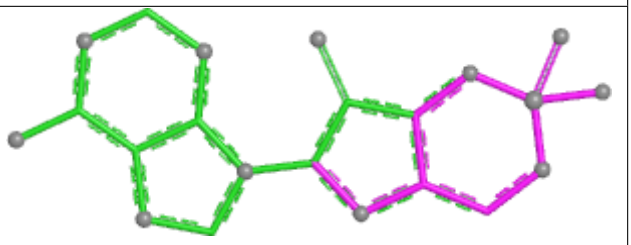
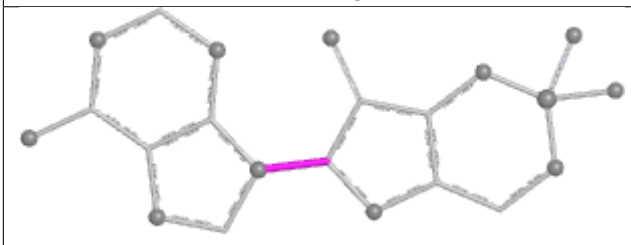
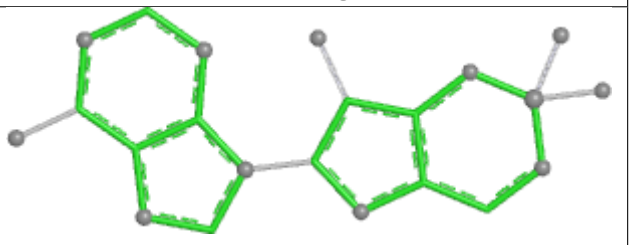


Torsions

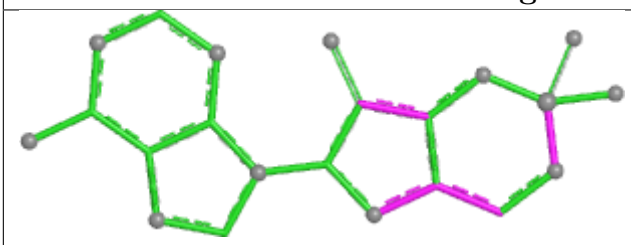


Rings

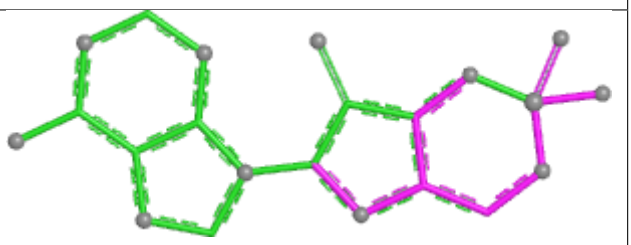
Ligand CMP A 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CMP B 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

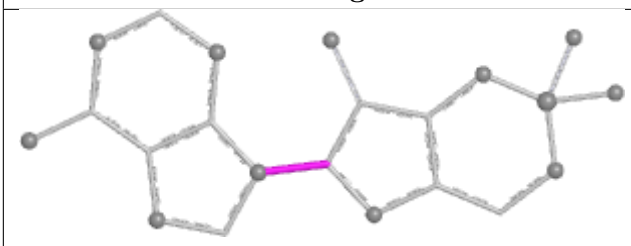
Ligand CMP C 903



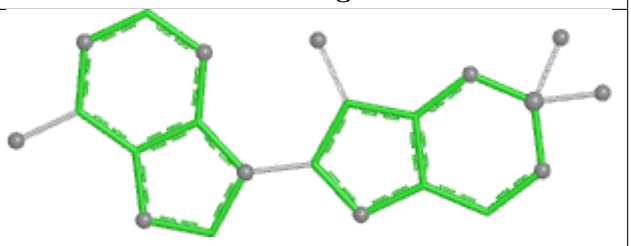
Bond lengths



Bond angles

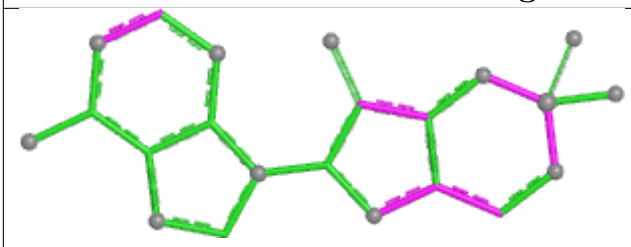


Torsions

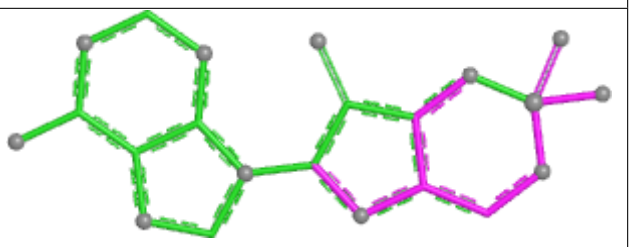


Rings

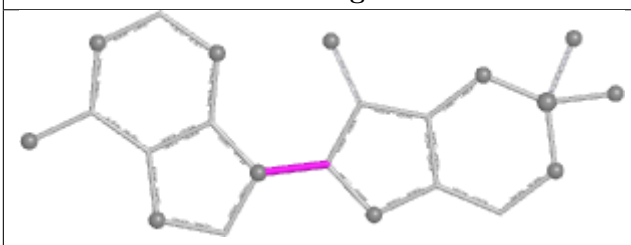
Ligand CMP D 904



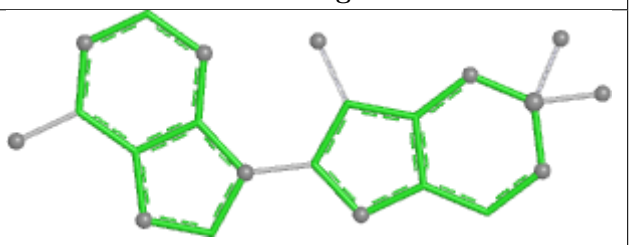
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	123:GLU	C	124:GLU	N	1.19

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	735/777 (94%)	-0.07	15 (2%)	65	49	18, 73, 128, 137	0
1	B	735/777 (94%)	-0.07	17 (2%)	61	46	18, 73, 128, 138	0
1	C	735/777 (94%)	-0.07	13 (1%)	67	53	17, 73, 128, 138	0
1	D	735/777 (94%)	-0.06	20 (2%)	56	42	17, 73, 127, 137	0
1	E	735/777 (94%)	-0.06	16 (2%)	62	47	17, 72, 127, 137	0
1	F	735/777 (94%)	-0.07	15 (2%)	65	49	18, 73, 127, 138	0
2	O	146/149 (97%)	-0.06	5 (3%)	48	35	17, 60, 119, 124	0
2	P	146/149 (97%)	-0.08	2 (1%)	73	59	17, 60, 119, 124	0
2	Q	146/149 (97%)	-0.04	3 (2%)	63	48	17, 60, 119, 123	0
2	R	146/149 (97%)	-0.04	4 (2%)	56	42	16, 60, 119, 123	0
2	S	146/149 (97%)	-0.09	2 (1%)	73	59	17, 60, 119, 123	0
2	T	146/149 (97%)	-0.05	3 (2%)	63	48	16, 60, 119, 124	0
All	All	5286/5556 (95%)	-0.07	115 (2%)	62	47	16, 70, 126, 138	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	TYR	4.8
1	E	171	TYR	4.7
1	A	171	TYR	4.7
1	B	171	TYR	4.7
1	A	162	ASN	4.7
1	D	171	TYR	4.5
1	E	162	ASN	4.4
1	F	171	TYR	4.2
1	D	162	ASN	3.7
1	A	110	ASP	3.5
1	D	190	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	162	ASN	3.2
2	O	79	THR	3.1
1	F	220	LEU	3.0
1	E	229	PHE	3.0
1	D	220	LEU	3.0
2	O	55	VAL	3.0
1	A	220	LEU	2.9
1	C	180	ASP	2.9
1	F	162	ASN	2.9
1	D	184	LYS	2.9
1	A	184	LYS	2.8
1	E	190	PRO	2.8
1	F	161	ILE	2.7
1	B	180	ASP	2.6
1	A	190	PRO	2.6
1	C	162	ASN	2.6
1	C	229	PHE	2.6
1	F	256	VAL	2.6
1	B	161	ILE	2.6
1	A	180	ASP	2.6
1	C	220	LEU	2.6
2	Q	73	ALA	2.6
1	A	161	ILE	2.6
1	F	230	ILE	2.6
1	E	72	THR	2.6
1	E	225	ILE	2.5
1	D	110	ASP	2.5
2	Q	43	PRO	2.5
1	A	109	ILE	2.5
1	E	161	ILE	2.5
1	C	72	THR	2.5
1	B	110	ASP	2.4
1	D	787	THR	2.4
1	E	208	LEU	2.4
1	D	211	SER	2.4
2	Q	55	VAL	2.4
2	S	79	THR	2.4
1	E	684	ASP	2.4
1	B	160	ALA	2.4
1	A	229	PHE	2.4
1	D	262	PRO	2.4
1	A	165	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	787	THR	2.3
1	B	225	ILE	2.3
1	E	184	LYS	2.3
1	F	190	PRO	2.3
2	S	73	ALA	2.3
1	F	184	LYS	2.3
1	D	381	GLU	2.3
1	F	212	GLN	2.3
2	T	55	VAL	2.3
1	B	190	PRO	2.2
2	R	73	ALA	2.2
2	T	73	ALA	2.2
1	B	231	LYS	2.2
1	E	165	GLN	2.2
1	E	259	LEU	2.2
1	F	160	ALA	2.2
1	C	213	LYS	2.2
1	D	161	ILE	2.2
1	B	220	LEU	2.2
1	B	684	ASP	2.2
1	F	229	PHE	2.2
2	R	55	VAL	2.2
1	B	203	SER	2.2
1	F	205	SER	2.2
1	A	122	GLU	2.2
2	R	43	PRO	2.2
1	A	684	ASP	2.2
1	D	225	ILE	2.1
1	B	111	LEU	2.1
1	D	208	LEU	2.1
1	B	184	LYS	2.1
1	E	211	SER	2.1
2	O	73	ALA	2.1
1	C	262	PRO	2.1
1	D	798	ASP	2.1
1	B	256	VAL	2.1
2	P	55	VAL	2.1
2	P	79	THR	2.1
1	A	225	ILE	2.1
1	D	188	LEU	2.1
1	A	126	ASN	2.1
1	D	766	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	259	LEU	2.1
2	T	52	ILE	2.1
1	D	191	GLU	2.1
1	C	225	ILE	2.1
1	E	209	LEU	2.1
1	F	208	LEU	2.1
2	O	78	ASP	2.1
1	C	212	GLN	2.1
1	F	122	GLU	2.1
1	C	684	ASP	2.1
1	C	260	TYR	2.1
1	F	262	PRO	2.1
2	R	79	THR	2.0
1	B	191	GLU	2.0
1	E	111	LEU	2.0
1	D	109	ILE	2.0
1	E	203	SER	2.0
1	D	239	HIS	2.0
2	O	46	ALA	2.0
1	D	212	GLN	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CMP	C	903	22/22	0.80	0.12	48,63,81,92	0
4	CMP	D	904	22/22	0.80	0.12	48,62,81,86	0
4	CMP	A	901	22/22	0.81	0.12	48,65,85,93	0

Continued on next page...

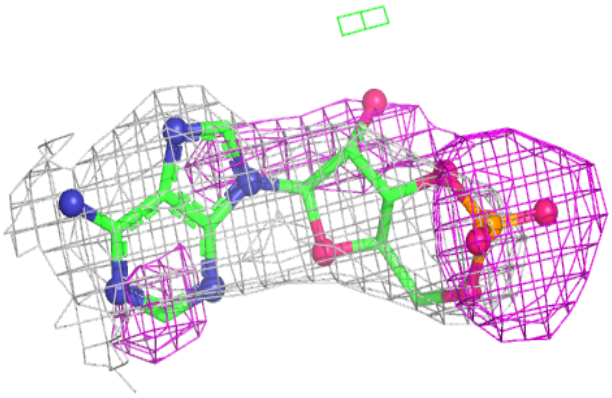
Continued from previous page...

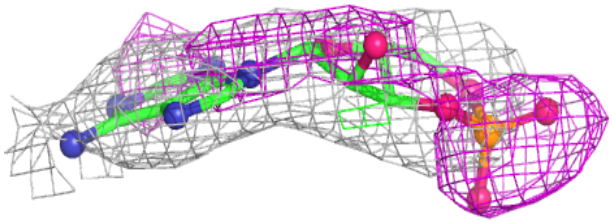
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CMP	B	902	22/22	0.82	0.11	49,63,81,89	0
4	CMP	E	905	22/22	0.83	0.10	47,63,84,91	0
4	CMP	F	906	22/22	0.83	0.11	48,63,84,93	0
5	CA	P	703	1/1	0.96	0.07	76,76,76,76	0
5	CA	R	707	1/1	0.96	0.10	69,69,69,69	0
5	CA	Q	705	1/1	0.97	0.05	76,76,76,76	0
5	CA	O	701	1/1	0.97	0.07	81,81,81,81	0
5	CA	S	709	1/1	0.97	0.07	78,78,78,78	0
5	CA	S	810	1/1	0.97	0.06	51,51,51,51	0
5	CA	T	711	1/1	0.97	0.07	79,79,79,79	0
5	CA	Q	806	1/1	0.98	0.04	51,51,51,51	0
5	CA	O	802	1/1	0.98	0.04	47,47,47,47	0
3	MG	E	904	1/1	0.98	0.05	17,17,17,17	0
5	CA	P	804	1/1	0.98	0.05	47,47,47,47	0
3	MG	D	903	1/1	0.98	0.04	14,14,14,14	0
5	CA	T	812	1/1	0.98	0.05	54,54,54,54	0
3	MG	F	905	1/1	0.99	0.04	15,15,15,15	0
3	MG	C	902	1/1	0.99	0.02	17,17,17,17	0
5	CA	R	807	1/1	0.99	0.03	29,29,29,29	0
5	CA	R	808	1/1	0.99	0.04	47,47,47,47	0
5	CA	P	803	1/1	0.99	0.02	30,30,30,30	0
5	CA	S	809	1/1	0.99	0.03	26,26,26,26	0
3	MG	A	900	1/1	0.99	0.03	13,13,13,13	0
3	MG	B	901	1/1	0.99	0.05	27,27,27,27	0
5	CA	Q	805	1/1	0.99	0.02	29,29,29,29	0
5	CA	T	811	1/1	1.00	0.02	26,26,26,26	0
5	CA	O	801	1/1	1.00	0.02	27,27,27,27	0

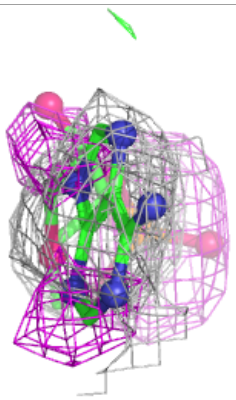
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CMP C 903:

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

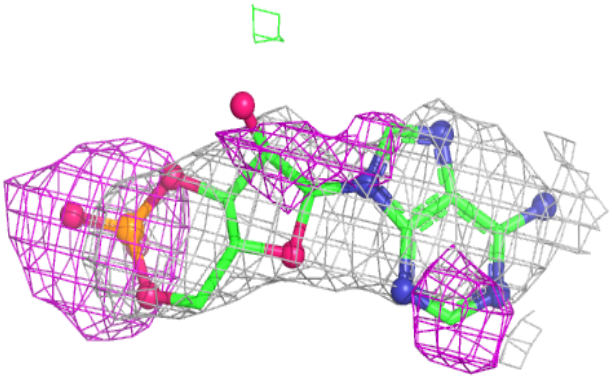


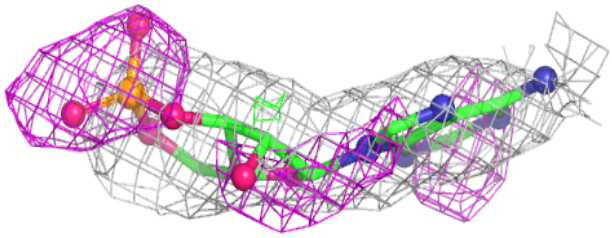


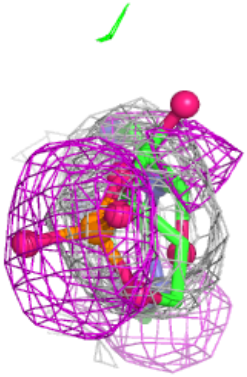


Electron density around CMP D 904:

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

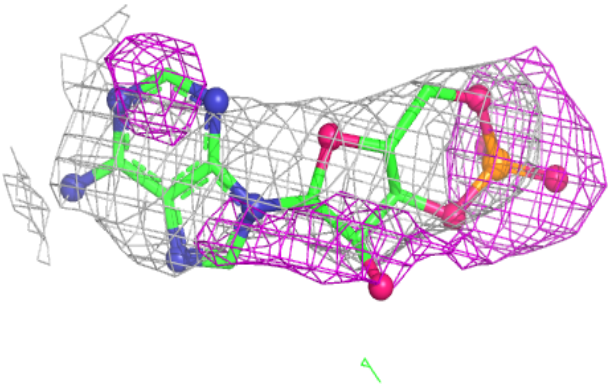


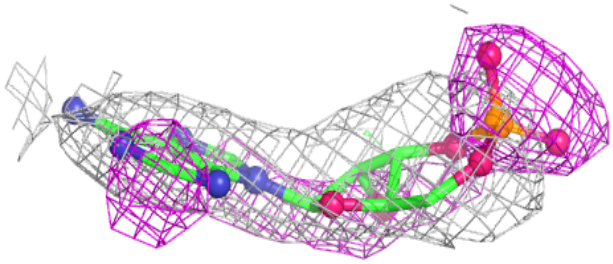


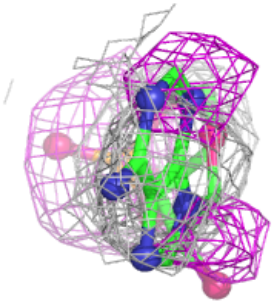


Electron density around CMP A 901:

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

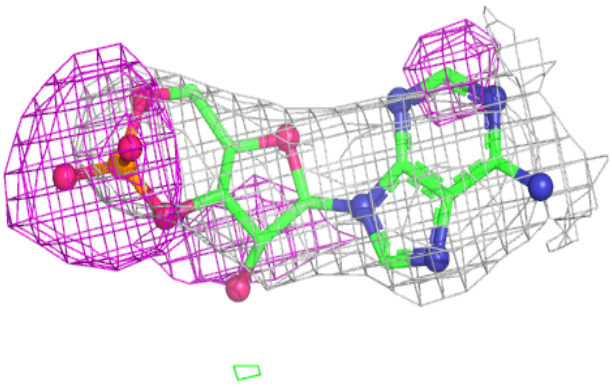


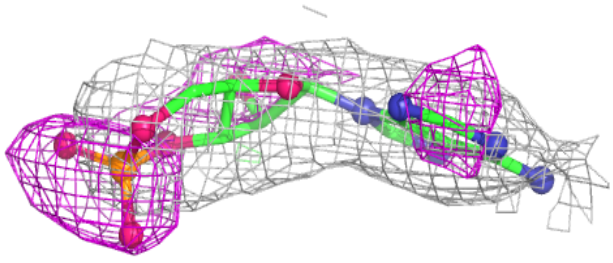


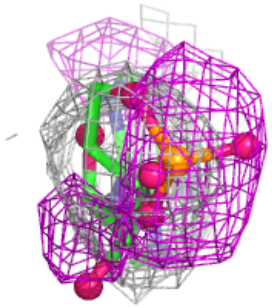


Electron density around CMP B 902:

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

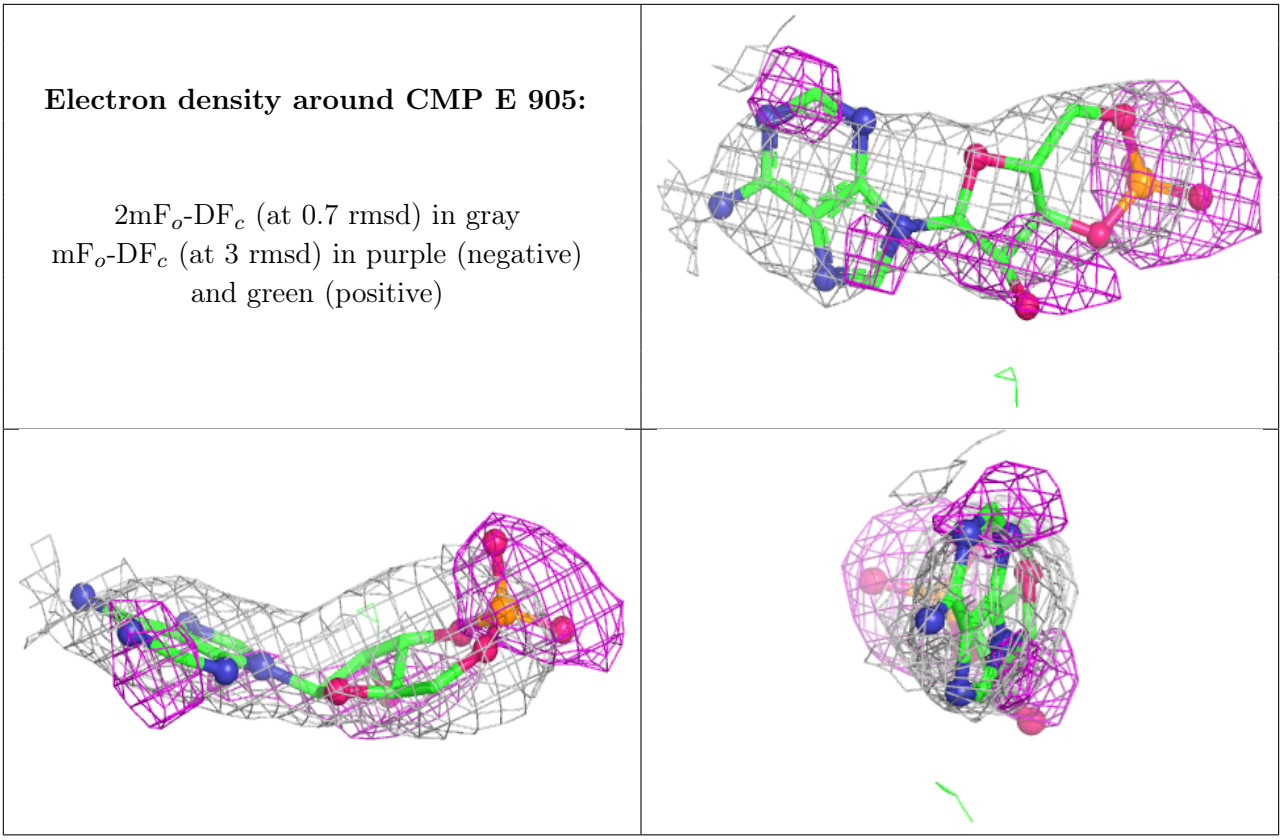






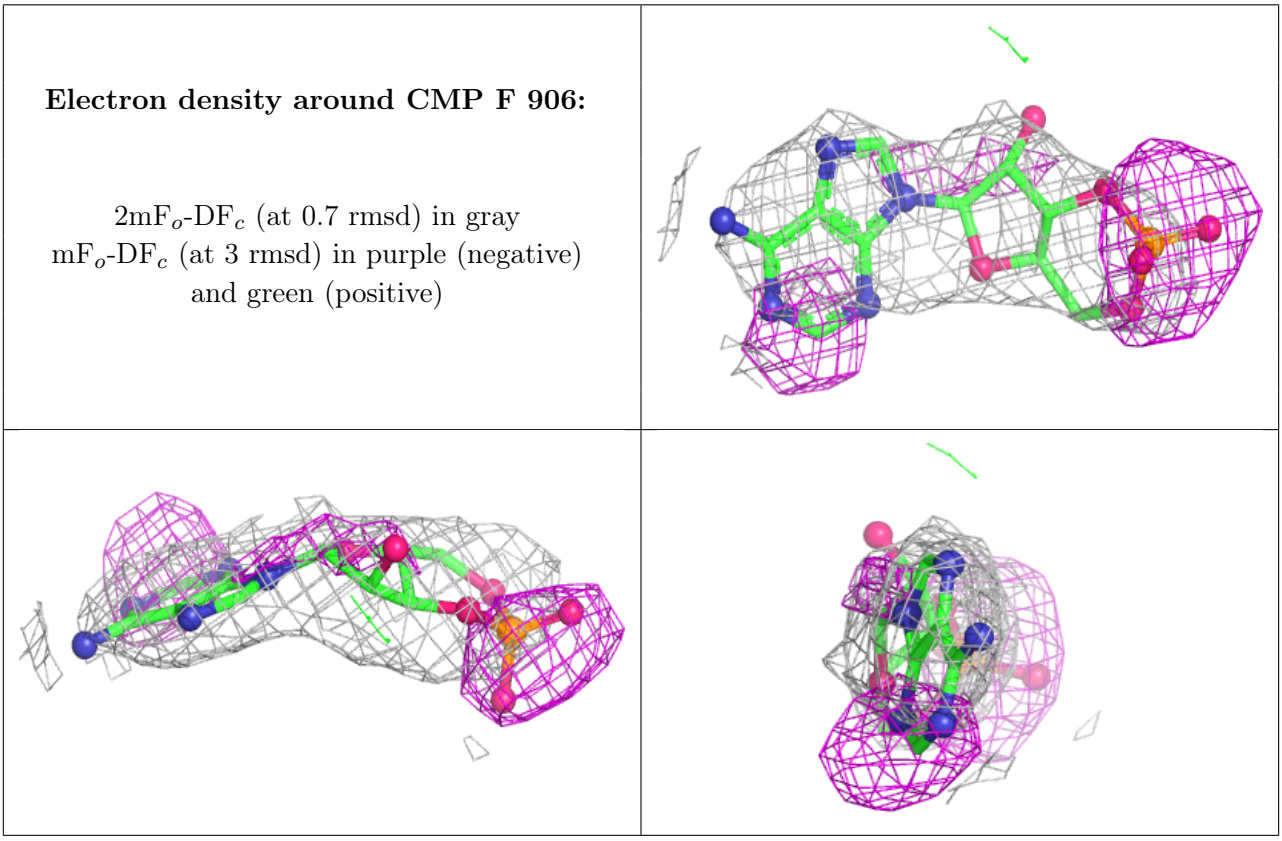
Electron density around CMP E 905:

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



Electron density around CMP F 906:

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



6.5 Other polymers (i)

There are no such residues in this entry.