



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:34 AM UTC

PDB ID : 3FKS / pdb_00003fks
Title : Yeast F1 ATPase in the absence of bound nucleotides
Authors : Kabaleeswaran, V.; Symersky, J.; Shen, H.; Walker, J.E.; Leslie, A.G.W.;
Mueller, D.M.
Deposited on : 2008-12-17
Resolution : 3.59 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
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

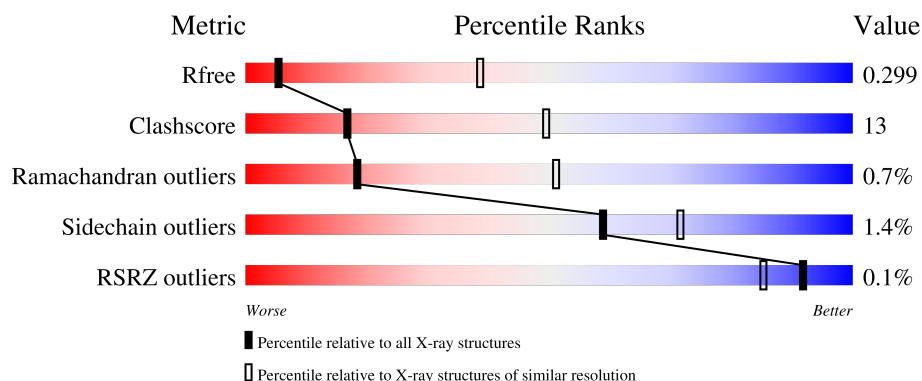
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	510	
1	B	510	
1	C	510	
1	J	510	
1	K	510	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	510	
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	138	
4	Q	138	
4	Z	138	
5	1	61	
5	I	61	
5	R	61	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 71793 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 ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3679	2322	650	704	3			
1	B	479	Total	C	N	O	S	0	0	0
			3645	2302	645	695	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3656	2309	646	698	3			
1	K	484	Total	C	N	O	S	0	0	0
			3659	2309	650	697	3			
1	L	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	S	481	Total	C	N	O	S	0	0	0
			3657	2310	646	698	3			
1	T	473	Total	C	N	O	S	0	0	0
			3596	2272	635	686	3			
1	U	477	Total	C	N	O	S	0	0	0
			3629	2296	643	687	3			

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	466	Total	C	N	O	S	0	0	0
			3517	2232	599	680	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	471	Total	C	N	O	S	0	0	0
			3558	2255	606	691	6			
2	M	469	Total	C	N	O	S	0	0	0
			3540	2244	603	687	6			
2	N	466	Total	C	N	O	S	0	0	0
			3522	2235	600	681	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	469	Total	C	N	O	S	0	0	0
			3539	2245	603	685	6			
2	V	455	Total	C	N	O	S	0	0	0
			3457	2192	589	670	6			
2	W	466	Total	C	N	O	S	0	0	0
			3526	2237	600	683	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	expression tag	UNP P00830
D	-4	SER	-	expression tag	UNP P00830
D	-3	HIS	-	expression tag	UNP P00830
D	-2	HIS	-	expression tag	UNP P00830
D	-1	HIS	-	expression tag	UNP P00830
D	0	HIS	-	expression tag	UNP P00830
D	1	HIS	-	expression tag	UNP P00830
D	2	HIS	-	expression tag	UNP P00830
E	-5	ALA	-	expression tag	UNP P00830
E	-4	SER	-	expression tag	UNP P00830
E	-3	HIS	-	expression tag	UNP P00830
E	-2	HIS	-	expression tag	UNP P00830
E	-1	HIS	-	expression tag	UNP P00830
E	0	HIS	-	expression tag	UNP P00830
E	1	HIS	-	expression tag	UNP P00830
E	2	HIS	-	expression tag	UNP P00830
F	-5	ALA	-	expression tag	UNP P00830
F	-4	SER	-	expression tag	UNP P00830
F	-3	HIS	-	expression tag	UNP P00830
F	-2	HIS	-	expression tag	UNP P00830
F	-1	HIS	-	expression tag	UNP P00830
F	0	HIS	-	expression tag	UNP P00830
F	1	HIS	-	expression tag	UNP P00830
F	2	HIS	-	expression tag	UNP P00830
M	-5	ALA	-	expression tag	UNP P00830
M	-4	SER	-	expression tag	UNP P00830
M	-3	HIS	-	expression tag	UNP P00830
M	-2	HIS	-	expression tag	UNP P00830
M	-1	HIS	-	expression tag	UNP P00830
M	0	HIS	-	expression tag	UNP P00830
M	1	HIS	-	expression tag	UNP P00830

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	2	HIS	-	expression tag	UNP P00830
N	-5	ALA	-	expression tag	UNP P00830
N	-4	SER	-	expression tag	UNP P00830
N	-3	HIS	-	expression tag	UNP P00830
N	-2	HIS	-	expression tag	UNP P00830
N	-1	HIS	-	expression tag	UNP P00830
N	0	HIS	-	expression tag	UNP P00830
N	1	HIS	-	expression tag	UNP P00830
N	2	HIS	-	expression tag	UNP P00830
O	-5	ALA	-	expression tag	UNP P00830
O	-4	SER	-	expression tag	UNP P00830
O	-3	HIS	-	expression tag	UNP P00830
O	-2	HIS	-	expression tag	UNP P00830
O	-1	HIS	-	expression tag	UNP P00830
O	0	HIS	-	expression tag	UNP P00830
O	1	HIS	-	expression tag	UNP P00830
O	2	HIS	-	expression tag	UNP P00830
V	-5	ALA	-	expression tag	UNP P00830
V	-4	SER	-	expression tag	UNP P00830
V	-3	HIS	-	expression tag	UNP P00830
V	-2	HIS	-	expression tag	UNP P00830
V	-1	HIS	-	expression tag	UNP P00830
V	0	HIS	-	expression tag	UNP P00830
V	1	HIS	-	expression tag	UNP P00830
V	2	HIS	-	expression tag	UNP P00830
W	-5	ALA	-	expression tag	UNP P00830
W	-4	SER	-	expression tag	UNP P00830
W	-3	HIS	-	expression tag	UNP P00830
W	-2	HIS	-	expression tag	UNP P00830
W	-1	HIS	-	expression tag	UNP P00830
W	0	HIS	-	expression tag	UNP P00830
W	1	HIS	-	expression tag	UNP P00830
W	2	HIS	-	expression tag	UNP P00830
X	-5	ALA	-	expression tag	UNP P00830
X	-4	SER	-	expression tag	UNP P00830
X	-3	HIS	-	expression tag	UNP P00830
X	-2	HIS	-	expression tag	UNP P00830
X	-1	HIS	-	expression tag	UNP P00830
X	0	HIS	-	expression tag	UNP P00830
X	1	HIS	-	expression tag	UNP P00830
X	2	HIS	-	expression tag	UNP P00830

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	268	Total	C	N	O	S	0	0	0
			2070	1300	357	403	10			
3	P	235	Total	C	N	O	S	0	0	0
			1766	1109	303	344	10			
3	Y	187	Total	C	N	O	S	0	0	0
			1444	901	257	277	9			

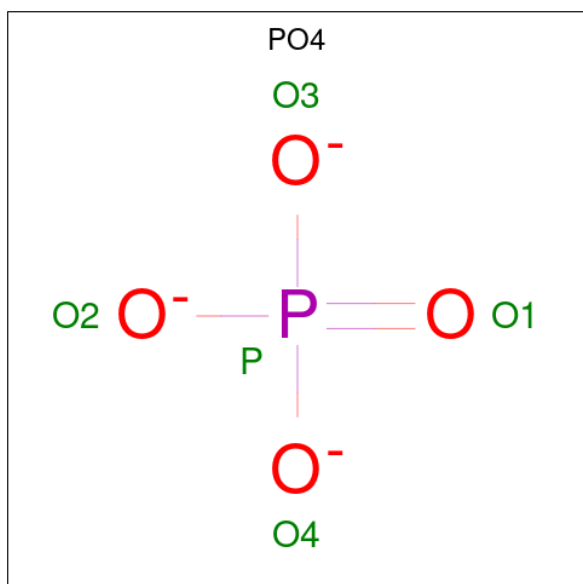
- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	116	Total	C	N	O	S	0	0	0
			849	539	140	168	2			
4	Q	68	Total	C	N	O		0	0	0
			339	203	68	68				
4	Z	11	Total	C	N	O		0	0	0
			55	33	11	11				

- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	46	Total	C	N	O	0	0	0
			326	209	51	66			
5	R	25	Total	C	N	O	0	0	0
			125	75	25	25			
5	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

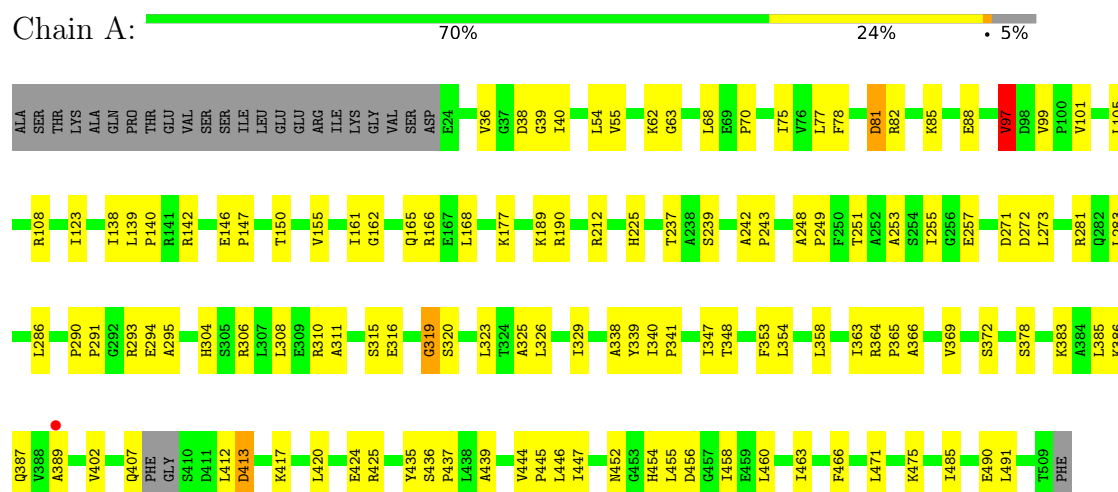


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	J	1	Total	O	P	0	0
			5	4	1		
6	K	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		
6	N	1	Total	O	P	0	0
			5	4	1		
6	O	1	Total	O	P	0	0
			5	4	1		
6	S	1	Total	O	P	0	0
			5	4	1		
6	T	1	Total	O	P	0	0
			5	4	1		
6	U	1	Total	O	P	0	0
			5	4	1		
6	X	1	Total	O	P	0	0
			5	4	1		

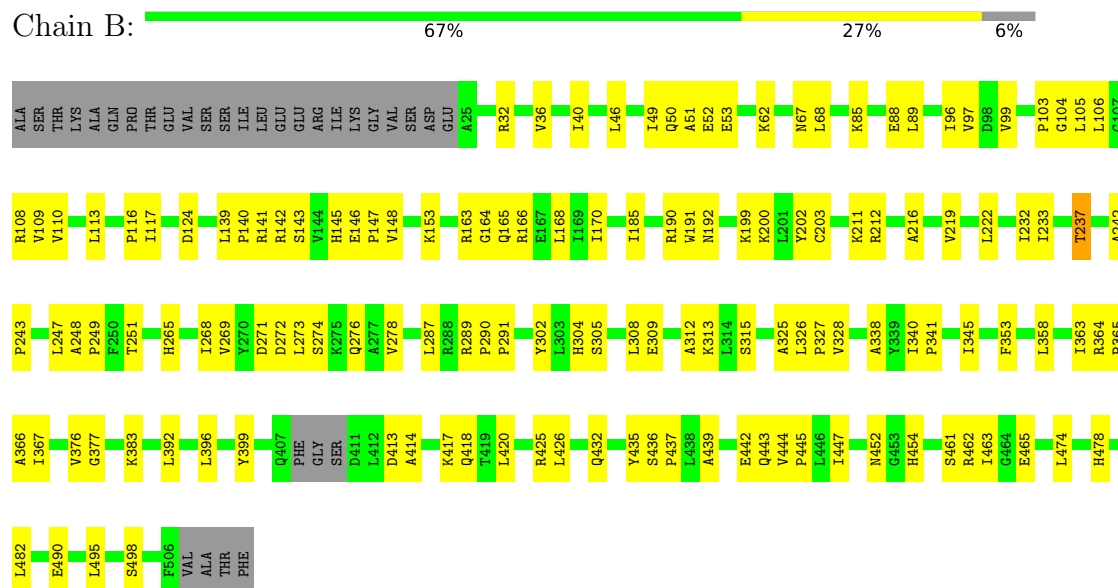
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: ATP synthase subunit alpha, mitochondrial

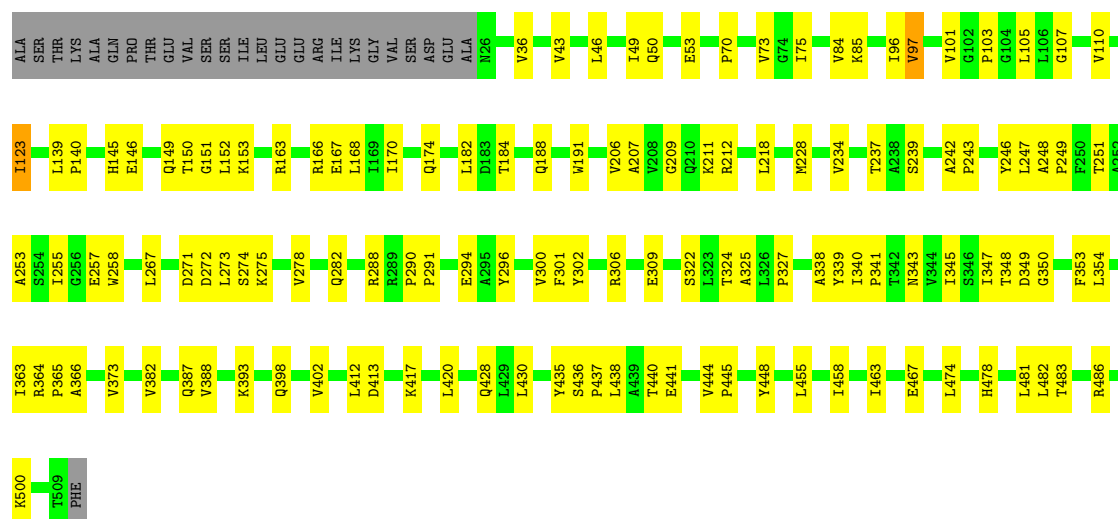


- Molecule 1: ATP synthase subunit alpha, mitochondrial



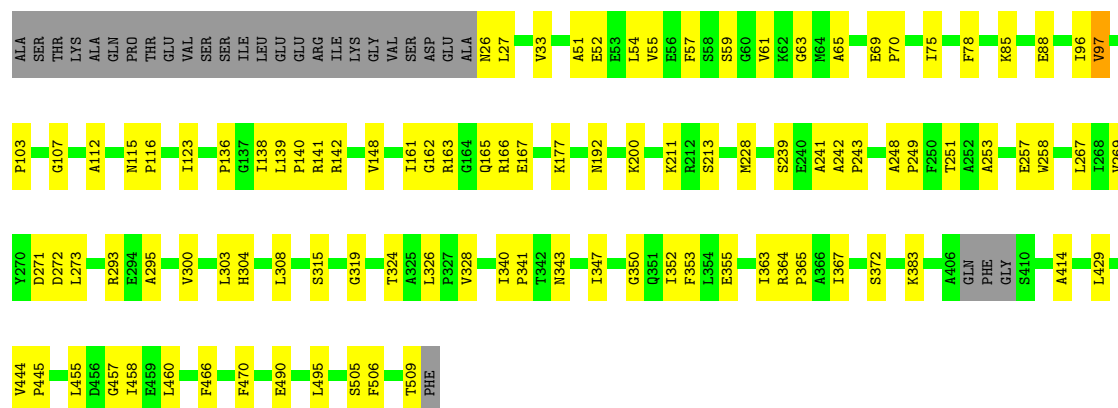
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:



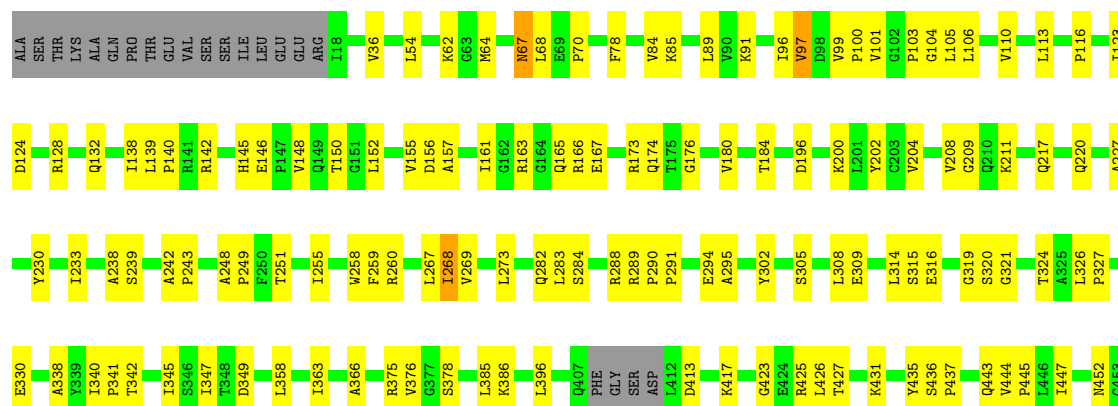
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain J:



- Molecule 1: ATP synthase subunit alpha, mitochondrial

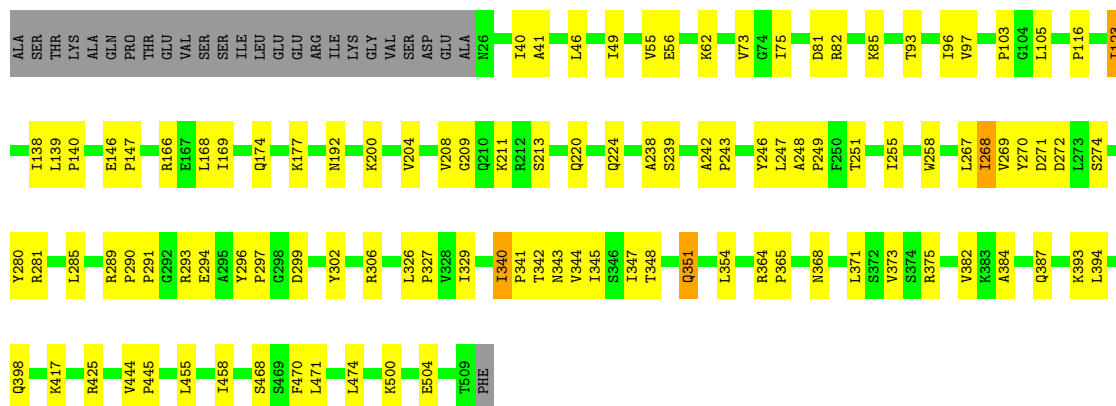
Chain K:





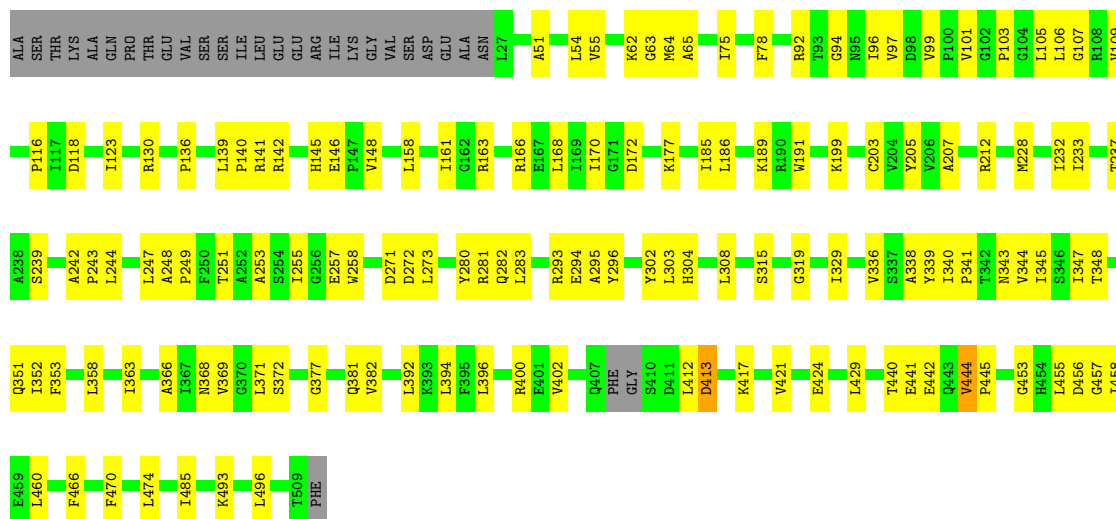
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain L: 74% 20% 5%



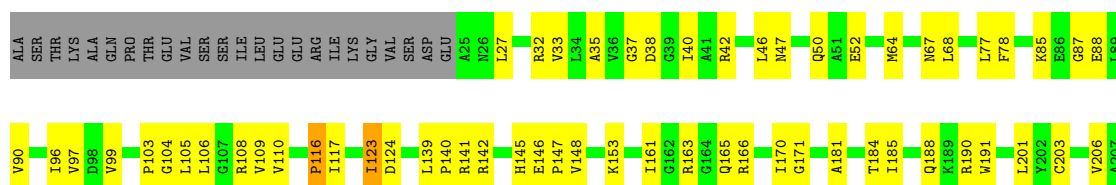
- Molecule 1: ATP synthase subunit alpha, mitochondrial

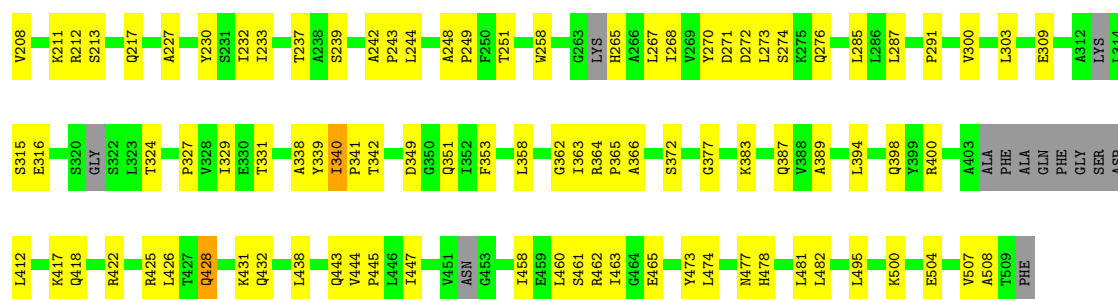
Chain S: 68% 26% 6%



- Molecule 1: ATP synthase subunit alpha, mitochondrial

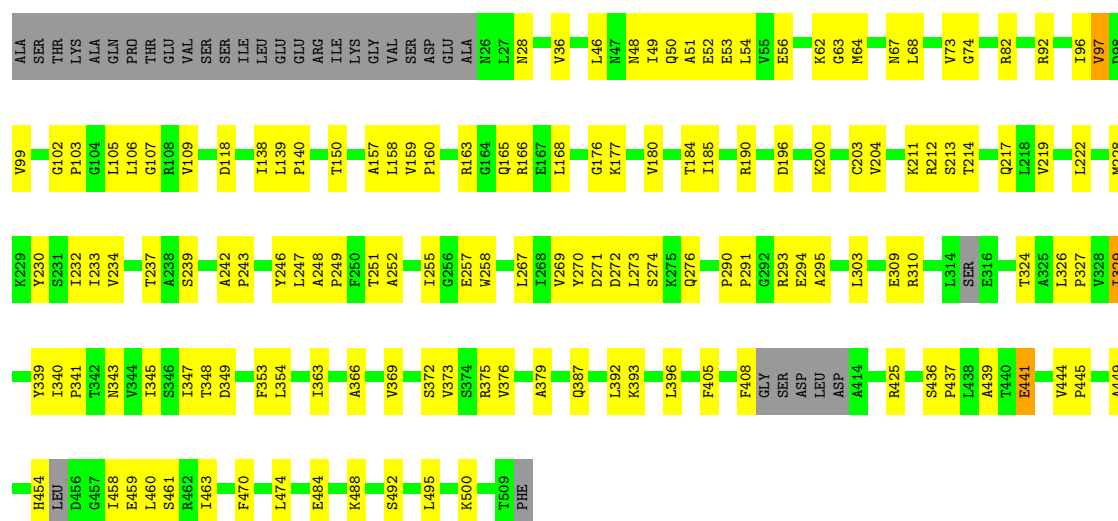
Chain T: 63% 29% 7%





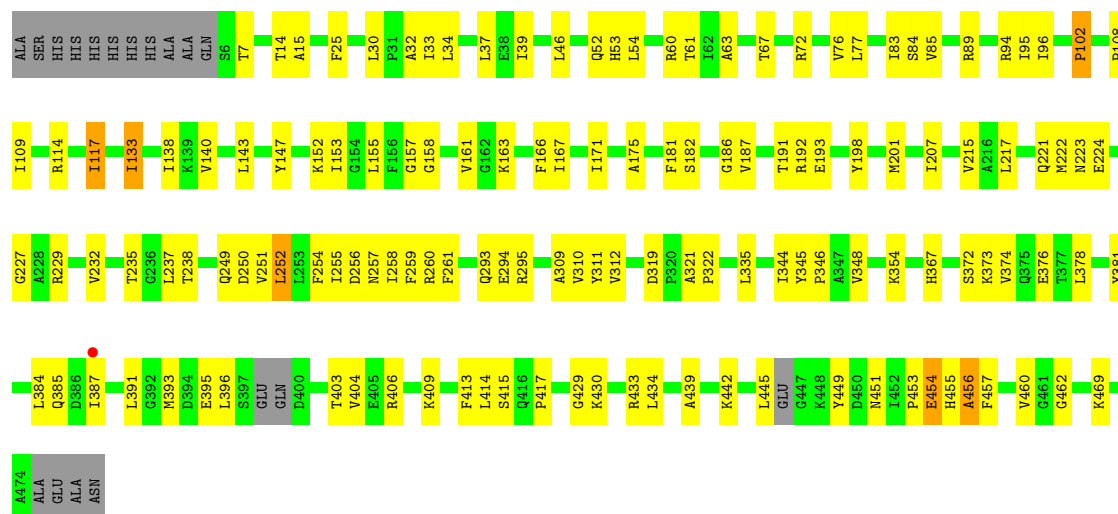
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain U: 66% 27% 6%



- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D: 68% 27% 5%



- Molecule 2: ATP synthase subunit beta, mitochondrial

E422	V307	M201	ALA
V423	Q308	T204	SER
F424	V310	L209	HIS
	D319	V215	HIS
R433	P320	F219	HIS
L473	A321	Q221	ALA
A474	P322	M222	ALA
A475	F326	N223	ALA
GLU	A327	E224	GLN
ALA	H328	P225	SER
ASN	L329	P226	P8
	T333	R229	V13
	I344	V232	T14
	Y345	T235	A15
	P346	G336	V16
	D349	L237	I109
	P350	T338	I114
	L357	Y242	I117
	V370	F243	F25
	V374	R244	E26
	L384	D245	Q27
	I387	L253	L30
	I388	F254	P31
	A389	I258	A32
	I390	T262	I33
	L391	E267	L34
	M393	D394	N35
	E395	L271	A36
	L396	V279	L37
	S397	D400	E38
	K401	L285	I39
	V404	Q293	R149
	E405	E294	K152
	R406	R295	I153
	A407	I296	V47
	R408	T297	L48
	K409	T298	E49
	I410	K301	V50
	Q411	G302	H53
	R412	V303	L54
	S415	V304	N57
	F418	T305	R60
		E306	T61
			M64
			T67
			L70
			L73

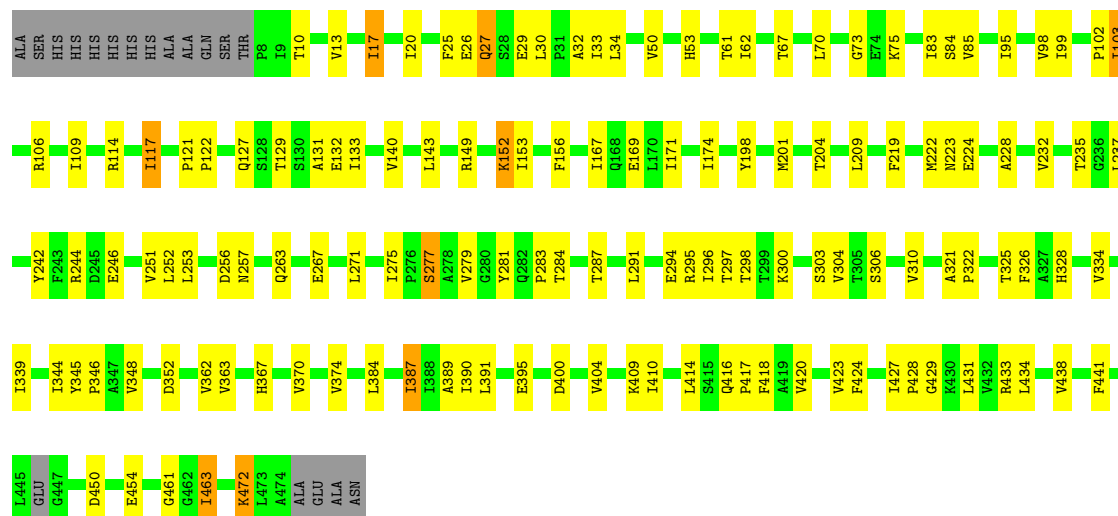
- [illegible]

- | | | |
|------|------|------|
| F254 | E101 | ALA |
| I258 | P102 | SER |
| G265 | I103 | HIS |
| S266 | D104 | HIS |
| E267 | P108 | HIS |
| V268 | | HIS |
| S269 | R114 | HIS |
| A270 | K115 | ALA |
| L271 | P116 | ALA |
| L272 | I117 | GLN |
| | P121 | SER |
| T275 | | T7 |
| P276 | I133 | I117 |
| S277 | | |
| A278 | G137 | F25 |
| V279 | D142 | E26 |
| G280 | | Q27 |
| V281 | | S28 |
| | I153 | E29 |
| L285 | G154 | L30 |
| E284 | L155 | P31 |
| R295 | G160 | A32 |
| T296 | V161 | I33 |
| L297 | G162 | L34 |
| T298 | | |
| | F181 | L37 |
| S303 | S182 | F38 |
| V307 | V183 | I39 |
| Q308 | E189 | Q43 |
| A309 | | G44 |
| V310 | | |
| Y311 | Y198 | V50 |
| | R199 | L54 |
| A314 | E200 | |
| | M201 | N57 |
| D319 | I207 | T58 |
| P320 | | V59 |
| A321 | L217 | A60 |
| P322 | | T61 |
| | G220 | I62 |
| L329 | Q221 | A63 |
| D330 | | M64 |
| | R229 | |
| S336 | A230 | R72 |
| | R231 | |
| I339 | V232 | V76 |
| I344 | | L77 |
| Y345 | T235 | D78 |
| P346 | G236 | V85 |
| A347 | L237 | P86 |
| | Q249 | |
| R356 | | L92 |
| | L252 | |
| D359 | T252 | I95 |



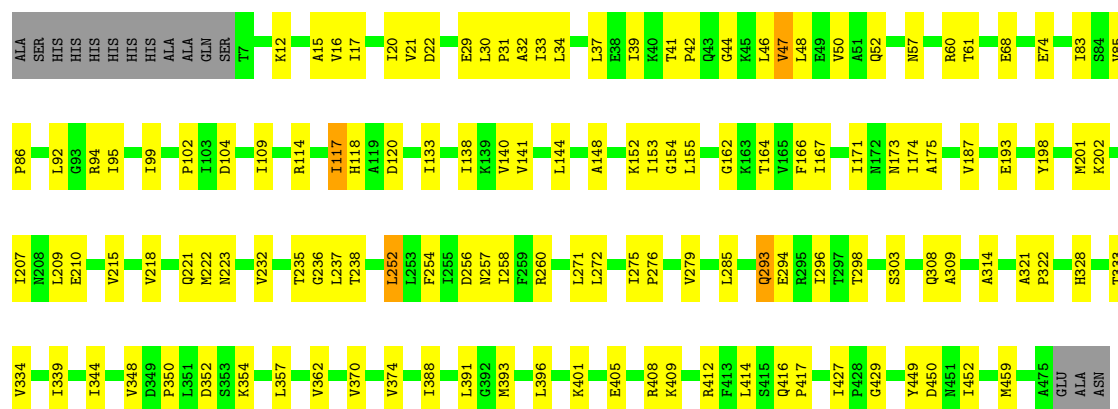
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain N: 68% 26% . .



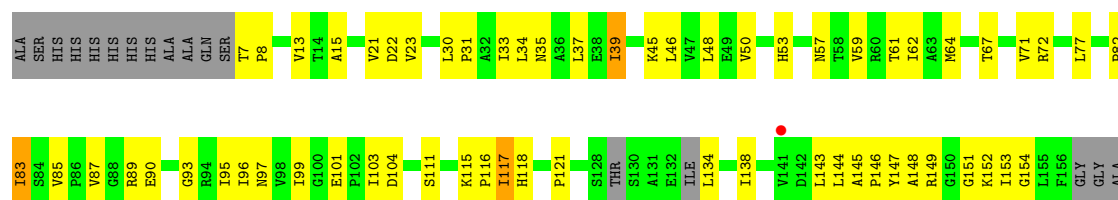
• Molecule 2: ATP synthase subunit beta, mitochondrial

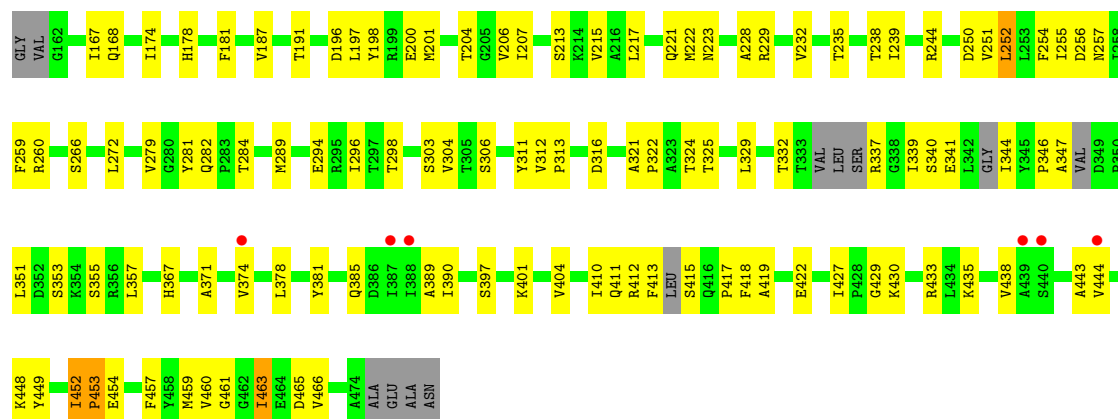
Chain O: 70% 26% . .



• Molecule 2: ATP synthase subunit beta, mitochondrial

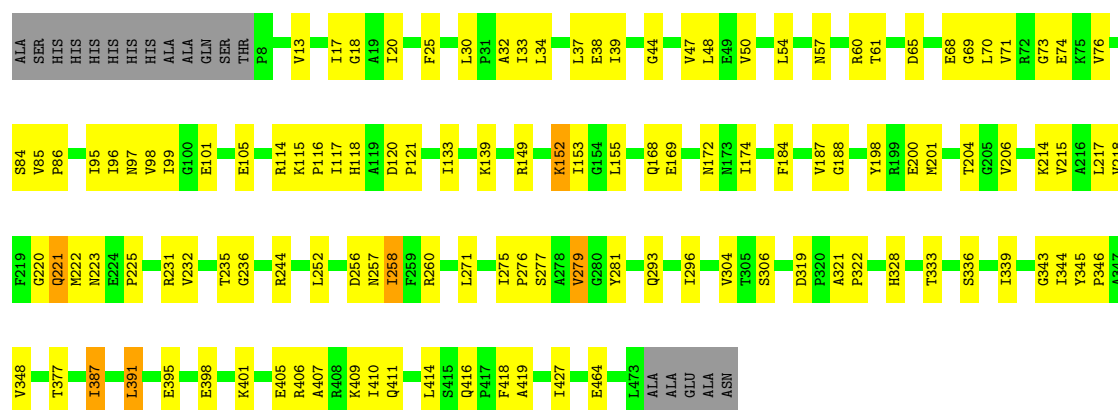
Chain V: % 58% 34% 6% . .





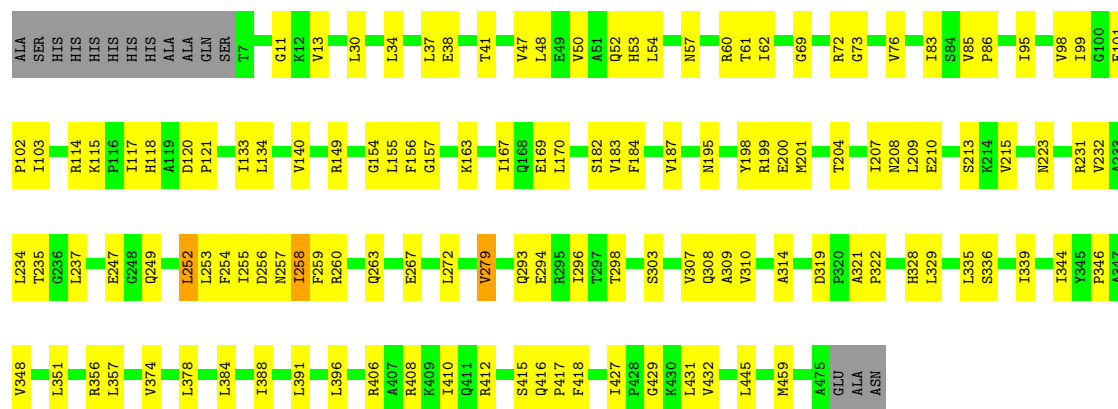
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain W: 71% 24%



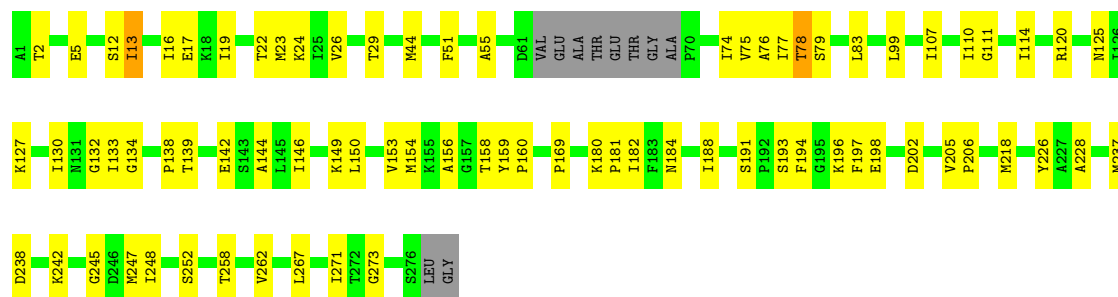
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain X: 70% 26%

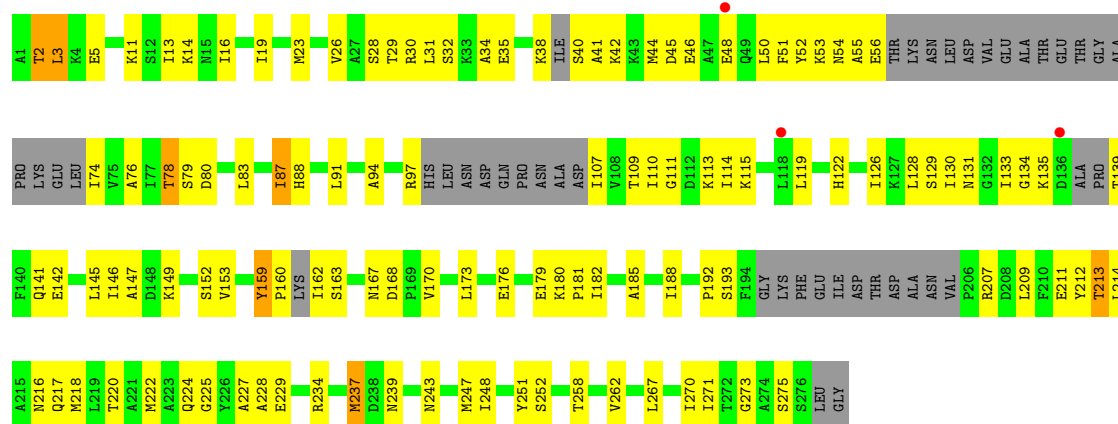


• Molecule 3: ATP synthase subunit gamma, mitochondrial

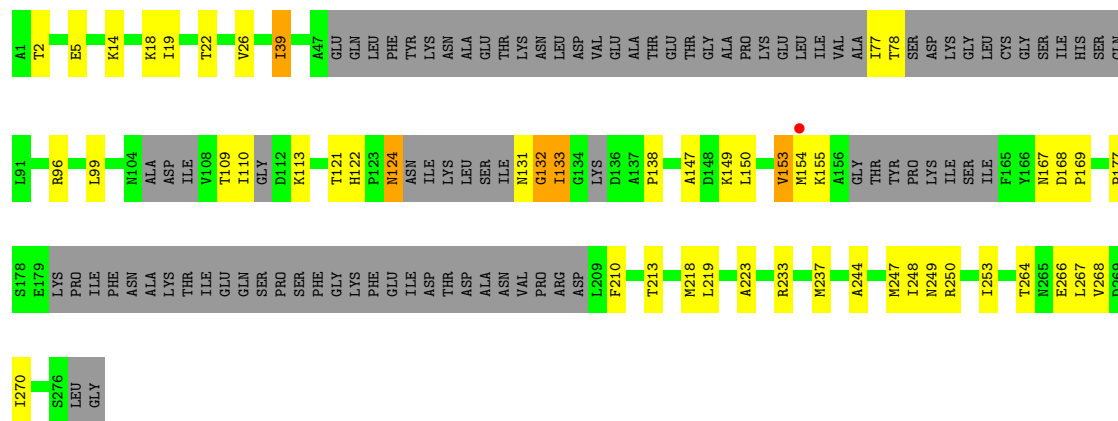
Chain G: 69% 27%



- Molecule 3: ATP synthase subunit gamma, mitochondrial

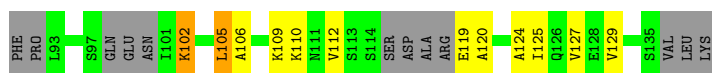


- Molecule 3: ATP synthase subunit gamma, mitochondrial



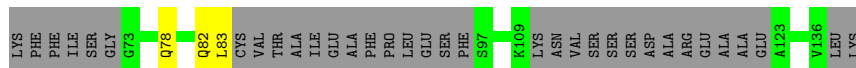
- Molecule 4: ATP synthase subunit delta, mitochondrial





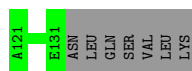
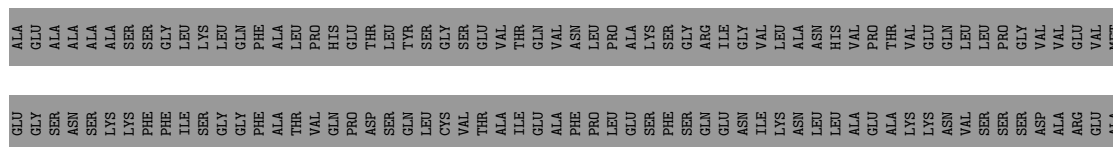
- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain Q: 40% 9% 51%



- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain Z: 8% 92%



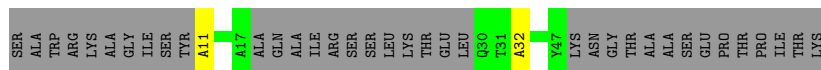
- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain I: 62% 11% 25%



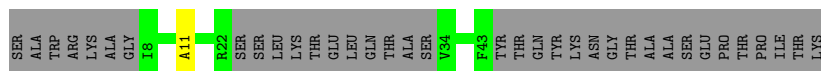
- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain R: 38% 59%



- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain 1: 39% 59%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.93Å 290.49Å 188.70Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	33.20 – 3.59 33.20 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.20-3.59) 98.0 (33.20-3.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.306 0.232 , 0.299	Depositor DCC
R_{free} test set	2727 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	111.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	71793	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	0/3733	0.70	0/5052
1	B	0.26	0/3699	0.69	0/5005
1	C	0.26	0/3736	0.71	0/5057
1	J	0.26	0/3710	0.70	0/5021
1	K	0.27	0/3712	0.70	0/5023
1	L	0.26	0/3736	0.69	1/5057 (0.0%)
1	S	0.28	0/3711	0.73	0/5022
1	T	0.25	0/3645	0.69	0/4929
1	U	0.25	0/3682	0.70	0/4979
2	D	0.28	0/3571	0.75	1/4840 (0.0%)
2	E	0.27	0/3592	0.73	2/4870 (0.0%)
2	F	0.27	0/3614	0.75	2/4901 (0.0%)
2	M	0.28	0/3596	0.75	0/4877
2	N	0.27	0/3577	0.72	0/4848
2	O	0.26	0/3595	0.75	2/4876 (0.0%)
2	V	0.26	0/3506	0.71	0/4742
2	W	0.25	0/3582	0.71	2/4856 (0.0%)
2	X	0.27	0/3599	0.76	4/4881 (0.1%)
3	G	0.27	0/2096	0.71	0/2822
3	P	0.31	0/1780	0.79	2/2388 (0.1%)
3	Y	0.26	0/1451	0.68	1/1939 (0.1%)
4	H	0.24	0/858	0.68	0/1161
4	Q	0.39	0/334	0.99	3/457 (0.7%)
4	Z	0.29	0/54	0.71	0/74
5	1	0.54	0/123	0.86	0/169
5	I	0.24	0/329	0.73	0/449
5	R	0.27	0/123	0.69	0/169
All	All	0.27	0/72744	0.72	20/98464 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	120	ASP	CA-C-N	7.51	125.14	119.66
2	F	120	ASP	C-N-CA	7.51	125.14	119.66
4	Q	78	GLN	CA-C-N	7.21	126.91	119.56
4	Q	78	GLN	C-N-CA	7.21	126.91	119.56
2	O	120	ASP	CA-C-N	6.88	124.69	119.66
2	O	120	ASP	C-N-CA	6.88	124.69	119.66
1	L	93	THR	N-CA-C	-6.36	107.38	114.62
3	P	122	HIS	CA-C-N	6.29	126.49	119.32
3	P	122	HIS	C-N-CA	6.29	126.49	119.32
2	X	120	ASP	CA-C-N	6.23	124.14	119.66
2	X	120	ASP	C-N-CA	6.23	124.14	119.66
3	Y	155	LYS	CB-CA-C	-5.40	110.37	116.63
4	Q	36	SER	CB-CA-C	-5.32	110.00	117.23
2	E	120	ASP	CA-C-N	5.19	123.40	119.66
2	E	120	ASP	C-N-CA	5.19	123.40	119.66
2	X	115	LYS	CA-C-N	5.18	125.12	119.78
2	X	115	LYS	C-N-CA	5.18	125.12	119.78
2	D	454	GLU	CB-CA-C	-5.10	110.29	117.23
2	W	115	LYS	CA-C-N	5.05	125.03	120.03
2	W	115	LYS	C-N-CA	5.05	125.03	120.03

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	3679	0	3762	84	0
1	B	3645	0	3730	96	0
1	C	3680	0	3764	98	0
1	J	3656	0	3743	67	0
1	K	3659	0	3732	102	0
1	L	3680	0	3764	84	0
1	S	3657	0	3745	104	0
1	T	3596	0	3681	111	0
1	U	3629	0	3710	92	0
2	D	3517	0	3594	111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3536	0	3610	100	0
2	F	3558	0	3629	109	0
2	M	3540	0	3607	79	0
2	N	3522	0	3598	104	0
2	O	3539	0	3612	91	0
2	V	3457	0	3510	122	0
2	W	3526	0	3600	88	0
2	X	3543	0	3616	86	0
3	G	2070	0	2128	55	0
3	P	1766	0	1794	97	0
3	Y	1444	0	1491	34	0
4	H	849	0	845	36	0
4	Q	339	0	160	5	0
4	Z	55	0	30	0	0
5	1	125	0	66	0	0
5	I	326	0	286	7	0
5	R	125	0	63	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
6	M	5	0	0	0	0
6	N	5	0	0	0	0
6	O	5	0	0	0	0
6	S	5	0	0	0	0
6	T	5	0	0	0	0
6	U	5	0	0	0	0
6	X	5	0	0	0	0
All	All	71793	0	72870	1852	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 13.

All (1852) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:444:VAL:HG23	1:S:445:PRO:HD3	1.47	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:HE2	2:D:32:ALA:HB2	1.47	0.96
1:U:73:VAL:HG22	2:V:72:ARG:HH22	1.33	0.93
4:H:102:LYS:HG2	4:H:105:LEU:HD11	1.49	0.93
2:M:237:LEU:HD11	2:M:296:ILE:HG12	1.53	0.90
2:E:95:ILE:HG22	2:E:103:ILE:HG13	1.56	0.88
3:P:38:LYS:C	3:P:40:SER:CA	2.48	0.87
3:P:110:ILE:HG12	3:P:130:ILE:HD13	1.56	0.87
2:W:188:GLY:HA3	2:W:260:ARG:HG2	1.55	0.86
2:E:50:VAL:HA	2:E:61:THR:HG22	1.58	0.86
3:P:38:LYS:HE3	3:P:42:LYS:HE2	1.56	0.85
3:G:198:GLU:HB3	4:H:48:THR:HG22	1.58	0.85
1:U:212:ARG:HG3	1:U:237:THR:HG21	1.57	0.85
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.59	0.84
2:V:83:ILE:HD11	2:V:99:ILE:HA	1.58	0.84
2:X:321:ALA:HB3	2:X:322:PRO:HD3	1.61	0.83
2:V:244:ARG:HD3	2:V:304:VAL:HG23	1.59	0.83
2:F:208:ASN:H	2:F:213:SER:HB3	1.42	0.83
2:V:413:PHE:HB2	2:V:457:PHE:HB3	1.59	0.82
2:V:201:MET:HE1	2:V:217:LEU:HD21	1.62	0.82
1:J:239:SER:HB2	2:M:294:GLU:HG3	1.62	0.82
3:Y:121:THR:HG22	3:Y:122:HIS:HD1	1.43	0.82
2:M:154:GLY:HA3	2:M:329:LEU:HD13	1.61	0.81
2:D:163:LYS:HG2	2:D:335:LEU:HD12	1.63	0.80
2:F:209:LEU:HD12	2:F:210:GLU:H	1.47	0.80
2:M:64:MET:HE1	2:M:231:ARG:HG3	1.62	0.80
3:P:182:ILE:HG21	3:P:214:LEU:HD12	1.63	0.79
1:S:347:ILE:HG12	2:W:222:MET:HE1	1.64	0.79
1:T:273:LEU:HD12	1:T:327:PRO:HB3	1.62	0.79
1:A:239:SER:HB2	2:D:294:GLU:HG3	1.63	0.79
1:K:85:LYS:HE2	2:N:32:ALA:HB2	1.63	0.78
1:L:239:SER:HB2	2:O:294:GLU:HG3	1.63	0.78
1:T:474:LEU:HD13	1:T:482:LEU:HD21	1.64	0.78
1:B:392:LEU:HD11	1:B:426:LEU:HD21	1.65	0.78
1:A:212:ARG:HG3	1:A:237:THR:HG21	1.65	0.78
1:L:55:VAL:HG21	1:L:75:ILE:HD13	1.65	0.78
1:S:116:PRO:HG3	1:S:123:ILE:HG12	1.66	0.78
1:C:239:SER:HB2	2:F:294:GLU:HG3	1.65	0.78
2:M:321:ALA:HB3	2:M:322:PRO:HD3	1.66	0.77
2:V:430:LYS:HD3	2:V:461:GLY:HA3	1.65	0.77
2:O:85:VAL:HG11	2:O:235:THR:HG23	1.64	0.77
2:W:387:ILE:HD13	2:W:387:ILE:H	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:273:LEU:HB3	1:S:304:HIS:CE1	2.19	0.77
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.63	0.77
2:W:20:ILE:HD11	2:W:271:LEU:HB3	1.65	0.77
2:O:334:VAL:HG21	2:O:352:ASP:HB3	1.66	0.77
3:P:239:ASN:O	3:P:243:ASN:HB2	1.84	0.77
2:F:30:LEU:HD21	2:F:57:ASN:HA	1.66	0.77
1:J:85:LYS:HE2	2:M:32:ALA:HB2	1.67	0.76
4:H:64:ASN:HD22	4:H:65:SER:N	1.83	0.76
2:F:334:VAL:HG23	2:F:349:ASP:HB3	1.66	0.76
1:S:54:LEU:CD1	1:S:97:VAL:HG22	2.15	0.75
1:J:293:ARG:HA	3:P:267:LEU:HD11	1.68	0.75
1:L:340:ILE:HD12	1:L:340:ILE:H	1.52	0.75
1:J:138:ILE:H	1:J:138:ILE:HD12	1.52	0.75
2:O:95:ILE:HD13	2:O:104:ASP:HB3	1.68	0.75
1:T:103:PRO:HG3	1:T:258:TRP:CH2	2.21	0.75
1:K:444:VAL:HG23	1:K:445:PRO:HD3	1.69	0.75
2:O:298:THR:HG23	2:O:303:SER:HA	1.68	0.75
2:X:417:PRO:HG3	2:X:459:MET:HG3	1.67	0.75
1:J:116:PRO:HG3	1:J:123:ILE:HG12	1.69	0.74
1:T:458:ILE:H	1:T:458:ILE:HD12	1.51	0.74
1:C:73:VAL:HG22	2:D:72:ARG:HH22	1.50	0.74
2:F:33:ILE:H	2:F:33:ILE:HD12	1.52	0.74
1:U:107:GLY:HA2	1:U:228:MET:HG3	1.68	0.74
2:E:13:VAL:HB	2:E:73:GLY:H	1.52	0.74
3:Y:247:MET:HA	3:Y:250:ARG:HD3	1.69	0.74
2:V:15:ALA:HB3	2:V:22:ASP:HB2	1.67	0.74
2:V:30:LEU:HD11	2:V:57:ASN:HA	1.68	0.74
2:N:244:ARG:HD3	2:N:304:VAL:HG23	1.69	0.74
1:U:458:ILE:H	1:U:458:ILE:HD12	1.52	0.74
2:D:138:ILE:H	2:D:138:ILE:HD12	1.52	0.73
2:E:25:PHE:HB2	2:E:30:LEU:HD23	1.71	0.73
1:B:413:ASP:HB3	1:B:417:LYS:HB2	1.70	0.73
1:B:444:VAL:HG23	1:B:445:PRO:HD3	1.71	0.73
2:O:37:LEU:HB2	2:O:48:LEU:HB2	1.69	0.73
1:S:191:TRP:HD1	1:S:199:LYS:HB3	1.53	0.73
1:C:338:ALA:HB3	1:C:341:PRO:HG2	1.71	0.73
2:M:25:PHE:O	2:M:57:ASN:HB3	1.88	0.73
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.69	0.73
1:U:269:VAL:HG22	1:U:326:LEU:HB2	1.70	0.72
2:O:144:LEU:HD13	2:O:350:PRO:HB3	1.70	0.72
2:E:133:ILE:HD12	2:E:146:PRO:HB2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:330:ASP:HB3	2:M:356:ARG:HD2	1.70	0.72
1:T:123:ILE:HD13	1:T:123:ILE:H	1.55	0.72
2:N:387:ILE:H	2:N:387:ILE:HD13	1.54	0.72
2:O:187:VAL:HG22	2:O:232:VAL:HG13	1.72	0.72
3:G:169:PRO:HG3	3:G:228:ALA:HB2	1.72	0.72
2:W:244:ARG:HD3	2:W:304:VAL:HG23	1.70	0.72
2:O:37:LEU:HD12	2:O:61:THR:HG21	1.71	0.72
2:X:37:LEU:HB2	2:X:48:LEU:HB2	1.71	0.72
1:J:353:PHE:H	1:J:372:SER:HB3	1.53	0.71
1:A:248:ALA:HB3	1:A:249:PRO:HD3	1.72	0.71
2:W:25:PHE:HB2	2:W:30:LEU:HD23	1.72	0.71
2:M:153:ILE:HD12	2:M:307:VAL:HG22	1.71	0.71
1:L:248:ALA:HB3	1:L:249:PRO:HD3	1.73	0.71
2:N:20:ILE:HD11	2:N:271:LEU:HB3	1.71	0.71
2:M:50:VAL:HA	2:M:61:THR:HG22	1.73	0.71
3:G:248:ILE:O	3:G:252:SER:HB2	1.91	0.71
1:T:85:LYS:HE2	2:W:32:ALA:HB2	1.71	0.71
3:P:44:MET:HE1	3:P:216:ASN:HD21	1.54	0.70
2:V:321:ALA:HB3	2:V:322:PRO:HD3	1.72	0.70
2:E:391:LEU:HD13	2:E:395:GLU:HG3	1.72	0.70
4:H:49:VAL:HG22	4:H:76:THR:HG23	1.74	0.70
2:X:85:VAL:HG11	2:X:235:THR:HG23	1.74	0.70
1:T:340:ILE:H	1:T:340:ILE:HD12	1.56	0.70
4:H:39:ILE:HD13	4:H:39:ILE:H	1.57	0.70
1:L:340:ILE:HB	1:L:341:PRO:HD3	1.74	0.70
1:L:375:ARG:HH21	2:M:160:GLY:HA2	1.56	0.70
2:W:85:VAL:HG11	2:W:235:THR:HG23	1.74	0.70
2:N:13:VAL:HB	2:N:73:GLY:H	1.57	0.70
3:P:111:GLY:O	3:P:114:ILE:HG22	1.90	0.70
1:U:248:ALA:HB3	1:U:249:PRO:HD3	1.72	0.70
2:X:201:MET:HA	2:X:201:MET:HE2	1.74	0.70
2:X:208:ASN:H	2:X:213:SER:HB3	1.56	0.70
3:P:212:TYR:O	3:P:216:ASN:HB2	1.91	0.69
1:C:478:HIS:HB3	1:C:481:LEU:HD23	1.73	0.69
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.74	0.69
1:T:145:HIS:CD2	1:T:146:GLU:HG3	2.27	0.69
2:X:298:THR:HG23	2:X:303:SER:HA	1.73	0.69
1:J:455:LEU:HA	1:J:458:ILE:HD13	1.74	0.69
3:P:2:THR:HG23	3:P:5:GLU:HB3	1.73	0.69
3:P:91:LEU:HD22	3:P:167:ASN:HD21	1.57	0.69
1:S:101:VAL:HG12	1:S:255:ILE:HD13	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:140:VAL:HG22	2:O:414:LEU:HB3	1.73	0.69
1:J:444:VAL:HG23	1:J:445:PRO:HD3	1.73	0.69
2:F:187:VAL:HG12	2:F:260:ARG:HB2	1.74	0.68
3:P:76:ALA:HB3	3:P:109:THR:HG22	1.75	0.68
1:B:358:LEU:HB2	1:B:366:ALA:HB1	1.74	0.68
3:P:149:LYS:O	3:P:153:VAL:HG12	1.93	0.68
2:E:244:ARG:HD3	2:E:304:VAL:HG23	1.74	0.68
2:N:132:GLU:HG3	2:N:149:ARG:HB3	1.76	0.68
3:P:170:VAL:HG23	3:P:176:GLU:HB2	1.76	0.68
2:E:102:PRO:HG3	2:E:109:ILE:HG13	1.75	0.68
1:T:108:ARG:HH21	1:T:116:PRO:HB3	1.59	0.68
2:F:298:THR:HG23	2:F:303:SER:HA	1.75	0.68
2:N:50:VAL:HA	2:N:61:THR:HG22	1.75	0.68
2:N:410:ILE:HG23	2:N:441:PHE:HE2	1.58	0.68
2:V:312:VAL:HG12	2:V:316:ASP:H	1.58	0.68
1:K:481:LEU:HD22	1:K:495:LEU:HD11	1.76	0.68
1:U:138:ILE:HD13	2:V:191:THR:HG23	1.74	0.68
2:E:390:ILE:HG21	3:G:29:THR:HA	1.75	0.68
1:A:460:LEU:HA	1:A:463:ILE:HG12	1.76	0.67
2:O:47:VAL:HG21	2:O:99:ILE:HG21	1.75	0.67
1:K:103:PRO:HG3	1:K:258:TRP:CH2	2.30	0.67
2:X:408:ARG:O	2:X:412:ARG:HG3	1.94	0.67
1:A:455:LEU:HD21	1:A:466:PHE:CE2	2.29	0.67
2:V:296:ILE:HG21	2:V:306:SER:HB2	1.77	0.67
2:D:33:ILE:HD12	2:D:33:ILE:H	1.60	0.67
1:A:385:LEU:HD11	1:A:447:ILE:HD12	1.77	0.66
2:D:454:GLU:HG3	2:D:455:HIS:N	2.10	0.66
1:T:342:THR:HG21	2:X:314:ALA:HA	1.77	0.66
1:L:139:LEU:HB3	1:L:140:PRO:HD3	1.77	0.66
1:C:248:ALA:HB3	1:C:249:PRO:HD3	1.76	0.66
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.78	0.66
1:K:89:LEU:HD21	1:K:91:LYS:HE3	1.76	0.66
1:S:168:LEU:HB2	1:S:348:THR:HG21	1.78	0.66
2:W:398:GLU:HA	2:W:401:LYS:HE2	1.78	0.66
1:B:36:VAL:HG12	2:E:53:HIS:HB2	1.78	0.66
1:L:123:ILE:HD13	1:L:123:ILE:H	1.61	0.66
1:A:455:LEU:HD23	1:A:458:ILE:HD12	1.77	0.66
1:C:455:LEU:HA	1:C:458:ILE:HD13	1.77	0.66
1:K:64:MET:HB2	1:K:78:PHE:HE1	1.61	0.66
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.78	0.66
2:V:444:VAL:HG13	2:V:449:TYR:HB2	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:MET:HE1	2:D:217:LEU:HD21	1.78	0.66
2:M:201:MET:HE1	2:M:217:LEU:HD21	1.78	0.66
2:D:25:PHE:HB2	2:D:30:LEU:HD23	1.78	0.65
2:M:345:TYR:HB2	2:M:459:MET:HE1	1.77	0.65
2:X:11:GLY:HA3	2:X:76:VAL:HB	1.76	0.65
1:C:168:LEU:HB2	1:C:348:THR:HG21	1.76	0.65
2:V:417:PRO:HG3	2:V:459:MET:HG3	1.77	0.65
4:H:109:LYS:O	4:H:112:VAL:HG12	1.97	0.65
1:J:248:ALA:HB3	1:J:249:PRO:HD3	1.79	0.65
2:O:138:ILE:H	2:O:138:ILE:HD12	1.60	0.65
1:B:338:ALA:HB3	1:B:341:PRO:HG2	1.77	0.65
1:B:108:ARG:HH21	1:B:116:PRO:HB3	1.61	0.65
2:M:102:PRO:HG2	2:M:108:PRO:HA	1.77	0.65
1:S:106:LEU:HD23	1:S:232:ILE:HD11	1.79	0.65
1:C:412:LEU:HD11	1:C:420:LEU:HD13	1.77	0.65
1:U:309:GLU:HG3	2:V:223:ASN:HB3	1.79	0.65
1:A:412:LEU:HD11	1:A:420:LEU:HD13	1.78	0.65
1:T:270:TYR:HB2	1:T:327:PRO:HA	1.77	0.64
2:W:187:VAL:HG22	2:W:232:VAL:HG23	1.79	0.64
1:C:139:LEU:HB3	1:C:140:PRO:HD3	1.79	0.64
3:G:191:SER:HB2	3:G:194:PHE:HB2	1.79	0.64
3:P:220:THR:O	3:P:224:GLN:HG2	1.96	0.64
2:X:391:LEU:HD23	2:X:391:LEU:H	1.60	0.64
1:A:460:LEU:H	1:A:460:LEU:HD12	1.61	0.64
2:O:417:PRO:HB2	2:O:429:GLY:HA2	1.80	0.64
2:X:417:PRO:HB2	2:X:429:GLY:HA2	1.79	0.64
2:F:98:VAL:HG13	2:F:99:ILE:HG23	1.80	0.64
3:G:130:ILE:HG12	3:G:146:ILE:HD12	1.79	0.64
3:G:142:GLU:O	3:G:146:ILE:HG12	1.97	0.64
2:W:96:ILE:HG22	2:W:97:ASN:H	1.63	0.64
1:B:413:ASP:H	1:B:417:LYS:HD3	1.62	0.64
1:K:96:ILE:HD12	1:K:96:ILE:H	1.62	0.64
3:P:13:ILE:HD13	3:P:247:MET:HG2	1.80	0.64
2:F:20:ILE:HD11	2:F:268:VAL:HB	1.79	0.64
1:S:394:LEU:H	1:S:394:LEU:HD12	1.63	0.64
4:H:32:LEU:HD11	4:H:83:LEU:HD21	1.79	0.63
3:Y:2:THR:HG22	3:Y:5:GLU:HG2	1.80	0.63
3:P:41:ALA:HB1	3:P:220:THR:HG22	1.79	0.63
2:W:98:VAL:HG13	2:W:99:ILE:HD12	1.80	0.63
1:B:273:LEU:HD12	1:B:327:PRO:HB3	1.79	0.63
1:K:54:LEU:HD21	1:K:62:LYS:HD3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:201:MET:HE3	2:M:207:ILE:HD11	1.81	0.63
1:A:138:ILE:HD12	1:A:138:ILE:H	1.64	0.63
1:L:85:LYS:HE2	2:O:32:ALA:HB2	1.80	0.63
2:O:393:MET:HA	2:O:396:LEU:HD13	1.79	0.63
3:P:141:GLN:O	3:P:145:LEU:HG	1.99	0.63
1:U:425:ARG:HG2	1:U:463:ILE:HD11	1.79	0.63
4:H:64:ASN:HD22	4:H:65:SER:H	1.46	0.63
1:L:82:ARG:HA	2:O:33:ILE:HB	1.80	0.63
1:U:177:LYS:HG2	1:U:354:LEU:HD12	1.81	0.62
1:B:40:ILE:HG21	1:B:287:LEU:HD21	1.81	0.62
1:J:136:PRO:HB2	1:J:141:ARG:HE	1.65	0.62
1:A:424:GLU:HG2	1:A:460:LEU:HD21	1.80	0.62
1:K:217:GLN:HE22	2:N:131:ALA:HB2	1.64	0.62
2:F:47:VAL:HG21	2:F:99:ILE:HG21	1.80	0.62
2:F:50:VAL:HA	2:F:61:THR:HG22	1.81	0.62
3:G:74:ILE:HB	3:G:107:ILE:HG12	1.80	0.62
1:U:103:PRO:HG3	1:U:258:TRP:CH2	2.34	0.62
1:U:109:VAL:HB	1:U:118:ASP:HB3	1.81	0.62
2:D:417:PRO:HB2	2:D:429:GLY:HA2	1.81	0.62
1:K:425:ARG:HB3	1:K:463:ILE:HD13	1.81	0.62
2:O:20:ILE:HD12	2:O:271:LEU:HB2	1.80	0.62
1:T:96:ILE:HG22	1:T:97:VAL:HG22	1.81	0.62
1:J:103:PRO:HG3	1:J:258:TRP:CH2	2.35	0.62
1:T:444:VAL:HG23	1:T:445:PRO:HD3	1.81	0.62
3:Y:121:THR:HG22	3:Y:122:HIS:ND1	2.13	0.62
1:A:168:LEU:HD11	1:A:329:ILE:HD13	1.81	0.62
1:C:149:GLN:HB2	1:C:191:TRP:HH2	1.64	0.62
2:D:222:MET:HA	2:D:229:ARG:HD2	1.81	0.62
2:N:346:PRO:HB2	2:N:348:VAL:HG23	1.82	0.62
1:S:191:TRP:CD1	1:S:199:LYS:HB3	2.34	0.62
1:C:103:PRO:HG3	1:C:258:TRP:CH2	2.35	0.61
1:C:174:GLN:HB3	2:F:354:LYS:HG3	1.82	0.61
2:F:83:ILE:HB	2:F:117:ILE:HD12	1.82	0.61
1:U:139:LEU:HB3	1:U:140:PRO:HD3	1.82	0.61
1:B:242:ALA:HB3	1:B:243:PRO:HD3	1.82	0.61
2:D:171:ILE:O	2:D:175:ALA:HB3	2.00	0.61
3:G:138:PRO:HD3	3:G:226:TYR:HD2	1.66	0.61
4:H:14:PHE:HE2	4:H:57:VAL:HG11	1.64	0.61
3:Y:77:ILE:N	3:Y:109:THR:HG1	1.98	0.61
1:B:309:GLU:OE1	2:F:223:ASN:HB3	2.00	0.61
1:C:211:LYS:HD3	2:F:328:HIS:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:293:ARG:HG2	1:L:294:GLU:HG3	1.81	0.61
3:P:94:ALA:HA	3:P:97:ARG:NH2	2.15	0.61
2:D:454:GLU:HG3	2:D:455:HIS:H	1.64	0.61
2:W:54:LEU:HD21	2:W:60:ARG:HE	1.65	0.61
1:A:63:GLY:HA2	1:A:78:PHE:CD2	2.36	0.61
2:F:209:LEU:HD12	2:F:210:GLU:N	2.15	0.61
1:S:248:ALA:HB3	1:S:249:PRO:HD3	1.80	0.61
2:V:281:TYR:OH	2:V:321:ALA:HB2	2.01	0.61
2:N:83:ILE:HB	2:N:117:ILE:HD12	1.82	0.61
2:N:345:TYR:HA	2:N:346:PRO:C	2.24	0.61
2:V:222:MET:HA	2:V:229:ARG:HD2	1.83	0.61
1:K:273:LEU:HD12	1:K:327:PRO:HB3	1.81	0.61
1:S:99:VAL:HG11	1:S:251:THR:HG23	1.82	0.61
2:V:85:VAL:HG11	2:V:235:THR:HG23	1.81	0.61
1:A:444:VAL:HG23	1:A:445:PRO:HD3	1.83	0.60
2:M:396:LEU:HB3	2:M:400:ASP:HB2	1.83	0.60
3:P:74:ILE:HB	3:P:107:ILE:HG12	1.82	0.60
2:D:157:GLY:H	2:D:312:VAL:HG23	1.66	0.60
2:D:460:VAL:HG12	2:D:469:LYS:HG3	1.83	0.60
3:P:2:THR:HG23	3:P:5:GLU:CB	2.31	0.60
2:X:154:GLY:HA3	2:X:329:LEU:HD13	1.83	0.60
2:O:201:MET:HE2	2:O:201:MET:HA	1.82	0.60
1:S:96:ILE:HD12	1:S:130:ARG:CZ	2.32	0.60
1:S:444:VAL:HG21	1:S:485:ILE:HG21	1.83	0.60
2:X:30:LEU:HD21	2:X:57:ASN:HA	1.82	0.60
2:E:224:GLU:O	2:E:229:ARG:HD3	2.02	0.60
2:F:417:PRO:HB2	2:F:429:GLY:HA2	1.82	0.60
1:K:305:SER:HB2	2:O:222:MET:HB2	1.82	0.60
1:T:170:ILE:HG23	1:T:353:PHE:HA	1.83	0.60
2:E:117:ILE:HA	2:E:238:THR:OG1	2.02	0.60
2:F:201:MET:HE2	2:F:201:MET:HA	1.82	0.60
1:K:248:ALA:HB3	1:K:249:PRO:HD3	1.84	0.60
2:N:310:VAL:HG11	2:N:326:PHE:HE1	1.67	0.60
1:K:100:PRO:HD3	1:K:128:ARG:HH21	1.66	0.60
3:G:17:GLU:HG3	3:G:248:ILE:HD13	1.83	0.60
1:S:412:LEU:HD22	1:S:417:LYS:HA	1.82	0.60
2:W:33:ILE:O	2:W:34:LEU:HB2	2.01	0.60
2:X:133:ILE:HD12	2:X:133:ILE:H	1.65	0.60
2:E:168:GLN:HE21	2:E:201:MET:HG2	1.67	0.60
1:K:104:GLY:HA3	1:K:124:ASP:HB3	1.82	0.60
1:K:413:ASP:HB3	1:K:417:LYS:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:GLU:HG2	1:L:62:LYS:HG2	1.84	0.60
1:T:363:ILE:H	1:T:363:ILE:HD12	1.65	0.60
1:L:105:LEU:HD13	1:L:255:ILE:HG23	1.84	0.60
1:L:455:LEU:HA	1:L:458:ILE:HD13	1.84	0.60
2:W:30:LEU:HD11	2:W:57:ASN:HA	1.82	0.60
2:D:373:LYS:HE3	2:D:406:ARG:HH22	1.66	0.59
1:U:369:VAL:HG11	1:U:396:LEU:HB2	1.84	0.59
2:X:62:ILE:HD11	2:X:272:LEU:HD21	1.84	0.59
2:X:95:ILE:HG22	2:X:103:ILE:HD12	1.84	0.59
1:A:389:ALA:HB2	1:A:447:ILE:HG21	1.84	0.59
2:D:403:THR:HG23	2:D:406:ARG:HH21	1.67	0.59
1:J:340:ILE:HB	1:J:341:PRO:HD3	1.82	0.59
2:O:102:PRO:HG3	2:O:109:ILE:HG13	1.84	0.59
1:A:353:PHE:H	1:A:372:SER:HB3	1.67	0.59
2:E:20:ILE:HD11	2:E:271:LEU:HB3	1.84	0.59
2:E:83:ILE:HB	2:E:117:ILE:HD12	1.83	0.59
1:K:67:ASN:HB3	2:O:17:ILE:HG23	1.84	0.59
2:M:115:LYS:NZ	2:M:115:LYS:HB3	2.18	0.59
1:S:294:GLU:O	1:S:295:ALA:HB3	2.03	0.59
2:X:50:VAL:HA	2:X:61:THR:HG22	1.83	0.59
1:A:378:SER:HB3	1:A:386:LYS:HE3	1.85	0.59
1:B:67:ASN:HB2	2:F:17:ILE:HG22	1.85	0.59
1:B:340:ILE:HB	1:B:341:PRO:HD3	1.85	0.59
1:K:101:VAL:HG12	1:K:255:ILE:HG12	1.84	0.59
1:J:269:VAL:HG22	1:J:326:LEU:HB2	1.85	0.59
2:V:417:PRO:HB2	2:V:429:GLY:HA2	1.85	0.59
3:P:44:MET:CE	3:P:216:ASN:HD21	2.15	0.59
2:D:396:LEU:HG	2:D:404:VAL:HG11	1.85	0.59
1:T:33:VAL:HB	1:T:87:GLY:H	1.68	0.59
2:D:187:VAL:HG22	2:D:232:VAL:HG13	1.84	0.58
2:N:102:PRO:HB3	2:N:109:ILE:HD11	1.85	0.58
2:X:374:VAL:HG23	2:X:445:LEU:HD11	1.85	0.58
1:B:190:ARG:HB2	1:B:191:TRP:CE3	2.38	0.58
1:L:375:ARG:HH22	2:M:162:GLY:H	1.49	0.58
1:S:55:VAL:HG21	1:S:75:ILE:HD13	1.85	0.58
1:U:204:VAL:HG22	1:U:232:ILE:HD13	1.84	0.58
1:C:73:VAL:HG22	2:D:72:ARG:NH2	2.19	0.58
1:T:104:GLY:HA3	1:T:124:ASP:HB3	1.85	0.58
2:W:152:LYS:NZ	2:W:293:GLN:HB3	2.18	0.58
2:F:83:ILE:H	2:F:83:ILE:HD12	1.69	0.58
2:F:171:ILE:O	2:F:175:ALA:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:51:ALA:HB3	2:W:69:GLY:H	1.67	0.58
2:V:201:MET:HA	2:V:204:THR:HG22	1.86	0.58
3:P:170:VAL:CG2	3:P:176:GLU:HB2	2.34	0.58
1:U:163:ARG:HA	1:U:324:THR:OG1	2.03	0.58
2:X:86:PRO:HG3	2:X:114:ARG:HE	1.69	0.58
3:P:53:LYS:O	3:P:56:GLU:HG3	2.03	0.58
1:T:239:SER:OG	2:W:121:PRO:HG2	2.03	0.58
1:B:462:ARG:HB3	1:B:465:GLU:HB2	1.86	0.58
2:F:63:ALA:O	2:F:227:GLY:HA3	2.04	0.58
1:J:455:LEU:HD21	1:J:466:PHE:CZ	2.38	0.58
2:V:340:SER:HB3	2:V:347:ALA:HA	1.86	0.58
2:W:321:ALA:HB3	2:W:322:PRO:HD3	1.84	0.58
2:X:357:LEU:HD22	2:X:357:LEU:H	1.68	0.58
2:O:202:LYS:HA	2:O:207:ILE:HB	1.86	0.58
1:A:70:PRO:HD3	2:E:15:ALA:HB2	1.86	0.57
2:D:319:ASP:O	2:D:322:PRO:HD2	2.03	0.57
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.86	0.57
2:O:148:ALA:HB2	2:O:357:LEU:HD11	1.85	0.57
2:W:97:ASN:HD21	2:W:101:GLU:HG3	1.69	0.57
1:K:96:ILE:O	1:K:97:VAL:C	2.47	0.57
2:F:96:ILE:HB	2:F:218:VAL:HG22	1.86	0.57
2:M:27:GLN:O	2:M:28:SER:OG	2.19	0.57
1:A:168:LEU:HB2	1:A:348:THR:HG21	1.86	0.57
1:B:62:LYS:HD2	1:B:113:LEU:HD13	1.86	0.57
2:D:147:TYR:CE2	2:D:153:ILE:HG21	2.39	0.57
3:P:142:GLU:O	3:P:146:ILE:HG12	2.03	0.57
2:F:152:LYS:HA	2:F:306:SER:OG	2.05	0.57
1:J:142:ARG:HB2	1:J:315:SER:HA	1.85	0.57
2:V:50:VAL:HA	2:V:61:THR:HG22	1.87	0.57
2:W:184:PHE:HB3	2:W:217:LEU:HD23	1.85	0.57
4:H:52:LEU:HD11	4:H:75:ALA:HB2	1.85	0.57
1:S:363:ILE:H	1:S:363:ILE:HD12	1.69	0.57
1:T:270:TYR:HB3	1:T:273:LEU:HG	1.85	0.57
2:W:406:ARG:O	2:W:410:ILE:HG12	2.05	0.57
1:B:413:ASP:CG	1:B:414:ALA:H	2.12	0.57
1:C:302:TYR:O	1:C:306:ARG:HG2	2.04	0.57
4:Q:82:GLN:O	4:Q:83:LEU:C	2.47	0.57
1:S:148:VAL:CG2	1:S:163:ARG:HG2	2.34	0.57
2:X:258:ILE:O	2:X:258:ILE:HD13	2.05	0.57
2:M:390:ILE:HG13	3:P:16:ILE:HD11	1.86	0.57
1:A:338:ALA:HB3	1:A:341:PRO:HG2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:413:ASP:H	1:K:417:LYS:HD3	1.70	0.57
2:O:50:VAL:HA	2:O:61:THR:HG22	1.87	0.57
3:P:29:THR:HG23	3:P:30:ARG:HG3	1.86	0.57
2:V:452:ILE:H	2:V:452:ILE:HD12	1.70	0.57
1:B:50:GLN:HB2	1:B:53:GLU:HB2	1.87	0.56
2:F:388:ILE:HD11	2:F:396:LEU:HD12	1.87	0.56
3:P:34:ALA:HB1	3:P:227:ALA:HB2	1.85	0.56
1:U:444:VAL:HB	1:U:445:PRO:HD3	1.85	0.56
1:C:373:VAL:HA	1:C:393:LYS:HZ1	1.70	0.56
1:U:217:GLN:HG2	2:X:356:ARG:HH21	1.70	0.56
1:C:85:LYS:HE2	2:F:32:ALA:HB2	1.87	0.56
2:M:86:PRO:HD3	2:M:114:ARG:NH2	2.20	0.56
2:N:33:ILE:O	2:N:34:LEU:HB2	2.04	0.56
1:U:274:SER:OG	1:U:329:ILE:HG12	2.06	0.56
1:U:484:GLU:O	1:U:488:LYS:HB2	2.05	0.56
1:A:142:ARG:HB2	1:A:315:SER:HA	1.86	0.56
1:B:165:GLN:HG2	1:B:166:ARG:N	2.21	0.56
2:E:152:LYS:HD2	2:E:152:LYS:N	2.20	0.56
1:J:460:LEU:H	1:J:460:LEU:HD12	1.69	0.56
1:S:343:ASN:O	1:S:347:ILE:HG13	2.06	0.56
1:B:97:VAL:HG11	1:B:247:LEU:HD21	1.86	0.56
1:C:291:PRO:HD2	3:G:273:GLY:HA2	1.88	0.56
2:E:397:SER:N	2:E:400:ASP:HB2	2.21	0.56
3:G:150:LEU:O	3:G:154:MET:HB2	2.05	0.56
4:H:15:ALA:HB3	4:H:86:THR:HG22	1.87	0.56
1:K:340:ILE:HB	1:K:341:PRO:HD3	1.87	0.56
1:T:474:LEU:HB3	1:T:482:LEU:HD11	1.85	0.56
1:A:358:LEU:HB2	1:A:366:ALA:HB1	1.88	0.56
1:A:444:VAL:CG2	1:A:445:PRO:HD3	2.34	0.56
2:M:276:PRO:HG3	3:P:273:GLY:HA3	1.88	0.56
2:W:427:ILE:H	2:W:427:ILE:HD12	1.70	0.56
2:D:117:ILE:HD13	2:D:117:ILE:H	1.69	0.56
2:O:83:ILE:HB	2:O:117:ILE:HD12	1.87	0.56
2:W:174:ILE:HD12	2:W:252:LEU:HD11	1.88	0.56
2:W:319:ASP:O	2:W:322:PRO:HD2	2.06	0.56
1:A:293:ARG:HD3	1:A:339:TYR:CD1	2.41	0.56
1:J:444:VAL:CG2	1:J:445:PRO:HD3	2.35	0.56
1:K:165:GLN:HG2	1:K:166:ARG:N	2.20	0.56
1:L:329:ILE:HD12	1:L:344:VAL:HG21	1.88	0.56
1:U:219:VAL:HA	1:U:228:MET:HE1	1.88	0.56
3:G:78:THR:OG1	3:G:114:ILE:HB	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:391:LEU:HD22	3:P:83:LEU:HD21	1.88	0.56
1:T:165:GLN:HG2	1:T:166:ARG:N	2.20	0.56
2:D:84:SER:OG	2:D:114:ARG:HB3	2.06	0.55
1:J:54:LEU:HD11	1:J:97:VAL:HG22	1.88	0.55
1:S:51:ALA:H	2:W:70:LEU:H	1.54	0.55
1:T:35:ALA:HB3	1:T:42:ARG:HD3	1.88	0.55
1:T:105:LEU:HB2	1:T:232:ILE:HD13	1.89	0.55
1:J:363:ILE:H	1:J:363:ILE:HD12	1.71	0.55
1:L:299:ASP:HA	2:M:267:GLU:HG2	1.87	0.55
2:N:169:GLU:HG2	2:N:418:PHE:CD1	2.41	0.55
5:I:46:GLN:C	5:I:56:PRO:HD2	2.31	0.55
1:J:239:SER:OG	2:M:121:PRO:HG3	2.06	0.55
2:M:33:ILE:O	2:M:34:LEU:HB2	2.05	0.55
1:T:166:ARG:NH1	1:T:309:GLU:HG2	2.21	0.55
1:U:376:VAL:HG12	1:U:379:ALA:HB3	1.88	0.55
2:F:357:LEU:HD22	2:F:362:VAL:HG11	1.88	0.55
1:K:64:MET:HB2	1:K:78:PHE:CE1	2.41	0.55
3:P:14:LYS:HD3	3:P:248:ILE:HD12	1.87	0.55
1:U:67:ASN:HB2	1:U:74:GLY:HA3	1.88	0.55
2:V:148:ALA:HB2	2:V:357:LEU:HD11	1.88	0.55
2:M:39:ILE:HG12	2:M:76:VAL:HG22	1.88	0.55
1:T:139:LEU:HB3	1:T:140:PRO:HD3	1.87	0.55
1:U:211:LYS:HZ3	1:U:213:SER:HB3	1.72	0.55
1:U:405:PHE:CE2	2:V:389:ALA:HA	2.42	0.55
1:B:452:ASN:HB2	1:B:454:HIS:CE1	2.41	0.55
2:E:397:SER:H	2:E:400:ASP:HB2	1.70	0.55
3:G:76:ALA:HB1	3:G:114:ILE:HG12	1.88	0.55
3:P:87:ILE:HD12	3:P:229:GLU:HB3	1.87	0.55
1:A:82:ARG:HB2	2:D:34:LEU:HD12	1.87	0.55
2:D:153:ILE:H	2:D:153:ILE:HD12	1.72	0.55
2:D:346:PRO:HB2	2:D:348:VAL:HG23	1.89	0.55
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.87	0.55
4:H:37:GLY:O	4:H:39:ILE:HG23	2.07	0.55
1:K:288:ARG:HD3	2:N:275:ILE:HD11	1.89	0.55
2:O:348:VAL:O	2:O:350:PRO:HD3	2.06	0.55
3:P:147:ALA:HB2	3:P:218:MET:HE2	1.89	0.55
1:A:354:LEU:HA	1:A:366:ALA:O	2.06	0.55
1:C:96:ILE:HD12	1:C:96:ILE:H	1.72	0.55
1:C:251:THR:O	1:C:255:ILE:HG12	2.07	0.55
2:F:86:PRO:HA	2:F:114:ARG:HG2	1.88	0.55
1:K:106:LEU:HD23	1:K:230:TYR:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:95:ILE:HD11	2:N:198:TYR:CE1	2.42	0.55
3:P:78:THR:HG23	3:P:91:LEU:HD23	1.88	0.55
1:T:170:ILE:HD11	1:T:331:THR:HG23	1.88	0.55
1:U:239:SER:OG	2:X:121:PRO:HG3	2.05	0.55
2:X:384:LEU:HB3	2:X:388:ILE:HD13	1.89	0.55
1:B:192:ASN:HA	1:B:200:LYS:HG2	1.89	0.55
2:M:298:THR:HG23	2:M:303:SER:HA	1.89	0.55
1:S:424:GLU:HG2	1:S:460:LEU:HD21	1.89	0.55
1:U:168:LEU:HB2	1:U:348:THR:HG21	1.89	0.55
2:V:134:LEU:HD13	2:V:149:ARG:HH21	1.72	0.55
2:W:345:TYR:HA	2:W:346:PRO:C	2.29	0.55
3:P:91:LEU:HD22	3:P:167:ASN:ND2	2.21	0.55
2:X:231:ARG:HA	2:X:234:LEU:HD12	1.88	0.55
1:B:143:SER:H	2:F:199:ARG:NH1	2.05	0.54
1:S:136:PRO:HB2	1:S:141:ARG:HE	1.71	0.54
1:S:242:ALA:HB3	1:S:243:PRO:HD3	1.89	0.54
1:T:40:ILE:HG21	1:T:287:LEU:HD21	1.88	0.54
2:V:463:ILE:O	2:V:463:ILE:HD13	2.07	0.54
3:Y:110:ILE:HG22	3:Y:131:ASN:HB3	1.89	0.54
1:B:444:VAL:CG2	1:B:445:PRO:HD3	2.37	0.54
2:D:52:GLN:HE21	2:D:54:LEU:HD21	1.71	0.54
1:K:444:VAL:CG2	1:K:445:PRO:HD3	2.38	0.54
1:S:54:LEU:HD11	1:S:97:VAL:HG22	1.86	0.54
1:T:443:GLN:O	1:T:447:ILE:HG12	2.07	0.54
2:D:384:LEU:HD11	2:D:396:LEU:HD11	1.88	0.54
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.89	0.54
2:F:387:ILE:H	2:F:387:ILE:HD12	1.72	0.54
1:L:166:ARG:O	1:L:348:THR:HB	2.07	0.54
1:L:168:LEU:HD12	1:L:327:PRO:O	2.07	0.54
1:L:192:ASN:HA	1:L:200:LYS:HG2	1.89	0.54
2:N:95:ILE:HG23	2:N:219:PHE:HD2	1.72	0.54
1:T:165:GLN:HG2	1:T:166:ARG:H	1.71	0.54
1:T:428:GLN:HA	1:T:431:LYS:HE3	1.90	0.54
2:E:33:ILE:O	2:E:34:LEU:HB2	2.08	0.54
1:S:142:ARG:HB2	1:S:315:SER:HA	1.89	0.54
1:S:148:VAL:HG23	1:S:163:ARG:HG2	1.90	0.54
1:A:306:ARG:O	1:A:310:ARG:HG3	2.07	0.54
2:D:455:HIS:O	2:D:456:ALA:HB2	2.08	0.54
2:V:89:ARG:NH1	2:V:181:PHE:HZ	2.05	0.54
1:L:268:ILE:HD12	1:L:270:TYR:CZ	2.43	0.54
2:O:218:VAL:HG21	2:O:236:GLY:HA2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:46:GLU:O	3:P:50:LEU:HB2	2.07	0.54
1:T:142:ARG:HB2	1:T:315:SER:HA	1.88	0.54
1:U:109:VAL:HG22	1:U:233:ILE:HB	1.90	0.54
2:V:430:LYS:HE2	2:V:465:ASP:OD1	2.08	0.54
1:B:364:ARG:HA	1:B:365:PRO:C	2.32	0.54
2:D:152:LYS:NZ	2:D:293:GLN:HB3	2.21	0.54
2:F:138:ILE:HD12	2:F:138:ILE:H	1.72	0.54
3:P:162:ILE:HB	3:P:182:ILE:HB	1.89	0.54
1:U:293:ARG:HG2	1:U:294:GLU:HG3	1.90	0.54
2:W:336:SER:HB3	2:W:339:ILE:HD13	1.89	0.54
2:X:431:LEU:HD23	2:X:432:VAL:N	2.23	0.54
2:F:37:LEU:HB2	2:F:48:LEU:HB2	1.89	0.54
3:G:19:ILE:O	3:G:22:THR:HG22	2.07	0.54
1:K:208:VAL:HG21	1:K:249:PRO:HG3	1.89	0.54
2:W:405:GLU:HG2	2:W:409:LYS:HE3	1.88	0.54
2:X:412:ARG:O	2:X:415:SER:HB3	2.07	0.54
2:D:373:LYS:HB3	2:D:445:LEU:HD13	1.90	0.54
1:T:242:ALA:HB3	1:T:243:PRO:HD3	1.90	0.54
2:X:388:ILE:HD11	2:X:396:LEU:HD11	1.88	0.54
2:F:237:LEU:HD21	2:F:295:ARG:HB2	1.89	0.54
2:N:339:ILE:HG22	2:N:344:ILE:HB	1.89	0.54
2:W:411:GLN:HA	2:W:414:LEU:HD12	1.90	0.54
1:A:166:ARG:HD3	1:A:308:LEU:O	2.07	0.53
2:E:84:SER:HB2	2:E:114:ARG:HG2	1.89	0.53
2:E:97:ASN:HD21	2:E:99:ILE:HG12	1.73	0.53
3:P:133:ILE:HG13	3:P:142:GLU:OE2	2.08	0.53
2:V:378:LEU:HD21	2:V:411:GLN:HB2	1.89	0.53
2:W:95:ILE:HD11	2:W:198:TYR:CE1	2.43	0.53
2:M:220:GLY:HA3	2:M:232:VAL:HG21	1.91	0.53
1:C:167:GLU:OE1	1:C:350:GLY:HA3	2.09	0.53
2:F:258:ILE:O	2:F:258:ILE:HD13	2.08	0.53
2:N:298:THR:HG23	2:N:303:SER:HB3	1.90	0.53
1:U:51:ALA:O	1:U:52:GLU:HB2	2.08	0.53
1:U:165:GLN:HG2	1:U:166:ARG:N	2.24	0.53
2:V:443:ALA:HB1	2:V:448:LYS:HD2	1.90	0.53
2:E:189:GLU:HG2	2:E:219:PHE:HE1	1.73	0.53
3:G:99:LEU:HD21	3:G:125:ASN:ND2	2.24	0.53
3:P:79:SER:HB2	3:P:134:GLY:HA3	1.91	0.53
2:F:33:ILE:O	2:F:34:LEU:HB2	2.08	0.53
1:K:242:ALA:HB3	1:K:243:PRO:HD3	1.89	0.53
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:117:ILE:H	2:N:117:ILE:HD13	1.74	0.53
1:S:63:GLY:HA2	1:S:78:PHE:CD2	2.44	0.53
1:T:212:ARG:HG3	1:T:237:THR:HG21	1.91	0.53
1:B:248:ALA:HB3	1:B:249:PRO:HD3	1.89	0.53
1:B:495:LEU:HD12	1:B:498:SER:HB3	1.90	0.53
2:E:319:ASP:O	2:E:322:PRO:HD2	2.08	0.53
2:F:95:ILE:HG22	2:F:103:ILE:HB	1.91	0.53
2:M:43:GLN:HG3	2:M:44:GLY:N	2.24	0.53
1:T:77:LEU:O	1:T:243:PRO:HG2	2.08	0.53
1:B:139:LEU:HB3	1:B:140:PRO:HD3	1.89	0.53
2:D:259:PHE:CD2	2:D:311:TYR:HB3	2.44	0.53
2:E:83:ILE:H	2:E:83:ILE:HD12	1.74	0.53
2:F:208:ASN:N	2:F:213:SER:HB3	2.19	0.53
3:G:133:ILE:HG13	3:G:142:GLU:OE2	2.09	0.53
2:N:62:ILE:HD12	2:N:62:ILE:O	2.09	0.53
3:P:224:GLN:O	3:P:228:ALA:HB2	2.09	0.53
2:N:84:SER:HB2	2:N:114:ARG:HG2	1.91	0.53
2:O:33:ILE:HD12	2:O:33:ILE:H	1.72	0.53
2:V:87:VAL:HG12	2:V:239:ILE:HD13	1.91	0.53
2:D:207:ILE:HD11	2:D:215:VAL:HG13	1.92	0.53
3:G:132:GLY:O	3:G:133:ILE:HD12	2.08	0.53
1:K:161:ILE:HD13	1:K:326:LEU:HD21	1.90	0.53
1:K:294:GLU:O	1:K:295:ALA:HB3	2.09	0.53
1:K:435:TYR:C	1:K:437:PRO:HD3	2.34	0.53
1:L:268:ILE:HD13	1:L:269:VAL:N	2.24	0.53
2:M:252:LEU:HD22	2:M:254:PHE:CE1	2.44	0.53
2:O:141:VAL:HG22	2:O:333:THR:HG21	1.91	0.53
1:S:444:VAL:CG2	1:S:445:PRO:HD3	2.30	0.53
1:A:316:GLU:HA	1:A:320:SER:OG	2.08	0.52
2:D:460:VAL:CG1	2:D:469:LYS:HG3	2.39	0.52
1:J:139:LEU:HB3	1:J:140:PRO:HD3	1.89	0.52
3:P:248:ILE:O	3:P:252:SER:HB2	2.08	0.52
2:V:82:PRO:HB2	2:V:116:PRO:HB3	1.91	0.52
2:X:187:VAL:HG12	2:X:260:ARG:HB2	1.91	0.52
3:P:52:TYR:HE2	3:P:213:THR:HG21	1.73	0.52
3:P:225:GLY:C	3:P:227:ALA:H	2.16	0.52
1:U:190:ARG:CZ	1:U:439:ALA:HB2	2.40	0.52
3:G:2:THR:HB	3:G:5:GLU:HB3	1.92	0.52
1:K:103:PRO:HG3	1:K:258:TRP:CZ2	2.45	0.52
2:V:144:LEU:HD23	2:V:371:ALA:HB1	1.90	0.52
1:B:165:GLN:HG2	1:B:166:ARG:H	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:HB2	1:B:328:VAL:O	2.09	0.52
2:F:169:GLU:HG2	2:F:418:PHE:CD1	2.44	0.52
1:L:168:LEU:HB2	1:L:348:THR:HG21	1.90	0.52
1:T:148:VAL:HB	1:T:161:ILE:HB	1.91	0.52
3:Y:167:ASN:HA	3:Y:177:PRO:HA	1.91	0.52
1:C:168:LEU:HD12	1:C:327:PRO:O	2.10	0.52
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.92	0.52
2:N:25:PHE:HB2	2:N:30:LEU:HD23	1.92	0.52
1:T:64:MET:HB2	1:T:78:PHE:HE1	1.73	0.52
1:T:211:LYS:HD2	2:W:328:HIS:HA	1.91	0.52
1:U:105:LEU:HD13	1:U:255:ILE:HD12	1.92	0.52
2:V:96:ILE:N	2:V:96:ILE:HD12	2.24	0.52
2:V:444:VAL:HG22	2:V:449:TYR:CD2	2.45	0.52
2:E:189:GLU:HG2	2:E:219:PHE:CE1	2.45	0.52
3:G:12:SER:O	3:G:13:ILE:HD12	2.09	0.52
1:L:174:GLN:HB3	2:O:354:LYS:HE2	1.92	0.52
3:P:19:ILE:O	3:P:23:MET:HG3	2.10	0.52
3:Y:19:ILE:O	3:Y:22:THR:HG22	2.10	0.52
2:E:132:GLU:HG3	2:E:149:ARG:HB3	1.92	0.52
2:E:387:ILE:HD12	2:E:388:ILE:N	2.25	0.52
3:G:245:GLY:C	3:G:247:MET:H	2.18	0.52
1:L:342:THR:HG22	2:M:311:TYR:OH	2.10	0.52
2:V:147:TYR:CE2	2:V:153:ILE:HG21	2.45	0.52
1:C:70:PRO:HD3	2:D:15:ALA:HB2	1.92	0.52
1:L:280:TYR:CD2	1:L:297:PRO:HG2	2.45	0.52
3:P:207:ARG:O	3:P:211:GLU:HG2	2.10	0.52
1:S:444:VAL:HG21	1:S:485:ILE:HD13	1.92	0.52
1:T:460:LEU:HD12	1:T:463:ILE:HD11	1.91	0.52
1:C:340:ILE:HB	1:C:341:PRO:HD3	1.92	0.52
2:E:279:VAL:O	2:E:279:VAL:HG12	2.10	0.52
5:I:48:LYS:O	5:I:53:ALA:HB1	2.09	0.52
2:M:95:ILE:HD11	2:M:198:TYR:CD1	2.44	0.52
2:N:67:THR:HB	2:N:70:LEU:HD12	1.92	0.52
2:N:244:ARG:HG3	2:N:303:SER:N	2.25	0.52
2:O:167:ILE:HD11	2:O:309:ALA:HB2	1.92	0.52
1:T:444:VAL:CG2	1:T:445:PRO:HD3	2.39	0.52
2:X:344:ILE:HG23	2:X:415:SER:HB2	1.91	0.52
2:D:372:SER:O	2:D:376:GLU:HG3	2.10	0.52
4:H:102:LYS:CG	4:H:105:LEU:HD11	2.31	0.52
1:J:166:ARG:HD3	1:J:308:LEU:O	2.10	0.52
3:P:159:TYR:CD2	3:P:160:PRO:HD2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:252:LEU:HD22	2:X:254:PHE:CE2	2.45	0.52
1:C:46:LEU:HB3	1:C:49:ILE:HB	1.92	0.51
1:C:428:GLN:HB3	1:C:463:ILE:HG21	1.92	0.51
1:K:396:LEU:HD21	1:K:426:LEU:HD23	1.92	0.51
2:O:39:ILE:HB	2:O:46:LEU:HB3	1.93	0.51
1:A:99:VAL:HG11	1:A:251:THR:HG23	1.92	0.51
2:E:106:ARG:HH21	2:E:209:LEU:HD22	1.75	0.51
2:O:41:THR:HG23	2:O:44:GLY:H	1.75	0.51
1:T:300:VAL:O	1:T:303:LEU:HB3	2.08	0.51
1:B:216:ALA:HA	2:E:124:PHE:CZ	2.46	0.51
2:E:155:LEU:HD12	2:E:333:THR:O	2.10	0.51
1:L:368:ASN:HD22	1:L:371:LEU:HB2	1.75	0.51
2:N:152:LYS:HD2	2:N:152:LYS:N	2.25	0.51
2:O:133:ILE:HD13	2:O:357:LEU:HD13	1.92	0.51
2:E:258:ILE:HG22	2:E:309:ALA:O	2.11	0.51
1:J:295:ALA:HB2	3:P:270:ILE:HD13	1.93	0.51
1:L:97:VAL:HG11	1:L:247:LEU:HD21	1.93	0.51
2:N:25:PHE:HB3	2:N:29:GLU:HB2	1.91	0.51
1:U:340:ILE:HB	1:U:341:PRO:HD3	1.92	0.51
2:V:367:HIS:HD2	2:V:438:VAL:HG22	1.75	0.51
2:W:258:ILE:HD13	2:W:258:ILE:O	2.11	0.51
1:B:148:VAL:CG2	1:B:163:ARG:HG2	2.41	0.51
2:M:258:ILE:O	2:M:258:ILE:HD13	2.10	0.51
2:N:228:ALA:O	2:N:232:VAL:HG13	2.11	0.51
2:O:39:ILE:HD12	2:O:46:LEU:HD23	1.92	0.51
1:U:102:GLY:HA2	1:U:258:TRP:CE2	2.45	0.51
2:V:89:ARG:HH11	2:V:181:PHE:HZ	1.56	0.51
2:W:152:LYS:HZ3	2:W:293:GLN:HB3	1.74	0.51
2:E:197:LEU:HD11	2:E:201:MET:HE3	1.92	0.51
2:F:275:ILE:H	2:F:275:ILE:HD12	1.76	0.51
3:G:158:THR:O	3:G:158:THR:HG22	2.10	0.51
1:L:270:TYR:HB2	1:L:327:PRO:HA	1.93	0.51
2:M:421:ALA:HA	2:M:424:PHE:HD2	1.75	0.51
2:N:417:PRO:HB2	2:N:429:GLY:HA2	1.92	0.51
2:N:463:ILE:O	2:N:463:ILE:HD13	2.10	0.51
1:S:273:LEU:HB3	1:S:304:HIS:HE1	1.74	0.51
1:U:349:ASP:HA	1:U:375:ARG:HD2	1.91	0.51
3:Y:14:LYS:O	3:Y:18:LYS:HG3	2.11	0.51
1:A:189:LYS:HD3	1:A:225:HIS:O	2.10	0.51
1:B:211:LYS:HD2	2:E:328:HIS:HA	1.92	0.51
2:N:277:SER:HB2	2:N:283:PRO:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:155:LEU:HD13	2:O:166:PHE:CD2	2.45	0.51
1:T:50:GLN:HB3	2:X:69:GLY:HA2	1.93	0.51
1:U:106:LEU:HD22	1:U:230:TYR:HA	1.93	0.51
1:U:449:ALA:HA	1:U:454:HIS:ND1	2.26	0.51
2:V:344:ILE:HG23	2:V:415:SER:HB3	1.93	0.51
1:C:212:ARG:NH1	2:F:123:SER:HA	2.26	0.51
1:C:483:THR:HG23	1:C:486:ARG:HH12	1.75	0.51
2:D:384:LEU:O	2:D:384:LEU:HD13	2.11	0.51
1:L:138:ILE:H	1:L:138:ILE:HD12	1.76	0.51
1:L:302:TYR:O	1:L:306:ARG:HG2	2.11	0.51
2:M:440:SER:OG	2:M:463:ILE:HB	2.11	0.51
3:P:267:LEU:O	3:P:271:ILE:HG12	2.10	0.51
1:U:96:ILE:O	1:U:97:VAL:C	2.54	0.51
1:U:257:GLU:OE2	1:U:310:ARG:HB3	2.10	0.51
1:A:101:VAL:HG12	1:A:255:ILE:HD13	1.93	0.51
1:C:168:LEU:HD23	1:C:345:ILE:HD13	1.92	0.51
1:C:412:LEU:HD13	1:C:417:LYS:HA	1.93	0.51
1:C:444:VAL:HB	1:C:445:PRO:HD3	1.93	0.51
2:E:95:ILE:HB	2:E:104:ASP:HB3	1.92	0.51
2:E:95:ILE:HD12	2:E:95:ILE:N	2.26	0.51
1:U:246:TYR:CD2	1:U:247:LEU:HD12	2.46	0.51
2:V:95:ILE:HD11	2:V:198:TYR:CE1	2.46	0.51
1:C:149:GLN:HB2	1:C:191:TRP:CH2	2.44	0.51
2:F:97:ASN:HD22	2:F:97:ASN:C	2.18	0.51
1:K:375:ARG:HH12	2:O:164:THR:HB	1.76	0.51
1:S:455:LEU:HA	1:S:458:ILE:HD13	1.92	0.51
1:C:182:LEU:HD13	1:C:218:LEU:HD11	1.92	0.50
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.41	0.50
1:J:148:VAL:HG22	1:J:163:ARG:HG2	1.94	0.50
1:L:280:TYR:CE2	1:L:297:PRO:HG2	2.46	0.50
2:O:339:ILE:HG22	2:O:344:ILE:HB	1.92	0.50
1:C:145:HIS:CD2	1:C:146:GLU:HG3	2.47	0.50
2:F:147:TYR:HB3	2:F:153:ILE:HD13	1.93	0.50
3:G:205:VAL:HB	3:G:206:PRO:HD3	1.92	0.50
1:K:363:ILE:H	1:K:363:ILE:HD12	1.77	0.50
1:T:412:LEU:HD22	1:T:417:LYS:HD2	1.93	0.50
2:V:143:LEU:HD12	2:V:367:HIS:NE2	2.25	0.50
2:V:351:LEU:C	2:V:353:SER:H	2.19	0.50
3:Y:22:THR:O	3:Y:26:VAL:HG23	2.11	0.50
1:A:293:ARG:HG2	1:A:294:GLU:HG3	1.93	0.50
1:B:110:VAL:HG12	1:B:116:PRO:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:ARG:HG3	2:D:193:GLU:N	2.25	0.50
1:K:217:GLN:NE2	2:N:131:ALA:HB2	2.26	0.50
2:O:237:LEU:HD13	2:O:296:ILE:HG12	1.94	0.50
2:V:33:ILE:O	2:V:34:LEU:HB2	2.10	0.50
1:C:242:ALA:HB3	1:C:243:PRO:HD3	1.94	0.50
2:N:409:LYS:HG2	2:N:454:GLU:HG2	1.93	0.50
2:W:50:VAL:HA	2:W:61:THR:HG22	1.94	0.50
1:B:166:ARG:HD3	1:B:308:LEU:O	2.12	0.50
1:B:191:TRP:CD1	1:B:199:LYS:HB3	2.46	0.50
1:T:248:ALA:HB3	1:T:249:PRO:HD3	1.94	0.50
2:V:257:ASN:HB3	2:V:260:ARG:HG2	1.92	0.50
2:W:99:ILE:HD12	2:W:99:ILE:H	1.76	0.50
1:K:138:ILE:H	1:K:138:ILE:HD12	1.76	0.50
2:M:62:ILE:HD11	2:M:272:LEU:HD21	1.93	0.50
2:O:409:LYS:NZ	2:O:450:ASP:HA	2.27	0.50
1:C:107:GLY:HA2	1:C:228:MET:O	2.11	0.50
1:C:300:VAL:HG11	1:C:339:TYR:HE2	1.75	0.50
2:E:39:ILE:HB	2:E:46:LEU:HB3	1.92	0.50
2:F:17:ILE:O	2:F:17:ILE:HG12	2.12	0.50
2:O:33:ILE:O	2:O:34:LEU:HB2	2.10	0.50
3:P:83:LEU:HB3	3:P:237:MET:HE1	1.93	0.50
3:P:110:ILE:HD12	3:P:222:MET:HE2	1.93	0.50
1:T:500:LYS:NZ	1:T:500:LYS:HB3	2.26	0.50
1:U:168:LEU:HD12	1:U:327:PRO:O	2.12	0.50
3:Y:96:ARG:HE	3:Y:121:THR:HG21	1.77	0.50
1:B:185:ILE:HG23	1:B:203:CYS:SG	2.52	0.50
2:D:33:ILE:O	2:D:34:LEU:HB2	2.12	0.50
3:Y:39:ILE:O	3:Y:39:ILE:HD13	2.12	0.50
1:A:311:ALA:HB1	1:A:323:LEU:O	2.12	0.49
1:B:153:LYS:HE2	1:B:432:GLN:HB2	1.94	0.49
1:B:269:VAL:HG22	1:B:326:LEU:HB2	1.93	0.49
2:E:242:TYR:CE2	2:E:246:GLU:HG3	2.47	0.49
4:H:16:LEU:HB2	4:H:19:GLU:O	2.12	0.49
1:U:196:ASP:O	1:U:200:LYS:HG3	2.11	0.49
2:X:95:ILE:HD11	2:X:198:TYR:CD1	2.47	0.49
1:A:190:ARG:CZ	1:A:439:ALA:HB2	2.42	0.49
1:K:165:GLN:HG2	1:K:166:ARG:H	1.77	0.49
2:N:156:PHE:HZ	2:N:326:PHE:HZ	1.60	0.49
2:D:155:LEU:HD23	2:D:155:LEU:H	1.76	0.49
2:F:187:VAL:HG22	2:F:232:VAL:HG13	1.93	0.49
2:F:189:GLU:O	2:F:221:GLN:HB3	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:54:LEU:HD13	1:U:97:VAL:HG22	1.93	0.49
1:C:363:ILE:H	1:C:363:ILE:HD12	1.77	0.49
2:F:217:LEU:HD22	2:F:219:PHE:HE1	1.77	0.49
1:K:142:ARG:HB2	1:K:315:SER:HA	1.93	0.49
1:K:267:LEU:HD12	1:K:324:THR:HB	1.93	0.49
3:P:28:SER:HA	3:P:31:LEU:HB2	1.93	0.49
1:A:165:GLN:HG2	1:A:166:ARG:N	2.27	0.49
1:B:439:ALA:HB3	1:B:442:GLU:HG3	1.94	0.49
2:N:281:TYR:CZ	2:N:321:ALA:HB2	2.48	0.49
2:O:30:LEU:HD21	2:O:57:ASN:HA	1.95	0.49
2:O:449:TYR:HB3	2:O:452:ILE:HD12	1.95	0.49
3:P:79:SER:CB	3:P:134:GLY:HA3	2.42	0.49
1:S:253:ALA:O	1:S:257:GLU:HB2	2.12	0.49
1:T:109:VAL:HG12	1:T:117:ILE:HD11	1.93	0.49
1:T:166:ARG:HH12	1:T:309:GLU:HG2	1.77	0.49
3:Y:77:ILE:HG13	3:Y:78:THR:HG22	1.93	0.49
1:J:300:VAL:O	1:J:303:LEU:HB3	2.13	0.49
1:K:227:ALA:HA	1:K:230:TYR:CE2	2.47	0.49
1:S:340:ILE:HB	1:S:341:PRO:HD3	1.95	0.49
1:S:470:PHE:O	1:S:474:LEU:HG	2.13	0.49
1:U:273:LEU:HD11	1:U:327:PRO:HB3	1.94	0.49
2:V:37:LEU:HD12	2:V:61:THR:HG21	1.95	0.49
1:C:163:ARG:HA	1:C:324:THR:OG1	2.13	0.49
2:D:258:ILE:HG21	2:D:310:VAL:HG22	1.94	0.49
1:J:455:LEU:HD11	1:J:466:PHE:CE1	2.48	0.49
1:L:246:TYR:CD2	1:L:247:LEU:HD12	2.48	0.49
3:P:79:SER:HB2	3:P:134:GLY:O	2.12	0.49
2:V:90:GLU:HG3	2:V:111:SER:HA	1.94	0.49
2:W:65:ASP:HA	2:W:225:PRO:HG3	1.94	0.49
2:X:13:VAL:HB	2:X:73:GLY:H	1.77	0.49
1:C:36:VAL:HG21	1:C:84:VAL:HB	1.95	0.49
2:N:95:ILE:N	2:N:95:ILE:HD12	2.27	0.49
2:W:95:ILE:H	2:W:95:ILE:HD12	1.78	0.49
1:A:340:ILE:HB	1:A:341:PRO:HD3	1.94	0.49
1:C:170:ILE:HG23	1:C:353:PHE:HD1	1.78	0.49
2:E:406:ARG:O	2:E:410:ILE:HG13	2.13	0.49
2:F:164:THR:HG21	2:F:193:GLU:OE1	2.13	0.49
1:K:152:LEU:HD22	1:K:155:VAL:HG23	1.95	0.49
1:L:329:ILE:HD13	1:L:341:PRO:HA	1.94	0.49
2:M:54:LEU:HD11	2:M:60:ARG:HB2	1.95	0.49
2:V:346:PRO:HG3	2:V:418:PHE:HE2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:13:VAL:HB	2:W:73:GLY:H	1.76	0.49
1:B:222:LEU:HD12	1:B:233:ILE:HD11	1.93	0.49
1:C:70:PRO:HG3	2:D:14:THR:HG22	1.94	0.49
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.42	0.49
2:F:141:VAL:HG22	2:F:333:THR:HG21	1.93	0.49
1:J:63:GLY:HA2	1:J:78:PHE:CD2	2.47	0.49
2:O:417:PRO:HG3	2:O:459:MET:HG3	1.95	0.49
1:A:82:ARG:HH11	2:D:34:LEU:HB2	1.77	0.48
1:A:455:LEU:HD21	1:A:466:PHE:CZ	2.48	0.48
2:D:95:ILE:HD11	2:D:198:TYR:CD1	2.48	0.48
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.95	0.48
2:D:417:PRO:HD2	2:D:430:LYS:HB2	1.95	0.48
2:F:95:ILE:CG2	2:F:103:ILE:HB	2.43	0.48
2:M:115:LYS:HB3	2:M:115:LYS:HZ2	1.78	0.48
3:P:2:THR:O	3:P:3:LEU:C	2.56	0.48
1:U:56:GLU:HG2	1:U:62:LYS:HG2	1.95	0.48
2:V:62:ILE:HD11	2:V:272:LEU:HD11	1.94	0.48
2:V:257:ASN:ND2	2:V:311:TYR:HB2	2.28	0.48
1:A:242:ALA:HB3	1:A:243:PRO:HD3	1.94	0.48
1:C:73:VAL:CG2	2:D:72:ARG:HH22	2.24	0.48
2:D:186:GLY:HA2	2:D:256:ASP:O	2.13	0.48
2:E:97:ASN:ND2	2:E:99:ILE:HG12	2.28	0.48
2:E:199:ARG:HB3	2:E:199:ARG:NH1	2.27	0.48
2:E:221:GLN:HB2	2:E:224:GLU:HG3	1.95	0.48
1:A:319:GLY:O	1:A:320:SER:HB2	2.13	0.48
1:A:425:ARG:HD2	1:A:456:ASP:HA	1.94	0.48
1:C:168:LEU:HD13	1:C:327:PRO:HB2	1.95	0.48
4:H:18:HIS:NE2	4:H:89:GLU:HG2	2.28	0.48
2:N:26:GLU:O	2:N:27:GLN:C	2.56	0.48
2:N:95:ILE:HG22	2:N:103:ILE:HD11	1.96	0.48
2:N:106:ARG:NH2	2:N:209:LEU:HB3	2.27	0.48
3:P:26:VAL:O	3:P:29:THR:HG22	2.12	0.48
1:S:64:MET:SD	1:S:247:LEU:HD11	2.54	0.48
1:S:457:GLY:C	1:S:458:ILE:HD12	2.39	0.48
2:V:37:LEU:HB2	2:V:48:LEU:HB2	1.94	0.48
1:B:142:ARG:HB2	1:B:315:SER:HA	1.95	0.48
3:G:127:LYS:HD3	3:G:154:MET:HE1	1.96	0.48
1:L:242:ALA:HB3	1:L:243:PRO:HD3	1.96	0.48
1:T:190:ARG:HB2	1:T:191:TRP:CE3	2.49	0.48
2:V:374:VAL:HG13	2:V:410:ILE:HG21	1.96	0.48
3:Y:233:ARG:O	3:Y:237:MET:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:378:SER:HB3	1:K:386:LYS:HD2	1.96	0.48
2:N:201:MET:HA	2:N:204:THR:HG22	1.96	0.48
1:S:172:ASP:O	1:S:177:LYS:HE3	2.14	0.48
1:S:282:GLN:NE2	2:V:284:THR:HG22	2.29	0.48
1:S:345:ILE:HG23	1:S:351:GLN:CD	2.39	0.48
2:V:154:GLY:O	2:V:332:THR:HA	2.13	0.48
2:X:184:PHE:HD1	2:X:254:PHE:HB2	1.78	0.48
1:B:443:GLN:O	1:B:447:ILE:HG12	2.13	0.48
2:D:54:LEU:HD11	2:D:60:ARG:HB2	1.95	0.48
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.96	0.48
2:E:226:PRO:HG3	2:E:267:GLU:OE1	2.13	0.48
2:F:103:ILE:O	2:F:103:ILE:HG22	2.14	0.48
4:H:105:LEU:O	4:H:109:LYS:HB2	2.13	0.48
1:J:51:ALA:O	1:J:52:GLU:HB2	2.13	0.48
2:M:43:GLN:HG3	2:M:44:GLY:H	1.78	0.48
2:N:98:VAL:HB	2:N:232:VAL:HG12	1.94	0.48
2:O:187:VAL:HG12	2:O:260:ARG:HB2	1.95	0.48
2:O:256:ASP:HA	2:O:257:ASN:HA	1.50	0.48
3:P:182:ILE:HG22	3:P:182:ILE:O	2.12	0.48
1:S:293:ARG:HD3	1:S:339:TYR:CD1	2.48	0.48
2:X:293:GLN:HG2	2:X:328:HIS:CG	2.49	0.48
1:K:358:LEU:HB2	1:K:366:ALA:HB1	1.94	0.48
2:O:164:THR:HG21	2:O:193:GLU:OE1	2.13	0.48
2:O:252:LEU:HD22	2:O:254:PHE:CE1	2.49	0.48
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.43	0.48
1:S:358:LEU:HB2	1:S:366:ALA:HB1	1.94	0.48
2:V:251:VAL:HB	2:V:304:VAL:HG22	1.96	0.48
2:W:155:LEU:HD12	2:W:333:THR:O	2.14	0.48
1:B:191:TRP:HD1	1:B:199:LYS:HB3	1.79	0.48
3:G:184:ASN:O	3:G:188:ILE:HG13	2.13	0.48
4:H:105:LEU:N	4:H:105:LEU:HD12	2.28	0.48
1:L:169:ILE:HD11	1:L:326:LEU:HD22	1.94	0.48
1:S:281:ARG:HD3	1:S:296:TYR:CD1	2.49	0.48
2:X:163:LYS:O	2:X:167:ILE:HG13	2.14	0.48
2:X:427:ILE:HD12	2:X:459:MET:HG2	1.96	0.48
2:D:52:GLN:HG2	2:D:60:ARG:HB3	1.96	0.48
5:I:59:ILE:HG22	5:I:60:THR:H	1.79	0.48
1:L:444:VAL:HB	1:L:445:PRO:HD3	1.95	0.48
2:O:95:ILE:HD12	2:O:95:ILE:N	2.29	0.48
3:P:55:ALA:O	3:P:56:GLU:HB2	2.14	0.48
3:P:115:LYS:O	3:P:119:LEU:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:92:ARG:HH21	1:S:94:GLY:HA2	1.79	0.48
1:S:381:GLN:HG2	1:S:382:VAL:N	2.29	0.48
1:B:51:ALA:HB3	2:F:69:GLY:H	1.79	0.48
2:D:140:VAL:HA	2:D:414:LEU:HD22	1.96	0.48
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.96	0.48
3:G:12:SER:O	3:G:16:ILE:HD13	2.12	0.48
1:J:272:ASP:HB2	1:J:328:VAL:O	2.14	0.48
1:S:239:SER:OG	2:V:121:PRO:HG3	2.14	0.48
1:U:239:SER:HB2	2:X:294:GLU:HG3	1.95	0.48
2:V:117:ILE:HA	2:V:238:THR:OG1	2.14	0.48
1:C:209:GLY:HA3	1:C:275:LYS:HD3	1.96	0.47
2:E:132:GLU:CD	2:E:149:ARG:HD3	2.39	0.47
2:F:384:LEU:HA	2:F:387:ILE:HD13	1.96	0.47
1:K:497:ALA:HA	1:K:500:LYS:NZ	2.29	0.47
2:N:133:ILE:HD11	2:N:362:VAL:HG12	1.95	0.47
2:N:222:MET:C	2:N:224:GLU:H	2.22	0.47
2:V:53:HIS:HA	2:V:59:VAL:HG12	1.96	0.47
2:V:115:LYS:NZ	2:V:115:LYS:HB3	2.29	0.47
2:W:71:VAL:HB	2:W:74:GLU:HG3	1.95	0.47
1:A:444:VAL:HG21	1:A:485:ILE:HG21	1.95	0.47
2:E:67:THR:HB	2:E:70:LEU:HD12	1.96	0.47
2:F:256:ASP:HA	2:F:257:ASN:HA	1.54	0.47
3:G:44:MET:HE3	4:H:86:THR:HB	1.96	0.47
1:K:145:HIS:CD2	1:K:146:GLU:HG3	2.49	0.47
2:M:25:PHE:HE2	2:M:59:VAL:HG22	1.79	0.47
2:O:209:LEU:HD12	2:O:210:GLU:N	2.29	0.47
1:T:106:LEU:HD12	1:T:232:ILE:HD11	1.96	0.47
1:T:383:LYS:O	1:T:387:GLN:HG3	2.14	0.47
1:U:36:VAL:HG12	2:X:53:HIS:HB2	1.96	0.47
1:U:441:GLU:CD	1:U:441:GLU:H	2.22	0.47
1:A:363:ILE:HD12	1:A:363:ILE:N	2.29	0.47
1:B:164:GLY:O	1:B:312:ALA:HA	2.13	0.47
1:J:242:ALA:HB3	1:J:243:PRO:HD3	1.95	0.47
1:L:116:PRO:HD3	1:L:123:ILE:HD12	1.96	0.47
2:M:189:GLU:O	2:M:221:GLN:HB3	2.14	0.47
3:P:44:MET:O	3:P:44:MET:HG2	2.13	0.47
1:S:205:TYR:HE1	1:S:207:ALA:HB2	1.79	0.47
1:U:271:ASP:HA	1:U:272:ASP:HA	1.50	0.47
2:V:147:TYR:CD2	2:V:153:ILE:HG21	2.49	0.47
2:W:133:ILE:H	2:W:133:ILE:HD12	1.78	0.47
2:X:83:ILE:HD12	2:X:83:ILE:H	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:336:SER:HB3	2:X:339:ILE:HG12	1.96	0.47
1:C:458:ILE:HD12	1:C:458:ILE:H	1.78	0.47
1:K:211:LYS:HD2	2:N:328:HIS:HA	1.96	0.47
2:O:258:ILE:HG22	2:O:309:ALA:O	2.15	0.47
1:U:294:GLU:O	1:U:295:ALA:HB3	2.15	0.47
1:U:436:SER:N	1:U:437:PRO:HD3	2.29	0.47
1:U:492:SER:H	1:U:495:LEU:HD12	1.78	0.47
2:W:220:GLY:CA	2:W:232:VAL:HG11	2.45	0.47
1:A:383:LYS:HB3	1:A:490:GLU:HG2	1.96	0.47
2:D:46:LEU:HD21	2:D:67:THR:HG22	1.97	0.47
2:F:147:TYR:HB3	2:F:153:ILE:CD1	2.44	0.47
4:H:65:SER:C	4:H:66:LYS:HD2	2.39	0.47
1:L:394:LEU:O	1:L:398:GLN:HG3	2.14	0.47
2:O:95:ILE:HD11	2:O:198:TYR:CE1	2.49	0.47
2:V:117:ILE:H	2:V:117:ILE:HD13	1.78	0.47
2:X:257:ASN:OD1	2:X:259:PHE:HB3	2.14	0.47
1:B:396:LEU:HA	1:B:399:TYR:HB3	1.97	0.47
1:C:309:GLU:HG3	2:D:223:ASN:HB3	1.95	0.47
2:D:191:THR:HA	2:D:221:GLN:HG3	1.97	0.47
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.97	0.47
1:U:54:LEU:HD12	1:U:63:GLY:O	2.14	0.47
2:W:139:LYS:HE2	2:W:416:GLN:HB2	1.97	0.47
2:W:256:ASP:HA	2:W:257:ASN:HA	1.54	0.47
1:A:460:LEU:HA	1:A:463:ILE:CG1	2.44	0.47
1:B:99:VAL:HG11	1:B:251:THR:HB	1.97	0.47
1:B:212:ARG:HA	1:B:237:THR:HG21	1.97	0.47
1:B:474:LEU:HD23	1:B:478:HIS:HB2	1.97	0.47
1:C:288:ARG:CZ	2:F:275:ILE:HD11	2.45	0.47
2:D:143:LEU:HD12	2:D:367:HIS:CE1	2.49	0.47
2:F:102:PRO:HG3	2:F:109:ILE:HG13	1.96	0.47
4:H:48:THR:H	4:H:77:VAL:HB	1.80	0.47
1:K:436:SER:N	1:K:437:PRO:HD3	2.29	0.47
1:L:177:LYS:HG2	1:L:354:LEU:HD12	1.97	0.47
2:M:406:ARG:NH2	2:M:447:GLY:HA3	2.30	0.47
2:N:133:ILE:HG12	2:N:363:VAL:HG12	1.97	0.47
2:N:387:ILE:HB	2:N:391:LEU:HD12	1.96	0.47
2:N:433:ARG:NH1	2:N:433:ARG:HB3	2.30	0.47
2:O:92:LEU:O	2:O:94:ARG:HG2	2.15	0.47
3:P:211:GLU:HB3	5:R:11:ALA:HA	1.97	0.47
1:S:417:LYS:O	1:S:421:VAL:HG23	2.14	0.47
2:V:87:VAL:HG21	2:V:115:LYS:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:138:ILE:HG12	2:V:418:PHE:CE1	2.49	0.47
2:V:259:PHE:CE1	2:V:313:PRO:HG3	2.49	0.47
2:V:298:THR:HG23	2:V:303:SER:HB3	1.97	0.47
2:W:38:GLU:C	2:W:39:ILE:HD12	2.40	0.47
2:W:117:ILE:HG13	2:W:118:HIS:CD2	2.50	0.47
2:X:351:LEU:HD21	2:X:378:LEU:HB2	1.97	0.47
3:Y:210:PHE:HB2	3:Y:213:THR:HB	1.97	0.47
1:A:38:ASP:O	1:A:286:LEU:HD13	2.15	0.47
1:B:425:ARG:HH11	1:B:463:ILE:HD11	1.79	0.47
1:C:500:LYS:HD3	1:C:500:LYS:C	2.40	0.47
2:E:135:GLU:HB2	2:E:178:HIS:NE2	2.30	0.47
2:F:5:GLN:C	2:F:7:THR:H	2.23	0.47
2:F:279:VAL:O	2:F:279:VAL:HG12	2.15	0.47
2:F:399:GLN:HA	2:F:399:GLN:HE21	1.80	0.47
3:G:83:LEU:HB3	3:G:237:MET:HE3	1.95	0.47
1:L:271:ASP:HA	1:L:272:ASP:HA	1.57	0.47
2:M:319:ASP:O	2:M:322:PRO:HD2	2.15	0.47
2:W:37:LEU:HB2	2:W:48:LEU:HB2	1.96	0.47
1:A:452:ASN:HB3	1:A:454:HIS:HE1	1.80	0.47
2:D:167:ILE:O	2:D:171:ILE:HG13	2.15	0.47
2:E:400:ASP:O	2:E:404:VAL:HG23	2.15	0.47
2:E:422:GLU:C	2:E:424:PHE:H	2.23	0.47
2:F:17:ILE:HD13	2:F:17:ILE:N	2.30	0.47
1:L:103:PRO:C	1:L:105:LEU:H	2.23	0.47
1:L:470:PHE:CE2	1:L:474:LEU:HD11	2.50	0.47
3:P:107:ILE:O	3:P:126:ILE:HA	2.15	0.47
1:U:242:ALA:HB3	1:U:243:PRO:HD3	1.95	0.47
2:V:204:THR:HG23	2:V:206:VAL:HG23	1.96	0.47
2:X:52:GLN:NE2	2:X:60:ARG:HD2	2.30	0.47
1:C:474:LEU:HB3	1:C:482:LEU:HD11	1.96	0.47
2:E:94:ARG:CZ	2:E:109:ILE:HG12	2.45	0.47
1:J:364:ARG:HA	1:J:365:PRO:C	2.40	0.47
1:K:106:LEU:HD21	1:K:202:TYR:CD2	2.49	0.47
1:K:209:GLY:O	1:K:238:ALA:HB2	2.14	0.47
1:L:382:VAL:HG12	1:L:384:ALA:H	1.80	0.47
1:S:239:SER:HB2	2:V:294:GLU:HG3	1.96	0.47
1:T:309:GLU:OE1	2:X:223:ASN:HB3	2.15	0.47
1:U:82:ARG:HD2	2:X:34:LEU:HD12	1.96	0.47
1:B:273:LEU:CD1	1:B:327:PRO:HB3	2.45	0.46
1:C:123:ILE:HD12	1:C:123:ILE:O	2.15	0.46
1:C:300:VAL:HG11	1:C:339:TYR:CE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:258:ILE:HG21	2:E:310:VAL:HG22	1.97	0.46
2:F:398:GLU:HG3	3:G:120:ARG:CZ	2.45	0.46
1:J:33:VAL:HB	1:J:88:GLU:H	1.80	0.46
1:J:161:ILE:HD12	1:J:167:GLU:HG2	1.95	0.46
1:K:173:ARG:HB2	1:K:330:GLU:OE2	2.15	0.46
2:N:167:ILE:O	2:N:171:ILE:HG13	2.16	0.46
3:P:139:THR:HG23	3:P:142:GLU:HB2	1.97	0.46
1:S:440:THR:O	1:S:444:VAL:HG22	2.14	0.46
1:T:27:LEU:HD22	1:T:47:ASN:HD21	1.79	0.46
2:V:93:GLY:HA3	2:V:213:SER:HB3	1.96	0.46
2:X:167:ILE:HD11	2:X:309:ALA:HB2	1.97	0.46
1:A:54:LEU:HD11	1:A:97:VAL:HA	1.96	0.46
1:B:85:LYS:H	1:B:88:GLU:CD	2.23	0.46
1:B:145:HIS:HE1	1:B:313:LYS:HE2	1.80	0.46
1:C:43:VAL:HG21	1:C:75:ILE:HD12	1.97	0.46
2:E:326:PHE:HA	2:E:329:LEU:HD12	1.96	0.46
1:L:500:LYS:O	1:L:504:GLU:HG3	2.15	0.46
2:M:281:TYR:CE1	2:M:321:ALA:HB2	2.50	0.46
3:P:44:MET:HE3	4:Q:16:LEU:O	2.16	0.46
1:S:368:ASN:HD22	1:S:371:LEU:HD12	1.79	0.46
2:X:256:ASP:HA	2:X:257:ASN:HA	1.53	0.46
1:B:474:LEU:HD13	1:B:482:LEU:HD21	1.98	0.46
2:D:391:LEU:HD13	2:D:395:GLU:CD	2.40	0.46
1:K:196:ASP:O	1:K:200:LYS:HG3	2.15	0.46
1:L:220:GLN:O	1:L:224:GLN:HG3	2.15	0.46
1:S:302:TYR:HE1	2:W:223:ASN:O	1.97	0.46
1:S:493:LYS:H	1:S:493:LYS:HD2	1.81	0.46
2:W:201:MET:HE2	2:W:206:VAL:HG21	1.98	0.46
2:X:319:ASP:O	2:X:322:PRO:HD2	2.16	0.46
1:K:290:PRO:HA	1:K:291:PRO:HD3	1.79	0.46
1:L:274:SER:OG	1:L:329:ILE:HG13	2.15	0.46
2:M:95:ILE:HB	2:M:104:ASP:HB3	1.97	0.46
4:Q:34:ALA:HB2	4:Q:52:LEU:HA	1.97	0.46
1:T:188:GLN:HG3	1:T:201:LEU:HD23	1.97	0.46
1:U:222:LEU:HB2	1:U:228:MET:HE2	1.97	0.46
2:V:46:LEU:HD21	2:V:67:THR:HG22	1.98	0.46
2:W:86:PRO:HD3	2:W:114:ARG:CZ	2.46	0.46
2:E:20:ILE:N	2:E:20:ILE:HD12	2.30	0.46
2:F:37:LEU:HD12	2:F:61:THR:HG21	1.96	0.46
2:V:64:MET:O	2:V:228:ALA:HB2	2.14	0.46
2:W:276:PRO:HB2	3:Y:267:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:377:THR:HG22	2:W:407:ALA:HB2	1.98	0.46
2:X:157:GLY:HA3	2:X:335:LEU:HB2	1.97	0.46
3:Y:150:LEU:HD11	3:Y:218:MET:HE1	1.98	0.46
1:A:62:LYS:HB2	1:A:62:LYS:NZ	2.30	0.46
1:B:106:LEU:HD21	1:B:202:TYR:CE1	2.51	0.46
2:D:439:ALA:HA	2:D:442:LYS:HD3	1.97	0.46
2:E:473:LEU:HD23	2:E:473:LEU:O	2.16	0.46
2:F:17:ILE:HD13	2:F:17:ILE:H	1.80	0.46
4:H:14:PHE:HB3	4:H:21:LEU:HB2	1.98	0.46
1:K:260:ARG:O	1:K:321:GLY:HA3	2.16	0.46
1:L:373:VAL:HA	1:L:393:LYS:HZ2	1.80	0.46
2:N:140:VAL:HG22	2:N:414:LEU:HB3	1.97	0.46
1:S:394:LEU:HD12	1:S:394:LEU:N	2.30	0.46
2:V:452:ILE:HG22	2:V:453:PRO:HD2	1.97	0.46
2:X:169:GLU:HG2	2:X:418:PHE:CD1	2.50	0.46
1:C:184:THR:O	1:C:188:GLN:HG2	2.16	0.46
2:F:184:PHE:HB3	2:F:217:LEU:HD23	1.97	0.46
1:J:470:PHE:HD1	1:J:506:PHE:CD2	2.34	0.46
1:L:281:ARG:O	1:L:285:LEU:HG	2.16	0.46
2:N:127:GLN:HE22	2:N:297:THR:HG21	1.81	0.46
2:N:384:LEU:HD23	2:N:387:ILE:HD11	1.97	0.46
3:P:78:THR:HB	3:P:79:SER:H	1.58	0.46
2:V:178:HIS:HE1	2:V:250:ASP:O	1.98	0.46
2:W:168:GLN:HE22	2:W:200:GLU:HG2	1.81	0.46
1:A:177:LYS:HB2	1:A:177:LYS:NZ	2.31	0.46
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.83	0.46
1:J:365:PRO:O	1:J:367:ILE:HG12	2.16	0.46
1:L:290:PRO:HA	1:L:291:PRO:HD3	1.77	0.46
1:S:271:ASP:HA	1:S:272:ASP:HA	1.65	0.46
1:T:249:PRO:HG2	1:T:276:GLN:NE2	2.30	0.46
2:W:133:ILE:HD12	2:W:133:ILE:N	2.31	0.46
2:W:321:ALA:HB3	2:W:322:PRO:CD	2.45	0.46
1:B:106:LEU:HD21	1:B:202:TYR:CD1	2.51	0.46
1:B:436:SER:N	1:B:437:PRO:HD3	2.30	0.46
2:D:387:ILE:HD11	3:G:19:ILE:HD11	1.98	0.46
2:F:117:ILE:H	2:F:117:ILE:HD13	1.80	0.46
4:H:106:ALA:O	4:H:110:LYS:HB3	2.16	0.46
1:L:267:LEU:HD21	1:L:326:LEU:HD12	1.97	0.46
2:M:183:VAL:O	2:M:253:LEU:HD12	2.15	0.46
2:O:279:VAL:O	2:O:279:VAL:HG12	2.16	0.46
1:T:153:LYS:HG3	1:T:438:LEU:HD12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:391:LEU:HB3	2:W:395:GLU:HG3	1.97	0.46
3:Y:133:ILE:HD13	3:Y:133:ILE:N	2.30	0.46
1:A:253:ALA:O	1:A:257:GLU:HB2	2.16	0.46
1:C:271:ASP:HA	1:C:272:ASP:HA	1.55	0.46
3:G:267:LEU:O	3:G:271:ILE:HG12	2.16	0.46
1:L:103:PRO:HG3	1:L:258:TRP:CH2	2.50	0.46
1:L:289:ARG:HH21	2:M:17:ILE:HG13	1.80	0.46
1:L:417:LYS:O	1:L:417:LYS:HD3	2.16	0.46
2:M:92:LEU:HD11	2:M:181:PHE:CE1	2.50	0.46
2:N:98:VAL:HG13	2:N:99:ILE:HG23	1.98	0.46
2:N:275:ILE:HD12	2:N:275:ILE:N	2.31	0.46
3:P:74:ILE:HA	3:P:163:SER:O	2.16	0.46
1:T:142:ARG:HD2	1:T:316:GLU:HG3	1.98	0.46
2:V:33:ILE:HD12	2:V:33:ILE:N	2.31	0.46
2:V:83:ILE:HG23	2:V:117:ILE:HD12	1.98	0.46
2:V:187:VAL:HG22	2:V:232:VAL:HG13	1.98	0.46
2:V:452:ILE:H	2:V:452:ILE:CD1	2.29	0.46
2:E:120:ASP:HA	2:E:121:PRO:HD3	1.85	0.45
2:E:201:MET:HA	2:E:204:THR:HG22	1.98	0.45
3:G:149:LYS:O	3:G:153:VAL:HG12	2.16	0.45
4:H:102:LYS:HD3	4:H:105:LEU:HD21	1.99	0.45
5:I:59:ILE:HG22	5:I:60:THR:N	2.31	0.45
1:L:96:ILE:N	1:L:96:ILE:HD12	2.31	0.45
2:W:68:GLU:O	2:W:68:GLU:HG2	2.17	0.45
2:X:117:ILE:HG13	2:X:118:HIS:CD2	2.51	0.45
2:X:140:VAL:HG11	2:X:348:VAL:HB	1.98	0.45
2:E:27:GLN:HG2	2:E:57:ASN:HD21	1.81	0.45
2:O:152:LYS:NZ	2:O:293:GLN:HG3	2.30	0.45
1:A:146:GLU:HA	1:A:147:PRO:HD3	1.73	0.45
3:G:55:ALA:HB2	3:G:197:PHE:HE2	1.80	0.45
1:J:460:LEU:HD12	1:J:460:LEU:N	2.31	0.45
3:P:87:ILE:HD12	3:P:229:GLU:CA	2.47	0.45
2:W:201:MET:HE1	2:W:215:VAL:HG11	1.99	0.45
1:A:243:PRO:HG3	1:A:283:LEU:HD21	1.96	0.45
1:B:341:PRO:O	1:B:345:ILE:HG13	2.15	0.45
1:C:302:TYR:CZ	1:C:306:ARG:HD3	2.52	0.45
2:D:155:LEU:HD13	2:D:166:PHE:CD2	2.51	0.45
2:F:33:ILE:H	2:F:33:ILE:CD1	2.27	0.45
1:K:302:TYR:HA	1:K:305:SER:OG	2.17	0.45
1:T:40:ILE:O	1:T:40:ILE:HD12	2.17	0.45
1:T:267:LEU:HD12	1:T:324:THR:HB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:271:ASP:HA	1:T:272:ASP:HA	1.57	0.45
1:C:343:ASN:O	1:C:347:ILE:HG12	2.15	0.45
2:F:12:LYS:HZ3	2:F:73:GLY:HA2	1.80	0.45
1:L:96:ILE:HD12	1:L:96:ILE:H	1.82	0.45
2:M:285:LEU:HD23	2:M:285:LEU:C	2.41	0.45
2:N:409:LYS:NZ	2:N:450:ASP:HA	2.32	0.45
2:O:293:GLN:HG2	2:O:328:HIS:HB3	1.99	0.45
3:P:11:LYS:HE3	3:P:11:LYS:HB2	1.76	0.45
1:T:170:ILE:HG13	1:T:171:GLY:N	2.32	0.45
1:T:213:SER:O	1:T:217:GLN:HG3	2.17	0.45
2:V:279:VAL:O	2:V:279:VAL:HG12	2.16	0.45
1:B:232:ILE:HD12	1:B:232:ILE:N	2.32	0.45
1:B:249:PRO:HG2	1:B:276:GLN:NE2	2.32	0.45
2:D:393:MET:HA	2:D:396:LEU:HD23	1.98	0.45
2:E:199:ARG:HB3	2:E:199:ARG:HH11	1.82	0.45
1:T:148:VAL:HG22	1:T:163:ARG:HG2	1.99	0.45
1:U:28:ASN:HB3	1:U:48:ASN:ND2	2.31	0.45
2:V:13:VAL:HG22	2:V:23:VAL:HG12	1.97	0.45
1:B:49:ILE:HG13	1:B:50:GLN:N	2.32	0.45
1:B:413:ASP:CG	1:B:414:ALA:N	2.74	0.45
1:C:363:ILE:HD12	1:C:363:ILE:N	2.32	0.45
1:C:382:VAL:HG11	1:C:440:THR:HG21	1.98	0.45
2:D:249:GLN:HG3	2:D:250:ASP:N	2.32	0.45
2:D:258:ILE:HG22	2:D:309:ALA:O	2.17	0.45
2:E:34:LEU:HD22	2:E:118:HIS:CE1	2.52	0.45
2:E:95:ILE:HD13	2:E:104:ASP:HB3	1.99	0.45
2:E:262:THR:HG23	2:E:285:LEU:HD11	1.98	0.45
2:E:370:VAL:O	2:E:374:VAL:HG23	2.17	0.45
2:F:377:THR:HG22	2:F:407:ALA:HB2	1.99	0.45
4:H:32:LEU:HA	4:H:33:PRO:HD3	1.78	0.45
1:K:338:ALA:HB3	1:K:341:PRO:HG2	1.98	0.45
1:K:341:PRO:O	1:K:345:ILE:HG13	2.15	0.45
1:K:497:ALA:HA	1:K:500:LYS:HZ2	1.81	0.45
2:N:389:ALA:C	2:N:390:ILE:HD12	2.42	0.45
2:O:12:LYS:HA	2:O:74:GLU:O	2.16	0.45
2:O:29:GLU:C	2:O:30:LEU:HD12	2.41	0.45
1:S:329:ILE:HD11	1:S:344:VAL:HG21	1.97	0.45
1:S:382:VAL:HG11	1:S:440:THR:HG21	1.98	0.45
1:T:233:ILE:HD12	1:T:233:ILE:N	2.31	0.45
1:U:211:LYS:HZ3	1:U:213:SER:CB	2.29	0.45
1:U:246:TYR:HE1	1:U:303:LEU:HD11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:31:PRO:HB3	2:V:35:ASN:HD22	1.82	0.45
2:V:34:LEU:HD22	2:V:118:HIS:NE2	2.32	0.45
2:V:191:THR:HA	2:V:221:GLN:HG3	1.99	0.45
2:V:346:PRO:HG3	2:V:418:PHE:CE2	2.52	0.45
4:H:73:GLY:HA3	4:H:86:THR:O	2.16	0.45
1:J:96:ILE:HD12	1:J:96:ILE:N	2.32	0.45
1:K:204:VAL:HB	1:K:268:ILE:HG12	1.99	0.45
3:P:209:LEU:HD23	3:P:209:LEU:C	2.42	0.45
4:Q:33:PRO:HB3	4:Q:38:ARG:HA	1.98	0.45
1:S:105:LEU:H	1:S:105:LEU:HD12	1.81	0.45
1:T:206:VAL:HG12	1:T:208:VAL:HG23	1.97	0.45
1:T:462:ARG:HB3	1:T:465:GLU:HB2	1.98	0.45
2:V:460:VAL:HG21	2:V:466:VAL:HG22	1.99	0.45
2:W:391:LEU:HD13	2:W:395:GLU:HG3	1.98	0.45
1:A:36:VAL:HG12	2:D:53:HIS:HB2	1.99	0.45
2:D:258:ILE:CG2	2:D:310:VAL:HG22	2.46	0.45
2:D:449:TYR:HB3	2:D:457:PHE:HZ	1.82	0.45
2:E:152:LYS:C	2:E:153:ILE:HD12	2.41	0.45
2:F:156:PHE:HB2	2:F:334:VAL:HG12	1.97	0.45
1:K:62:LYS:HD2	1:K:113:LEU:HD13	1.97	0.45
1:K:103:PRO:C	1:K:105:LEU:H	2.24	0.45
1:K:305:SER:HA	1:K:347:ILE:HD13	1.99	0.45
1:L:73:VAL:HG22	2:M:72:ARG:HH12	1.81	0.45
1:L:341:PRO:O	1:L:345:ILE:HG13	2.17	0.45
1:L:343:ASN:O	1:L:347:ILE:HG13	2.17	0.45
2:N:83:ILE:O	2:N:117:ILE:HG23	2.17	0.45
2:N:472:LYS:HB2	2:N:472:LYS:NZ	2.31	0.45
2:O:117:ILE:HA	2:O:238:THR:OG1	2.17	0.45
3:P:3:LEU:HD12	3:P:3:LEU:H	1.82	0.45
3:P:41:ALA:O	3:P:45:ASP:N	2.49	0.45
1:S:139:LEU:HB3	1:S:140:PRO:HD3	1.98	0.45
1:S:363:ILE:HD12	1:S:363:ILE:N	2.31	0.45
1:S:402:VAL:O	1:S:402:VAL:HG12	2.17	0.45
2:V:146:PRO:O	2:V:357:LEU:HD12	2.17	0.45
2:V:397:SER:O	2:V:401:LYS:HB2	2.17	0.45
1:C:212:ARG:HG2	1:C:237:THR:HG21	1.99	0.45
1:C:341:PRO:O	1:C:345:ILE:HG12	2.16	0.45
1:C:398:GLN:O	1:C:402:VAL:HG23	2.16	0.45
2:E:182:SER:O	2:E:215:VAL:HA	2.17	0.45
2:F:157:GLY:HA3	2:F:335:LEU:HB2	1.99	0.45
4:H:125:ILE:O	4:H:129:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:26:ASN:O	1:J:27:LEU:HB2	2.17	0.45
1:K:284:SER:HB2	1:K:289:ARG:HB2	1.99	0.45
1:L:208:VAL:HG21	1:L:249:PRO:HG3	1.98	0.45
2:M:384:LEU:HD23	2:M:387:ILE:HD12	1.99	0.45
1:T:99:VAL:HG11	1:T:251:THR:HB	1.99	0.45
1:T:300:VAL:CG1	1:T:339:TYR:HE2	2.29	0.45
2:X:255:ILE:HD12	2:X:308:GLN:HG2	1.99	0.45
1:A:446:LEU:HD11	1:A:471:LEU:HD11	1.99	0.44
1:B:67:ASN:CB	2:F:17:ILE:HG22	2.46	0.44
1:C:96:ILE:O	1:C:97:VAL:C	2.60	0.44
1:C:273:LEU:HD12	1:C:327:PRO:HB3	1.98	0.44
1:K:342:THR:HG21	2:O:314:ALA:HA	1.99	0.44
1:K:443:GLN:O	1:K:447:ILE:HG12	2.18	0.44
2:O:408:ARG:O	2:O:412:ARG:HG3	2.17	0.44
1:S:158:LEU:HD21	1:S:392:LEU:HG	1.99	0.44
1:S:296:TYR:CD1	1:S:296:TYR:N	2.85	0.44
2:V:427:ILE:HD12	2:V:427:ILE:H	1.82	0.44
2:V:435:LYS:H	2:V:435:LYS:HD2	1.82	0.44
2:X:34:LEU:HD22	2:X:118:HIS:CE1	2.53	0.44
2:X:279:VAL:HG12	2:X:279:VAL:O	2.16	0.44
2:D:257:ASN:HB3	2:D:260:ARG:HG2	1.98	0.44
2:E:152:LYS:HZ3	2:E:293:GLN:HB3	1.82	0.44
4:H:51:GLN:H	4:H:51:GLN:HG2	1.56	0.44
1:J:211:LYS:HZ3	1:J:213:SER:HB2	1.83	0.44
2:N:256:ASP:HA	2:N:257:ASN:HA	1.50	0.44
3:P:46:GLU:O	3:P:50:LEU:N	2.50	0.44
3:P:87:ILE:CD1	3:P:229:GLU:HB3	2.47	0.44
3:P:214:LEU:HD23	3:P:214:LEU:C	2.42	0.44
1:T:338:ALA:HB3	1:T:341:PRO:HG2	2.00	0.44
2:V:325:THR:O	2:V:329:LEU:HG	2.16	0.44
1:A:166:ARG:HG2	1:A:325:ALA:HB3	1.99	0.44
1:C:325:ALA:C	1:C:327:PRO:HD3	2.42	0.44
1:C:388:VAL:HG12	1:C:448:TYR:HD1	1.82	0.44
2:D:409:LYS:HE3	2:D:409:LYS:HB2	1.83	0.44
2:E:16:VAL:HG22	2:E:21:VAL:HG22	1.98	0.44
2:F:97:ASN:C	2:F:97:ASN:ND2	2.74	0.44
1:K:239:SER:OG	2:N:121:PRO:HG2	2.16	0.44
1:L:271:ASP:OD1	1:L:272:ASP:HB2	2.17	0.44
1:L:468:SER:HA	1:L:471:LEU:HD12	2.00	0.44
2:N:321:ALA:HB3	2:N:322:PRO:CD	2.47	0.44
1:T:78:PHE:HD2	1:T:244:LEU:HD23	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:285:LEU:CD2	1:T:291:PRO:HG3	2.47	0.44
2:W:275:ILE:HA	2:W:276:PRO:HD2	1.85	0.44
2:W:427:ILE:HD12	2:W:427:ILE:N	2.33	0.44
3:Y:124:ASN:C	3:Y:124:ASN:HD22	2.25	0.44
1:B:219:VAL:HG22	1:B:233:ILE:HD12	1.99	0.44
1:B:365:PRO:HB2	1:B:367:ILE:HG13	2.00	0.44
1:C:96:ILE:HD12	1:C:96:ILE:N	2.32	0.44
1:C:436:SER:N	1:C:437:PRO:HD3	2.33	0.44
2:D:94:ARG:HH21	2:D:102:PRO:HB3	1.83	0.44
2:E:253:LEU:O	2:E:306:SER:HA	2.18	0.44
2:F:83:ILE:HD12	2:F:83:ILE:N	2.30	0.44
1:K:96:ILE:HD12	1:K:96:ILE:N	2.30	0.44
2:N:251:VAL:HG12	2:N:252:LEU:N	2.33	0.44
2:N:287:THR:O	2:N:291:LEU:HG	2.17	0.44
1:S:460:LEU:H	1:S:460:LEU:HD12	1.83	0.44
1:T:181:ALA:O	1:T:185:ILE:HD12	2.16	0.44
1:T:351:GLN:O	1:T:372:SER:HA	2.18	0.44
1:T:358:LEU:HB2	1:T:366:ALA:HB1	1.98	0.44
1:T:458:ILE:HD12	1:T:458:ILE:N	2.26	0.44
3:Y:96:ARG:O	3:Y:99:LEU:HB3	2.18	0.44
3:Y:244:ALA:O	3:Y:248:ILE:HG13	2.17	0.44
1:A:39:GLY:C	1:A:40:ILE:HD12	2.42	0.44
1:A:161:ILE:HD13	1:A:326:LEU:HD21	2.00	0.44
1:A:290:PRO:HA	1:A:291:PRO:HD3	1.86	0.44
1:C:246:TYR:CD2	1:C:247:LEU:HD12	2.52	0.44
3:G:51:PHE:HB2	4:H:76:THR:HG21	2.00	0.44
1:K:148:VAL:HG23	1:K:163:ARG:HG2	2.00	0.44
2:M:37:LEU:HD23	2:M:78:ASP:HA	1.99	0.44
2:O:221:GLN:OE1	2:O:221:GLN:HA	2.18	0.44
3:P:167:ASN:O	3:P:224:GLN:HB3	2.18	0.44
1:U:211:LYS:HG3	1:U:214:THR:H	1.83	0.44
2:V:256:ASP:HA	2:V:257:ASN:HA	1.51	0.44
2:D:252:LEU:HD22	2:D:254:PHE:CE1	2.53	0.44
1:K:167:GLU:O	1:K:327:PRO:HD2	2.17	0.44
1:K:176:GLY:O	1:K:180:VAL:HG23	2.17	0.44
1:K:375:ARG:NH2	2:O:162:GLY:HA2	2.32	0.44
1:L:97:VAL:HG11	1:L:247:LEU:CD2	2.47	0.44
2:M:137:GLY:HA2	2:M:432:VAL:O	2.17	0.44
2:M:446:GLU:OE1	2:M:448:LYS:HE3	2.18	0.44
2:N:204:THR:OG1	2:N:420:VAL:HB	2.17	0.44
2:N:237:LEU:HD21	2:N:295:ARG:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:154:GLY:HA2	2:O:308:GLN:O	2.17	0.44
2:O:391:LEU:HD22	3:P:83:LEU:CD2	2.47	0.44
3:P:88:HIS:CD2	3:P:113:LYS:HB2	2.52	0.44
1:S:280:TYR:CD2	1:S:303:LEU:HD22	2.53	0.44
1:T:32:ARG:HA	1:T:88:GLU:O	2.18	0.44
1:U:354:LEU:HA	1:U:366:ALA:O	2.17	0.44
2:W:279:VAL:O	2:W:279:VAL:HG12	2.18	0.44
1:A:150:THR:HG21	1:A:155:VAL:HG11	2.00	0.44
1:C:388:VAL:HG11	1:C:444:VAL:HG13	2.00	0.44
1:C:435:TYR:C	1:C:437:PRO:HD3	2.43	0.44
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.99	0.44
2:D:391:LEU:HD12	3:G:23:MET:HE1	2.00	0.44
2:D:454:GLU:CG	2:D:455:HIS:H	2.27	0.44
4:H:119:GLU:HG3	4:H:120:ALA:N	2.32	0.44
5:I:21:ILE:O	5:I:21:ILE:HG22	2.17	0.44
1:K:106:LEU:HD11	1:K:259:PHE:HZ	1.83	0.44
1:T:110:VAL:HG12	1:T:116:PRO:HA	2.00	0.44
1:A:55:VAL:HG21	1:A:75:ILE:HG12	2.00	0.44
2:F:174:ILE:HD12	2:F:174:ILE:N	2.33	0.44
1:J:69:GLU:HB3	1:J:70:PRO:HD2	2.00	0.44
1:J:107:GLY:HA2	1:J:228:MET:O	2.18	0.44
1:K:316:GLU:HA	1:K:320:SER:OG	2.17	0.44
2:M:265:GLY:O	2:M:269:SER:HB2	2.17	0.44
2:M:359:ASP:O	2:M:363:VAL:HG22	2.18	0.44
1:S:243:PRO:HG3	1:S:283:LEU:HD21	2.00	0.44
1:S:338:ALA:HB3	1:S:341:PRO:HG2	1.99	0.44
1:S:442:GLU:O	1:S:445:PRO:HD2	2.18	0.44
1:U:500:LYS:C	1:U:500:LYS:HD3	2.43	0.44
2:V:266:SER:HA	2:V:282:GLN:HB3	1.99	0.44
2:X:209:LEU:HD12	2:X:210:GLU:N	2.32	0.44
2:D:413:PHE:CD1	2:D:457:PHE:HB3	2.53	0.44
1:J:59:SER:OG	1:J:61:VAL:HG12	2.18	0.44
1:J:383:LYS:HD3	1:J:490:GLU:OE2	2.18	0.44
1:L:46:LEU:HD13	1:L:49:ILE:HD12	1.98	0.44
1:L:103:PRO:HD3	1:L:258:TRP:CZ2	2.52	0.44
2:N:253:LEU:HB3	2:N:306:SER:OG	2.17	0.44
2:O:33:ILE:HG22	2:O:34:LEU:HG	1.99	0.44
2:O:167:ILE:O	2:O:171:ILE:HG13	2.17	0.44
1:S:109:VAL:HB	1:S:118:ASP:HB3	2.00	0.44
1:T:201:LEU:HD12	1:T:265:HIS:O	2.18	0.44
2:V:412:ARG:HG2	2:V:454:GLU:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:206:VAL:HA	2:W:214:LYS:HE3	2.00	0.44
3:Y:99:LEU:HD22	3:Y:122:HIS:CE1	2.53	0.44
1:C:50:GLN:HB2	1:C:53:GLU:HB2	2.00	0.43
2:E:221:GLN:HB3	2:E:223:ASN:OD1	2.18	0.43
1:J:253:ALA:O	1:J:257:GLU:HB2	2.18	0.43
1:J:343:ASN:O	1:J:347:ILE:HG13	2.18	0.43
1:J:353:PHE:HE2	1:J:355:GLU:HG2	1.82	0.43
1:K:243:PRO:HG3	1:K:283:LEU:HD21	2.00	0.43
2:O:173:ASN:HB2	2:O:174:ILE:HD12	2.00	0.43
1:S:185:ILE:HG23	1:S:203:CYS:SG	2.58	0.43
1:S:186:LEU:O	1:S:189:LYS:HE2	2.18	0.43
1:T:364:ARG:HA	1:T:365:PRO:C	2.43	0.43
1:U:68:LEU:HD22	2:V:72:ARG:HH21	1.83	0.43
1:U:293:ARG:HD2	1:U:339:TYR:HB2	2.00	0.43
2:V:143:LEU:HG	2:V:371:ALA:HB2	2.00	0.43
2:W:296:ILE:HD13	2:W:306:SER:OG	2.17	0.43
3:Y:264:THR:O	3:Y:268:VAL:HG23	2.18	0.43
1:A:471:LEU:O	1:A:475:LYS:HG3	2.17	0.43
2:D:117:ILE:HA	2:D:238:THR:OG1	2.18	0.43
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.40	0.43
2:E:167:ILE:O	2:E:171:ILE:HG13	2.17	0.43
2:F:138:ILE:HD12	2:F:138:ILE:N	2.32	0.43
4:H:55:GLY:H	4:H:70:ILE:HG22	1.82	0.43
3:P:258:THR:O	3:P:262:VAL:HG23	2.18	0.43
2:V:77:LEU:HD23	2:V:77:LEU:H	1.83	0.43
2:W:204:THR:HG23	2:W:206:VAL:H	1.83	0.43
1:A:402:VAL:O	1:A:402:VAL:HG12	2.18	0.43
1:B:273:LEU:HD13	1:B:304:HIS:HD2	1.84	0.43
1:C:207:ALA:HA	1:C:271:ASP:O	2.18	0.43
1:C:253:ALA:O	1:C:257:GLU:HG3	2.18	0.43
2:D:454:GLU:CG	2:D:455:HIS:N	2.75	0.43
2:F:33:ILE:HD12	2:F:33:ILE:N	2.28	0.43
2:F:38:GLU:HG2	2:F:47:VAL:HG12	2.00	0.43
2:F:159:ALA:HB2	2:F:311:TYR:HE1	1.83	0.43
1:J:55:VAL:HG21	1:J:75:ILE:HG12	2.01	0.43
1:K:150:THR:HG22	1:K:184:THR:HG23	2.01	0.43
1:L:342:THR:HG21	2:M:314:ALA:H	1.83	0.43
1:L:364:ARG:HA	1:L:365:PRO:C	2.42	0.43
2:M:377:THR:HG23	2:M:403:THR:HG23	2.00	0.43
2:N:416:GLN:HA	2:N:417:PRO:HD3	1.85	0.43
3:P:135:LYS:HE2	3:P:135:LYS:HB3	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:146:GLU:O	1:S:163:ARG:HG3	2.18	0.43
1:T:227:ALA:HA	1:T:230:TYR:CE2	2.54	0.43
2:X:183:VAL:O	2:X:253:LEU:HD12	2.18	0.43
2:X:184:PHE:CD1	2:X:254:PHE:HB2	2.54	0.43
2:X:346:PRO:HB3	2:X:418:PHE:HE2	1.83	0.43
3:Y:138:PRO:HG3	3:Y:223:ALA:HA	2.00	0.43
1:B:148:VAL:HG23	1:B:163:ARG:HG2	2.00	0.43
1:C:151:GLY:HA2	1:C:438:LEU:O	2.19	0.43
1:C:364:ARG:HA	1:C:365:PRO:C	2.42	0.43
2:D:221:GLN:OE1	2:D:221:GLN:HA	2.18	0.43
2:E:54:LEU:HD21	2:E:60:ARG:HE	1.83	0.43
1:J:167:GLU:OE1	1:J:350:GLY:HA3	2.17	0.43
1:J:192:ASN:HA	1:J:200:LYS:HG2	2.01	0.43
1:J:273:LEU:HB3	1:J:304:HIS:NE2	2.33	0.43
1:L:375:ARG:HH22	2:M:162:GLY:N	2.16	0.43
2:M:181:PHE:HE2	2:M:249:GLN:HG3	1.84	0.43
1:T:170:ILE:HD11	1:T:331:THR:CG2	2.48	0.43
2:W:17:ILE:HD12	2:W:17:ILE:N	2.34	0.43
2:X:155:LEU:HD23	2:X:155:LEU:H	1.84	0.43
3:Y:168:ASP:HA	3:Y:169:PRO:HD3	1.84	0.43
1:A:436:SER:N	1:A:437:PRO:HD3	2.34	0.43
1:B:271:ASP:HA	1:B:272:ASP:HA	1.56	0.43
1:B:290:PRO:HA	1:B:291:PRO:HD3	1.80	0.43
1:B:302:TYR:HA	1:B:305:SER:OG	2.18	0.43
2:E:433:ARG:HB3	2:E:433:ARG:NH1	2.34	0.43
3:G:180:LYS:HA	3:G:181:PRO:HD3	1.81	0.43
4:H:16:LEU:HD11	4:H:90:ALA:HB3	2.01	0.43
1:K:268:ILE:HD13	1:K:269:VAL:N	2.34	0.43
1:K:282:GLN:CD	2:N:284:THR:HG22	2.43	0.43
2:O:86:PRO:HG3	2:O:114:ARG:HH21	1.83	0.43
1:S:455:LEU:HD21	1:S:466:PHE:CZ	2.54	0.43
1:T:139:LEU:C	1:T:141:ARG:H	2.26	0.43
1:T:394:LEU:O	1:T:398:GLN:HG2	2.19	0.43
3:Y:153:VAL:HG13	3:Y:154:MET:HG3	2.01	0.43
1:B:32:ARG:NH1	1:B:89:LEU:HA	2.33	0.43
1:B:109:VAL:O	1:B:117:ILE:HG12	2.18	0.43
2:D:258:ILE:O	2:D:261:PHE:HB3	2.19	0.43
3:G:77:ILE:CD1	3:G:110:ILE:HD12	2.49	0.43
2:M:77:LEU:HD23	2:M:77:LEU:H	1.83	0.43
2:N:423:VAL:HG23	2:N:424:PHE:CD1	2.53	0.43
3:P:78:THR:OG1	3:P:114:ILE:HB	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:182:ILE:HD11	3:P:217:GLN:CB	2.49	0.43
1:U:157:ALA:O	1:U:158:LEU:HD23	2.18	0.43
1:U:234:VAL:HG11	1:U:252:ALA:HB2	2.00	0.43
2:V:207:ILE:HD11	2:V:215:VAL:HG12	2.00	0.43
1:B:200:LYS:O	1:B:265:HIS:HB2	2.18	0.43
1:C:458:ILE:HD12	1:C:458:ILE:N	2.34	0.43
3:G:159:TYR:HA	3:G:160:PRO:HD3	1.79	0.43
2:N:133:ILE:N	2:N:133:ILE:HD12	2.34	0.43
2:N:174:ILE:HG12	2:N:252:LEU:HD11	2.00	0.43
2:O:427:ILE:N	2:O:427:ILE:HD12	2.33	0.43
3:P:168:ASP:HB3	3:P:176:GLU:HB3	2.01	0.43
1:S:243:PRO:HA	1:S:283:LEU:HD11	2.00	0.43
1:A:139:LEU:N	1:A:140:PRO:CD	2.82	0.43
1:A:281:ARG:HD2	1:A:295:ALA:HB3	2.01	0.43
1:A:347:ILE:HG12	2:E:222:MET:HE1	2.01	0.43
1:A:364:ARG:HA	1:A:365:PRO:C	2.44	0.43
1:B:268:ILE:O	1:B:325:ALA:HA	2.19	0.43
2:D:52:GLN:NE2	2:D:60:ARG:HD2	2.34	0.43
2:F:452:ILE:HD12	2:F:452:ILE:N	2.34	0.43
3:G:193:SER:OG	3:G:196:LYS:HD2	2.18	0.43
1:K:452:ASN:HB2	1:K:454:HIS:CE1	2.53	0.43
3:P:128:LEU:HD12	3:P:129:SER:H	1.84	0.43
1:S:294:GLU:O	1:S:295:ALA:CB	2.67	0.43
1:T:185:ILE:HG23	1:T:203:CYS:SG	2.59	0.43
1:T:273:LEU:HD23	1:T:273:LEU:HA	1.87	0.43
1:T:460:LEU:HD12	1:T:463:ILE:CD1	2.48	0.43
2:V:151:GLY:C	2:V:152:LYS:HG3	2.44	0.43
2:V:427:ILE:HD12	2:V:427:ILE:N	2.34	0.43
2:W:37:LEU:O	2:W:47:VAL:HA	2.19	0.43
2:X:101:GLU:HA	2:X:102:PRO:HD3	1.92	0.43
1:A:162:GLY:O	1:A:165:GLN:HB3	2.18	0.43
1:B:46:LEU:HB3	1:B:49:ILE:HB	1.99	0.43
1:C:282:GLN:NE2	2:F:284:THR:HG22	2.34	0.43
1:C:354:LEU:HA	1:C:366:ALA:O	2.18	0.43
2:D:94:ARG:NH2	2:D:109:ILE:HG12	2.34	0.43
2:F:252:LEU:HD22	2:F:254:PHE:CE2	2.54	0.43
2:F:411:GLN:HA	2:F:414:LEU:HD12	2.00	0.43
4:H:14:PHE:H	4:H:22:TYR:HB2	1.84	0.43
1:K:138:ILE:HD12	1:K:138:ILE:N	2.34	0.43
1:K:156:ASP:O	1:K:385:LEU:HD13	2.18	0.43
2:M:372:SER:O	2:M:376:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:30:LEU:HB3	2:N:53:HIS:HE1	1.84	0.43
1:S:107:GLY:HA2	1:S:228:MET:O	2.18	0.43
1:T:153:LYS:HE3	1:T:432:GLN:HB2	2.00	0.43
2:V:34:LEU:HD22	2:V:118:HIS:CE1	2.53	0.43
1:B:435:TYR:C	1:B:437:PRO:HD3	2.44	0.43
2:D:413:PHE:HA	2:D:457:PHE:O	2.19	0.43
2:E:384:LEU:HD22	2:E:387:ILE:HD11	2.00	0.43
1:J:241:ALA:HB1	1:J:243:PRO:HD2	2.01	0.43
1:L:458:ILE:N	1:L:458:ILE:HD12	2.33	0.43
2:M:101:GLU:HA	2:M:102:PRO:HD3	1.90	0.43
2:M:417:PRO:HD3	2:M:459:MET:HG3	2.01	0.43
2:N:251:VAL:HG12	2:N:252:LEU:H	1.84	0.43
3:P:31:LEU:HD23	3:P:31:LEU:C	2.44	0.43
1:T:146:GLU:HA	1:T:147:PRO:HD3	1.71	0.43
1:U:176:GLY:O	1:U:180:VAL:HG23	2.19	0.43
2:V:252:LEU:HD22	2:V:254:PHE:CE1	2.54	0.43
2:X:98:VAL:HG23	2:X:232:VAL:HA	2.00	0.43
3:Y:113:LYS:O	3:Y:113:LYS:HD3	2.18	0.43
3:Y:266:GLU:O	3:Y:270:ILE:HG12	2.19	0.43
1:A:273:LEU:HB3	1:A:304:HIS:CE1	2.54	0.42
2:D:152:LYS:HZ1	2:D:293:GLN:HB3	1.84	0.42
2:D:182:SER:O	2:D:215:VAL:HG23	2.18	0.42
2:D:345:TYR:HA	2:D:346:PRO:C	2.43	0.42
2:D:439:ALA:HA	2:D:442:LYS:CD	2.48	0.42
2:F:431:LEU:HD23	2:F:431:LEU:C	2.44	0.42
1:J:352:ILE:HA	1:J:372:SER:HB2	2.00	0.42
2:O:174:ILE:HD12	2:O:174:ILE:N	2.34	0.42
3:P:42:LYS:O	3:P:46:GLU:HG3	2.18	0.42
3:P:173:LEU:HD23	3:P:234:ARG:HH22	1.84	0.42
1:T:428:GLN:HG2	1:T:431:LYS:NZ	2.34	0.42
2:V:95:ILE:HD12	2:V:104:ASP:HB3	2.00	0.42
2:W:152:LYS:N	2:W:152:LYS:HD2	2.34	0.42
2:W:169:GLU:HG2	2:W:418:PHE:CD1	2.54	0.42
2:W:281:TYR:CE2	2:W:321:ALA:HB2	2.54	0.42
1:A:108:ARG:NH1	1:A:123:ILE:HG12	2.34	0.42
1:B:104:GLY:HA3	1:B:124:ASP:HB3	2.01	0.42
1:C:274:SER:O	1:C:278:VAL:HG23	2.18	0.42
2:F:188:GLY:O	2:F:260:ARG:HG3	2.19	0.42
3:G:139:THR:HG23	3:G:142:GLU:H	1.84	0.42
3:G:242:LYS:C	3:G:242:LYS:HD3	2.44	0.42
1:L:294:GLU:C	1:L:296:TYR:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:142:ASP:HB3	2:M:434:LEU:HD13	2.00	0.42
2:N:143:LEU:O	2:N:367:HIS:HE1	2.02	0.42
1:T:97:VAL:HG23	1:T:97:VAL:O	2.19	0.42
2:V:145:ALA:HB1	2:V:355:SER:HB2	2.01	0.42
2:W:118:HIS:HE1	2:W:231:ARG:NH1	2.17	0.42
1:B:168:LEU:HD12	1:B:327:PRO:O	2.18	0.42
2:E:387:ILE:HB	2:E:391:LEU:HD12	2.01	0.42
1:K:99:VAL:HG11	1:K:251:THR:HB	2.00	0.42
1:L:425:ARG:HD3	1:L:455:LEU:O	2.20	0.42
2:N:103:ILE:HD13	2:N:103:ILE:N	2.34	0.42
2:N:296:ILE:HD13	2:N:306:SER:OG	2.19	0.42
1:T:285:LEU:HD21	1:T:291:PRO:HG3	2.00	0.42
1:U:50:GLN:HG2	2:V:71:VAL:HG22	1.99	0.42
2:X:38:GLU:HG2	2:X:47:VAL:HG12	2.01	0.42
2:X:182:SER:O	2:X:215:VAL:HA	2.19	0.42
1:C:46:LEU:O	1:C:49:ILE:HG22	2.20	0.42
3:G:22:THR:O	3:G:26:VAL:HG23	2.19	0.42
4:H:88:ILE:HD12	4:H:88:ILE:N	2.34	0.42
1:K:99:VAL:HA	1:K:100:PRO:HD3	1.92	0.42
3:P:51:PHE:C	3:P:51:PHE:CD2	2.96	0.42
3:P:180:LYS:HA	3:P:181:PRO:HD3	1.78	0.42
1:S:65:ALA:HB2	1:S:75:ILE:HG12	2.00	0.42
1:S:429:LEU:HD23	1:S:429:LEU:O	2.20	0.42
1:T:444:VAL:N	1:T:445:PRO:CD	2.82	0.42
1:U:249:PRO:HB3	1:U:270:TYR:CD2	2.54	0.42
2:V:7:THR:HA	2:V:8:PRO:HD3	1.72	0.42
2:V:196:ASP:O	2:V:200:GLU:HG2	2.19	0.42
2:V:339:ILE:HD13	2:V:411:GLN:NE2	2.34	0.42
2:W:464:GLU:H	2:W:464:GLU:CD	2.27	0.42
3:Y:219:LEU:HD13	3:Y:219:LEU:C	2.44	0.42
2:D:133:ILE:HD13	2:D:133:ILE:C	2.44	0.42
2:E:30:LEU:HA	2:E:31:PRO:HD3	1.84	0.42
2:F:285:LEU:HD23	2:F:285:LEU:C	2.45	0.42
1:J:267:LEU:HD12	1:J:324:THR:HB	2.00	0.42
1:K:452:ASN:HB2	1:K:454:HIS:HE1	1.85	0.42
1:L:138:ILE:HD12	1:L:138:ILE:N	2.34	0.42
2:N:17:ILE:HD13	2:N:17:ILE:N	2.34	0.42
2:N:427:ILE:HA	2:N:428:PRO:HD2	1.87	0.42
2:O:275:ILE:HA	2:O:276:PRO:HD2	1.85	0.42
1:S:78:PHE:HD1	1:S:244:LEU:HG	1.84	0.42
1:S:96:ILE:O	1:S:97:VAL:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:458:ILE:H	1:T:458:ILE:CD1	2.27	0.42
1:U:353:PHE:H	1:U:372:SER:HB3	1.84	0.42
2:W:343:GLY:C	2:W:344:ILE:HD12	2.44	0.42
2:X:263:GLN:O	2:X:267:GLU:HG3	2.20	0.42
3:Y:147:ALA:HA	3:Y:150:LEU:HD12	2.01	0.42
1:C:110:VAL:O	1:C:234:VAL:HA	2.20	0.42
2:D:94:ARG:HH22	2:D:108:PRO:C	2.28	0.42
2:E:98:VAL:HB	2:E:232:VAL:HG13	2.01	0.42
3:G:23:MET:HB2	3:G:237:MET:SD	2.59	0.42
1:K:308:LEU:HD22	1:K:327:PRO:HG3	2.01	0.42
1:L:290:PRO:HB2	2:M:270:ALA:HB1	2.01	0.42
2:M:30:LEU:HA	2:M:31:PRO:HD3	1.74	0.42
2:N:122:PRO:HB2	2:N:127:GLN:NE2	2.34	0.42
1:S:212:ARG:CG	1:S:237:THR:HG21	2.49	0.42
1:T:504:GLU:O	1:T:507:VAL:HG23	2.19	0.42
1:U:341:PRO:O	1:U:345:ILE:HG13	2.20	0.42
2:V:33:ILE:HD12	2:V:33:ILE:H	1.83	0.42
2:X:201:MET:HB3	2:X:207:ILE:HG13	2.01	0.42
2:X:357:LEU:HD22	2:X:357:LEU:N	2.34	0.42
1:A:435:TYR:C	1:A:437:PRO:HD3	2.43	0.42
2:D:344:ILE:H	2:D:344:ILE:HD12	1.85	0.42
2:D:374:VAL:O	2:D:378:LEU:HG	2.20	0.42
2:E:301:LYS:HE3	2:N:300:LYS:O	2.19	0.42
1:J:55:VAL:N	1:J:63:GLY:O	2.50	0.42
1:J:363:ILE:HD12	1:J:363:ILE:N	2.34	0.42
1:L:56:GLU:OE2	1:L:62:LYS:HE3	2.20	0.42
1:L:96:ILE:O	1:L:97:VAL:C	2.62	0.42
2:O:370:VAL:O	2:O:374:VAL:HG23	2.20	0.42
1:S:103:PRO:HG3	1:S:258:TRP:CH2	2.55	0.42
1:T:389:ALA:HB2	1:T:447:ILE:HG21	2.02	0.42
1:T:422:ARG:O	1:T:426:LEU:HB2	2.20	0.42
1:U:185:ILE:HD12	1:U:203:CYS:HB3	2.02	0.42
2:V:134:LEU:HD21	2:V:174:ILE:HD12	2.01	0.42
2:W:95:ILE:HD11	2:W:198:TYR:CD1	2.54	0.42
2:E:32:ALA:O	2:E:35:ASN:HB2	2.20	0.42
2:E:40:LYS:HG3	1:T:508:ALA:HB3	2.00	0.42
2:F:47:VAL:HG23	2:F:64:MET:HB2	2.02	0.42
2:F:120:ASP:HA	2:F:121:PRO:HD2	1.87	0.42
3:G:51:PHE:CE1	4:H:49:VAL:HG21	2.55	0.42
3:G:77:ILE:O	3:G:78:THR:HG23	2.19	0.42
3:G:258:THR:O	3:G:262:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:GLU:OE1	2:O:223:ASN:HB3	2.19	0.42
2:M:96:ILE:HD12	2:M:96:ILE:O	2.20	0.42
2:N:242:TYR:CZ	2:N:246:GLU:HG2	2.55	0.42
2:N:434:LEU:O	2:N:438:VAL:HG23	2.20	0.42
1:S:296:TYR:CD2	1:S:340:ILE:HD11	2.55	0.42
1:T:358:LEU:HD21	1:T:400:ARG:HH21	1.85	0.42
1:T:473:TYR:O	1:T:477:ASN:HB2	2.19	0.42
1:U:408:PHE:CD1	2:V:390:ILE:HG13	2.54	0.42
2:V:39:ILE:HD12	2:V:46:LEU:O	2.19	0.42
1:C:166:ARG:O	1:C:348:THR:HB	2.20	0.42
2:E:349:ASP:HA	2:E:350:PRO:HD3	1.84	0.42
1:K:67:ASN:ND2	1:K:67:ASN:N	2.68	0.42
1:K:139:LEU:HB3	1:K:140:PRO:HD3	2.01	0.42
1:K:423:GLY:HA2	1:K:426:LEU:HB3	2.02	0.42
2:N:121:PRO:HG3	2:N:295:ARG:HG3	2.02	0.42
2:N:391:LEU:HD13	2:N:395:GLU:HG3	2.01	0.42
3:P:83:LEU:HD22	3:P:237:MET:HE1	2.01	0.42
1:S:442:GLU:C	1:S:445:PRO:HD2	2.45	0.42
1:T:363:ILE:HG22	1:T:366:ALA:HA	2.02	0.42
2:V:200:GLU:HA	2:V:200:GLU:OE1	2.19	0.42
2:X:416:GLN:HA	2:X:417:PRO:HD3	1.91	0.42
1:A:363:ILE:HD12	1:A:363:ILE:H	1.84	0.42
1:B:96:ILE:O	1:B:97:VAL:C	2.61	0.42
1:B:170:ILE:O	1:B:353:PHE:HA	2.19	0.42
2:D:251:VAL:HG12	2:D:252:LEU:N	2.35	0.42
2:E:169:GLU:HG2	2:E:418:PHE:CD1	2.55	0.42
3:G:156:ALA:HA	3:G:159:TYR:CD1	2.55	0.42
1:J:505:SER:O	1:J:509:THR:HG22	2.20	0.42
1:L:146:GLU:HA	1:L:147:PRO:HD3	1.73	0.42
2:M:279:VAL:O	2:M:279:VAL:HG12	2.20	0.42
2:M:384:LEU:HA	2:M:387:ILE:HD12	2.01	0.42
3:P:32:SER:HA	3:P:35:GLU:HB2	2.02	0.42
3:P:54:ASN:O	3:P:193:SER:HB3	2.20	0.42
1:T:481:LEU:HD22	1:T:495:LEU:HD11	2.02	0.42
1:U:46:LEU:HD13	1:U:49:ILE:HD12	2.01	0.42
1:U:158:LEU:C	1:U:160:PRO:HD3	2.45	0.42
1:U:459:GLU:HG2	1:U:461:SER:H	1.85	0.42
2:W:218:VAL:HG21	2:W:236:GLY:HA2	2.01	0.42
2:W:221:GLN:HB2	2:W:223:ASN:OD1	2.20	0.42
3:Y:99:LEU:HD22	3:Y:122:HIS:NE2	2.35	0.42
1:A:105:LEU:HD22	1:A:255:ILE:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:OE1	1:A:491:LEU:HB2	2.20	0.41
1:A:413:ASP:O	1:A:417:LYS:HD2	2.20	0.41
1:C:163:ARG:HB3	1:C:322:SER:OG	2.20	0.41
2:E:37:LEU:HB2	2:E:48:LEU:HB2	2.02	0.41
3:G:75:VAL:HG11	3:G:218:MET:HE2	2.02	0.41
3:G:181:PRO:C	3:G:182:ILE:HD12	2.45	0.41
1:K:239:SER:HB2	2:N:294:GLU:HG3	2.02	0.41
2:N:410:ILE:HG23	2:N:441:PHE:CE2	2.45	0.41
2:O:153:ILE:HD12	2:O:153:ILE:N	2.35	0.41
2:O:285:LEU:C	2:O:285:LEU:HD23	2.45	0.41
2:V:257:ASN:HD21	2:V:311:TYR:HB2	1.85	0.41
2:W:37:LEU:HD12	2:W:61:THR:HG21	2.02	0.41
2:W:153:ILE:HD12	2:W:153:ILE:N	2.35	0.41
2:X:195:ASN:O	2:X:199:ARG:HG3	2.20	0.41
1:C:105:LEU:CD1	1:C:255:ILE:HD12	2.50	0.41
1:C:294:GLU:C	1:C:296:TYR:H	2.28	0.41
2:D:117:ILE:H	2:D:117:ILE:CD1	2.32	0.41
2:E:298:THR:HG23	2:E:303:SER:HB3	2.01	0.41
3:G:79:SER:CB	3:G:134:GLY:HA3	2.50	0.41
1:J:457:GLY:C	1:J:458:ILE:HD12	2.44	0.41
1:K:173:ARG:O	1:K:174:GLN:HB2	2.21	0.41
1:L:209:GLY:O	1:L:238:ALA:HB2	2.20	0.41
2:N:152:LYS:C	2:N:153:ILE:HD12	2.45	0.41
1:S:166:ARG:HD3	1:S:308:LEU:O	2.20	0.41
1:S:358:LEU:HD11	1:S:400:ARG:HH22	1.85	0.41
2:X:99:ILE:HG13	2:X:101:GLU:HG2	2.01	0.41
1:A:271:ASP:HA	1:A:272:ASP:HA	1.73	0.41
2:D:63:ALA:O	2:D:227:GLY:HA3	2.21	0.41
2:E:357:LEU:HD23	2:E:357:LEU:HA	1.90	0.41
1:S:62:LYS:HB2	1:S:62:LYS:NZ	2.35	0.41
1:U:53:GLU:OE2	1:U:92:ARG:HB3	2.20	0.41
1:U:363:ILE:N	1:U:363:ILE:HD12	2.35	0.41
1:U:373:VAL:HA	1:U:393:LYS:HZ1	1.85	0.41
1:C:441:GLU:H	1:C:441:GLU:CD	2.28	0.41
2:D:321:ALA:CB	2:D:322:PRO:HD3	2.41	0.41
3:G:24:LYS:HD2	3:G:238:ASP:HA	2.02	0.41
1:K:110:VAL:HG12	1:K:116:PRO:HA	2.02	0.41
1:K:155:VAL:C	1:K:157:ALA:H	2.29	0.41
1:K:470:PHE:O	1:K:474:LEU:HG	2.20	0.41
2:N:370:VAL:O	2:N:374:VAL:HG23	2.20	0.41
2:O:416:GLN:HA	2:O:417:PRO:HD3	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:32:LEU:HA	4:Q:33:PRO:HD3	1.68	0.41
1:S:161:ILE:HD12	1:S:161:ILE:N	2.36	0.41
1:T:425:ARG:HH12	1:T:460:LEU:N	2.18	0.41
1:U:150:THR:HA	1:U:184:THR:HG23	2.02	0.41
1:U:249:PRO:HG2	1:U:276:GLN:NE2	2.35	0.41
2:V:168:GLN:HE21	2:V:197:LEU:HD12	1.85	0.41
2:W:120:ASP:HA	2:W:121:PRO:HD3	1.93	0.41
1:A:68:LEU:O	2:E:15:ALA:HA	2.19	0.41
2:D:224:GLU:O	2:D:229:ARG:HD3	2.21	0.41
2:F:207:ILE:HD11	2:F:215:VAL:HG13	2.03	0.41
1:L:192:ASN:O	1:L:200:LYS:HE2	2.19	0.41
1:L:285:LEU:CD2	1:L:291:PRO:HG3	2.51	0.41
2:O:401:LYS:O	2:O:405:GLU:HG3	2.20	0.41
3:P:79:SER:HB3	3:P:229:GLU:OE2	2.20	0.41
1:S:139:LEU:CD2	2:W:105:GLU:HB2	2.51	0.41
2:X:134:LEU:HD13	2:X:149:ARG:HG2	2.01	0.41
2:X:406:ARG:O	2:X:410:ILE:HG13	2.20	0.41
1:B:268:ILE:HG23	1:B:325:ALA:HA	2.03	0.41
1:C:301:PHE:CZ	1:C:347:ILE:HD11	2.56	0.41
1:C:500:LYS:HD3	1:C:500:LYS:O	2.21	0.41
2:E:47:VAL:HB	2:E:64:MET:HB2	2.01	0.41
2:E:397:SER:O	2:E:401:LYS:HG2	2.20	0.41
2:F:12:LYS:HA	2:F:74:GLU:O	2.19	0.41
1:J:112:ALA:O	1:J:251:THR:HG21	2.21	0.41
1:K:282:GLN:NE2	2:N:284:THR:HG22	2.36	0.41
1:L:211:LYS:HZ3	1:L:213:SER:HB3	1.86	0.41
2:M:339:ILE:HG22	2:M:344:ILE:HB	2.01	0.41
2:M:392:GLY:O	2:M:395:GLU:HB3	2.21	0.41
2:O:171:ILE:O	2:O:175:ALA:HB3	2.20	0.41
3:P:247:MET:O	3:P:251:TYR:HB2	2.21	0.41
2:V:255:ILE:N	2:V:255:ILE:HD12	2.36	0.41
2:X:37:LEU:HD12	2:X:61:THR:HG21	2.02	0.41
1:A:407:GLN:HG3	2:D:395:GLU:O	2.20	0.41
2:D:83:ILE:HG23	2:D:83:ILE:O	2.21	0.41
2:D:381:TYR:O	2:D:385:GLN:HB3	2.20	0.41
2:F:422:GLU:CD	2:F:428:PRO:HA	2.45	0.41
4:H:45:HIS:HD2	4:H:77:VAL:HG21	1.85	0.41
1:J:115:ASN:HA	1:J:116:PRO:HD3	1.91	0.41
2:N:20:ILE:HD12	2:N:20:ILE:N	2.36	0.41
3:P:48:GLU:O	3:P:52:TYR:HD2	2.04	0.41
1:S:296:TYR:N	1:S:296:TYR:HD1	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:338:ALA:HB3	1:S:341:PRO:HD2	2.02	0.41
1:S:352:ILE:HA	1:S:372:SER:CB	2.51	0.41
1:S:352:ILE:HA	1:S:372:SER:HB3	2.03	0.41
1:T:340:ILE:HB	1:T:341:PRO:HD3	2.02	0.41
2:V:13:VAL:HG13	2:V:21:VAL:HG13	2.03	0.41
2:X:170:LEU:HD13	2:X:307:VAL:HG11	2.02	0.41
2:X:417:PRO:HA	2:X:459:MET:HE3	2.02	0.41
1:B:413:ASP:N	1:B:417:LYS:HD3	2.33	0.41
1:C:153:LYS:HB3	1:C:430:LEU:HD23	2.03	0.41
1:C:246:TYR:HD2	1:C:247:LEU:HD12	1.86	0.41
1:J:211:LYS:NZ	1:J:213:SER:HB2	2.36	0.41
2:N:294:GLU:OE1	2:N:294:GLU:HA	2.21	0.41
2:O:16:VAL:HG22	2:O:21:VAL:HG22	2.02	0.41
2:O:41:THR:OG1	2:O:42:PRO:HD2	2.21	0.41
1:S:233:ILE:N	1:S:233:ILE:HD12	2.36	0.41
1:T:27:LEU:HD23	1:T:27:LEU:O	2.20	0.41
1:U:103:PRO:HG3	1:U:258:TRP:HH2	1.85	0.41
2:W:172:ASN:ND2	2:W:419:ALA:HB3	2.35	0.41
2:X:237:LEU:CD1	2:X:296:ILE:HG12	2.51	0.41
2:X:247:GLU:HG3	2:X:249:GLN:HG2	2.02	0.41
1:A:444:VAL:N	1:A:445:PRO:CD	2.83	0.41
1:B:68:LEU:O	2:F:15:ALA:HA	2.20	0.41
1:B:103:PRO:C	1:B:105:LEU:H	2.29	0.41
1:B:444:VAL:N	1:B:445:PRO:CD	2.83	0.41
1:C:267:LEU:O	1:C:267:LEU:HD23	2.20	0.41
1:C:413:ASP:O	1:C:417:LYS:HB2	2.21	0.41
2:D:52:GLN:CG	2:D:60:ARG:HB3	2.50	0.41
2:D:89:ARG:NH1	2:D:181:PHE:HZ	2.18	0.41
2:E:296:ILE:HD13	2:E:306:SER:OG	2.21	0.41
2:E:345:TYR:HA	2:E:346:PRO:C	2.44	0.41
2:F:7:THR:HA	2:F:8:PRO:HD2	1.80	0.41
2:F:91:THR:HB	2:F:96:ILE:HD11	2.03	0.41
2:F:180:GLY:HA3	2:F:250:ASP:O	2.21	0.41
2:F:387:ILE:HD12	2:F:387:ILE:N	2.34	0.41
1:J:65:ALA:HB2	1:J:75:ILE:HG13	2.03	0.41
1:J:162:GLY:O	1:J:165:GLN:HB3	2.21	0.41
1:J:177:LYS:HB2	1:J:177:LYS:NZ	2.36	0.41
1:J:242:ALA:N	1:J:243:PRO:CD	2.84	0.41
1:J:271:ASP:HA	1:J:272:ASP:HA	1.78	0.41
1:K:68:LEU:N	1:K:68:LEU:HD12	2.36	0.41
1:K:220:GLN:HB2	2:N:129:THR:HB	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:233:ILE:N	1:K:233:ILE:HD12	2.35	0.41
1:K:260:ARG:HG2	1:K:314:LEU:HD12	2.03	0.41
1:K:273:LEU:HD23	1:K:273:LEU:HA	1.94	0.41
1:K:302:TYR:HA	1:K:305:SER:HG	1.86	0.41
1:L:251:THR:O	1:L:255:ILE:HG12	2.20	0.41
2:N:334:VAL:HG21	2:N:352:ASP:HB3	2.02	0.41
2:N:431:LEU:HD23	2:N:431:LEU:C	2.45	0.41
2:O:33:ILE:HD12	2:O:33:ILE:N	2.34	0.41
2:O:34:LEU:HD22	2:O:118:HIS:CD2	2.56	0.41
2:O:133:ILE:HD11	2:O:362:VAL:HG12	2.03	0.41
2:O:388:ILE:HG12	2:O:396:LEU:HD11	2.02	0.41
3:P:19:ILE:HD12	3:P:19:ILE:C	2.46	0.41
1:S:118:ASP:OD1	1:S:118:ASP:N	2.54	0.41
1:S:170:ILE:O	1:S:353:PHE:HA	2.20	0.41
1:S:212:ARG:HG2	1:S:237:THR:HG21	2.03	0.41
1:S:369:VAL:HG11	1:S:396:LEU:HB2	2.03	0.41
1:T:67:ASN:H	1:T:67:ASN:ND2	2.19	0.41
1:U:158:LEU:HD21	1:U:392:LEU:HB3	2.03	0.41
1:U:343:ASN:O	1:U:347:ILE:HG12	2.21	0.41
1:U:470:PHE:CE2	1:U:474:LEU:HD11	2.56	0.41
2:V:381:TYR:O	2:V:385:GLN:HB2	2.20	0.41
2:W:281:TYR:CZ	2:W:321:ALA:HB2	2.55	0.41
2:W:346:PRO:HB2	2:W:348:VAL:HG23	2.02	0.41
2:X:30:LEU:HD21	2:X:57:ASN:CA	2.51	0.41
2:X:52:GLN:HE21	2:X:54:LEU:HD21	1.86	0.41
3:Y:147:ALA:O	3:Y:150:LEU:HB2	2.21	0.41
1:B:274:SER:O	1:B:278:VAL:HG23	2.20	0.41
1:C:290:PRO:HA	1:C:291:PRO:HD3	1.75	0.41
2:D:158:GLY:O	2:D:161:VAL:HG22	2.21	0.41
2:D:319:ASP:HB3	2:D:322:PRO:HD2	2.03	0.41
2:D:433:ARG:HB3	2:D:434:LEU:H	1.77	0.41
2:F:221:GLN:OE1	2:F:221:GLN:HA	2.20	0.41
2:F:354:LYS:HE3	2:F:354:LYS:HB3	1.95	0.41
2:M:229:ARG:HA	2:M:232:VAL:HG12	2.03	0.41
2:N:400:ASP:O	2:N:404:VAL:HG23	2.20	0.41
1:S:453:GLY:HA2	1:S:456:ASP:OD1	2.22	0.41
1:T:184:THR:O	1:T:188:GLN:HG2	2.21	0.41
1:U:52:GLU:HB3	1:U:64:MET:HE3	2.02	0.41
1:U:203:CYS:HA	1:U:267:LEU:O	2.21	0.41
1:U:290:PRO:HA	1:U:291:PRO:HD3	1.87	0.41
2:V:419:ALA:O	2:V:422:GLU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:65:ASP:CA	2:W:225:PRO:HG3	2.51	0.41
1:A:452:ASN:HB3	1:A:454:HIS:CE1	2.56	0.40
1:B:139:LEU:C	1:B:141:ARG:H	2.29	0.40
1:B:383:LYS:HD2	1:B:490:GLU:CD	2.46	0.40
1:B:444:VAL:HG23	1:B:445:PRO:CD	2.48	0.40
2:F:97:ASN:HD21	2:F:101:GLU:N	2.19	0.40
2:F:330:ASP:HB3	2:F:356:ARG:HD3	2.02	0.40
1:K:427:THR:O	1:K:431:LYS:HG3	2.21	0.40
1:L:204:VAL:O	1:L:268:ILE:HG12	2.21	0.40
2:M:275:ILE:HA	2:M:276:PRO:HD2	1.91	0.40
1:S:232:ILE:HD12	1:S:232:ILE:N	2.36	0.40
1:T:274:SER:OG	1:T:329:ILE:HG23	2.21	0.40
2:V:337:ARG:O	2:V:341:GLU:HG3	2.20	0.40
2:X:156:PHE:CD1	2:X:310:VAL:HB	2.56	0.40
1:C:206:VAL:HG11	1:C:249:PRO:HA	2.03	0.40
2:D:37:LEU:HD12	2:D:61:THR:HG21	2.03	0.40
2:D:39:ILE:HD11	2:D:76:VAL:HG22	2.03	0.40
2:D:138:ILE:HG22	2:D:140:VAL:HG12	2.04	0.40
2:D:451:ASN:O	2:D:453:PRO:HD3	2.21	0.40
2:E:83:ILE:HD12	2:E:83:ILE:N	2.36	0.40
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.56	0.40
2:F:30:LEU:N	2:F:30:LEU:HD12	2.36	0.40
2:F:138:ILE:HA	2:F:416:GLN:OE1	2.20	0.40
3:G:111:GLY:O	3:G:114:ILE:HG22	2.21	0.40
3:G:130:ILE:N	3:G:130:ILE:HD12	2.36	0.40
4:H:124:ALA:O	4:H:127:VAL:HG22	2.21	0.40
1:J:57:PHE:HD1	1:J:61:VAL:O	2.03	0.40
2:M:336:SER:O	2:M:347:ALA:HB1	2.20	0.40
2:M:452:ILE:HA	2:M:453:PRO:HD3	1.89	0.40
2:N:10:THR:HG23	2:N:75:LYS:HG3	2.04	0.40
2:O:20:ILE:HD11	2:O:272:LEU:HG	2.03	0.40
1:T:46:LEU:HD11	1:T:90:VAL:CG1	2.51	0.40
1:T:52:GLU:O	1:T:96:ILE:HG23	2.21	0.40
1:T:117:ILE:C	1:T:117:ILE:HD12	2.46	0.40
2:V:45:LYS:HE2	2:V:101:GLU:OE2	2.21	0.40
3:Y:249:ASN:O	3:Y:253:ILE:HG12	2.21	0.40
1:B:51:ALA:O	1:B:52:GLU:HB2	2.22	0.40
1:C:438:LEU:HD11	1:C:467:GLU:OE2	2.22	0.40
2:E:49:GLU:HB2	2:E:64:MET:HE2	2.04	0.40
3:G:2:THR:HB	3:G:5:GLU:CB	2.51	0.40
2:N:263:GLN:O	2:N:267:GLU:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:30:LEU:HA	2:O:31:PRO:HD3	1.90	0.40
3:P:179:GLU:HG2	3:P:180:LYS:N	2.35	0.40
1:T:68:LEU:HD12	1:T:68:LEU:N	2.37	0.40
1:U:99:VAL:HG11	1:U:251:THR:HB	2.03	0.40
1:U:460:LEU:HD12	1:U:463:ILE:HD11	2.03	0.40
2:V:289:MET:HG2	2:V:324:THR:HG22	2.03	0.40
2:V:378:LEU:CD2	2:V:411:GLN:HB2	2.50	0.40
2:W:74:GLU:O	2:W:76:VAL:HG23	2.21	0.40
2:W:84:SER:HA	2:W:116:PRO:HA	2.03	0.40
1:A:77:LEU:HD13	1:A:81:ASP:HA	2.04	0.40
1:B:146:GLU:HA	1:B:147:PRO:HD3	1.76	0.40
1:B:289:ARG:HA	1:B:290:PRO:HD3	1.95	0.40
1:B:417:LYS:O	1:B:420:LEU:HB3	2.21	0.40
1:C:101:VAL:HG12	1:C:255:ILE:HD13	2.03	0.40
1:C:150:THR:C	1:C:152:LEU:H	2.28	0.40
2:E:35:ASN:O	2:E:50:VAL:HG23	2.21	0.40
2:F:408:ARG:O	2:F:412:ARG:HG3	2.21	0.40
3:G:144:ALA:HB1	5:I:11:ALA:HB1	2.03	0.40
1:K:36:VAL:HG11	1:K:84:VAL:O	2.21	0.40
2:M:408:ARG:O	2:M:412:ARG:HB2	2.22	0.40
2:N:156:PHE:HZ	2:N:326:PHE:CZ	2.39	0.40
2:N:242:TYR:CE2	2:N:246:GLU:HG2	2.56	0.40
2:N:279:VAL:HG12	2:N:279:VAL:O	2.21	0.40
2:O:52:GLN:HE21	2:O:60:ARG:HD2	1.87	0.40
3:P:185:ALA:HA	3:P:188:ILE:HD12	2.03	0.40
1:S:496:LEU:HD23	1:S:496:LEU:O	2.21	0.40
1:U:243:PRO:O	1:U:247:LEU:HD13	2.22	0.40
2:V:97:ASN:HB3	2:V:103:ILE:HD13	2.02	0.40
2:X:86:PRO:HG3	2:X:114:ARG:NE	2.35	0.40
2:E:408:ARG:HH11	2:E:412:ARG:HH21	1.69	0.40
2:F:34:LEU:HD22	2:F:118:HIS:CD2	2.57	0.40
2:F:288:ASP:C	2:F:290:GLY:H	2.29	0.40
5:I:46:GLN:HB2	5:I:56:PRO:HG2	2.04	0.40
1:J:455:LEU:HD21	1:J:466:PHE:CE2	2.57	0.40
1:L:40:ILE:HG22	1:L:41:ALA:N	2.37	0.40
1:L:345:ILE:HG23	1:L:351:GLN:HG2	2.03	0.40
2:M:155:LEU:HB3	2:M:309:ALA:HA	2.04	0.40
2:N:62:ILE:H	2:N:62:ILE:HG13	1.77	0.40
2:N:310:VAL:HG11	2:N:326:PHE:CE1	2.50	0.40
3:P:225:GLY:C	3:P:227:ALA:N	2.80	0.40
1:S:353:PHE:H	1:S:372:SER:HB3	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:37:GLY:O	1:T:38:ASP:HB2	2.21	0.40
1:T:68:LEU:HB3	2:X:72:ARG:HD3	2.04	0.40
2:V:167:ILE:HG13	2:V:168:GLN:N	2.36	0.40
2:W:25:PHE:HB2	2:W:30:LEU:CD2	2.47	0.40
2:X:200:GLU:O	2:X:204:THR:HG23	2.22	0.40
3:Y:132:GLY:H	3:Y:133:ILE:HD13	1.86	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	480/510 (94%)	437 (91%)	40 (8%)	3 (1%)	21	54
1	B	475/510 (93%)	430 (90%)	41 (9%)	4 (1%)	16	49
1	C	482/510 (94%)	449 (93%)	32 (7%)	1 (0%)	43	72
1	J	477/510 (94%)	447 (94%)	27 (6%)	3 (1%)	21	54
1	K	480/510 (94%)	442 (92%)	35 (7%)	3 (1%)	21	54
1	L	482/510 (94%)	453 (94%)	29 (6%)	0	100	100
1	S	477/510 (94%)	440 (92%)	32 (7%)	5 (1%)	12	44
1	T	461/510 (90%)	414 (90%)	43 (9%)	4 (1%)	14	46
1	U	469/510 (92%)	427 (91%)	41 (9%)	1 (0%)	43	72
2	D	460/484 (95%)	417 (91%)	40 (9%)	3 (1%)	18	51
2	E	466/484 (96%)	422 (91%)	41 (9%)	3 (1%)	21	54
2	F	469/484 (97%)	436 (93%)	32 (7%)	1 (0%)	43	72
2	M	467/484 (96%)	430 (92%)	35 (8%)	2 (0%)	30	60
2	N	462/484 (96%)	429 (93%)	30 (6%)	3 (1%)	21	54
2	O	467/484 (96%)	434 (93%)	32 (7%)	1 (0%)	43	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	439/484 (91%)	381 (87%)	55 (12%)	3 (1%)	18	51
2	W	464/484 (96%)	414 (89%)	43 (9%)	7 (2%)	8	37
2	X	467/484 (96%)	435 (93%)	31 (7%)	1 (0%)	43	72
3	G	264/278 (95%)	244 (92%)	19 (7%)	1 (0%)	30	60
3	P	221/278 (80%)	200 (90%)	17 (8%)	4 (2%)	6	34
3	Y	169/278 (61%)	153 (90%)	14 (8%)	2 (1%)	10	41
4	H	108/138 (78%)	92 (85%)	16 (15%)	0	100	100
4	Q	56/138 (41%)	40 (71%)	12 (21%)	4 (7%)	1	10
4	Z	9/138 (6%)	5 (56%)	4 (44%)	0	100	100
5	1	21/61 (34%)	14 (67%)	6 (29%)	1 (5%)	2	16
5	I	38/61 (62%)	34 (90%)	3 (8%)	1 (3%)	4	27
5	R	21/61 (34%)	15 (71%)	5 (24%)	1 (5%)	2	16
All	All	9351/10377 (90%)	8534 (91%)	755 (8%)	62 (1%)	18	51

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ASP
2	D	456	ALA
3	P	192	PRO
4	Q	17	PRO
4	Q	39	ILE
2	X	279	VAL
2	E	279	VAL
1	K	97	VAL
2	N	277	SER
2	O	68	GLU
3	P	3	LEU
3	P	275	SER
1	A	319	GLY
1	B	237	THR
1	B	461	SER
2	E	393	MET
3	G	202	ASP
1	J	414	ALA
2	M	277	SER
2	N	223	ASN
3	P	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	16	LEU
1	S	319	GLY
1	T	377	GLY
1	U	97	VAL
2	W	277	SER
5	1	11	ALA
2	D	462	GLY
2	F	68	GLU
1	K	319	GLY
4	Q	43	ALA
5	R	32	ALA
1	S	145	HIS
1	S	413	ASP
1	T	461	SER
2	W	18	GLY
2	W	149	ARG
2	W	391	LEU
1	A	97	VAL
5	I	21	ILE
1	J	319	GLY
2	M	461	GLY
1	S	377	GLY
2	V	433	ARG
1	T	362	GLY
2	V	453	PRO
2	W	221	GLN
3	Y	153	VAL
1	B	377	GLY
1	C	97	VAL
2	D	102	PRO
2	N	461	GLY
2	E	423	VAL
1	J	97	VAL
1	K	70	PRO
1	S	336	VAL
1	T	116	PRO
2	W	44	GLY
2	W	279	VAL
1	B	363	ILE
2	V	83	ILE
3	Y	132	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/412 (95%)	386 (99%)	4 (1%)	68	75
1	B	386/412 (94%)	384 (100%)	2 (0%)	81	80
1	C	390/412 (95%)	387 (99%)	3 (1%)	73	77
1	J	388/412 (94%)	386 (100%)	2 (0%)	81	80
1	K	384/412 (93%)	378 (98%)	6 (2%)	55	69
1	L	390/412 (95%)	384 (98%)	6 (2%)	57	70
1	S	388/412 (94%)	385 (99%)	3 (1%)	73	77
1	T	382/412 (93%)	375 (98%)	7 (2%)	51	68
1	U	382/412 (93%)	378 (99%)	4 (1%)	68	75
2	D	377/390 (97%)	370 (98%)	7 (2%)	50	67
2	E	378/390 (97%)	375 (99%)	3 (1%)	73	77
2	F	381/390 (98%)	374 (98%)	7 (2%)	51	68
2	M	378/390 (97%)	372 (98%)	6 (2%)	55	69
2	N	377/390 (97%)	368 (98%)	9 (2%)	43	63
2	O	378/390 (97%)	373 (99%)	5 (1%)	61	72
2	V	370/390 (95%)	364 (98%)	6 (2%)	55	69
2	W	378/390 (97%)	375 (99%)	3 (1%)	73	77
2	X	379/390 (97%)	376 (99%)	3 (1%)	73	77
3	G	228/236 (97%)	226 (99%)	2 (1%)	70	76
3	P	188/236 (80%)	180 (96%)	8 (4%)	26	52
3	Y	157/236 (66%)	153 (98%)	4 (2%)	42	63
4	H	92/112 (82%)	89 (97%)	3 (3%)	33	58
4	Q	1/112 (1%)	1 (100%)	0	100	100
5	I	29/48 (60%)	29 (100%)	0	100	100
All	All	7571/8198 (92%)	7468 (99%)	103 (1%)	59	71

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	88	GLU
1	A	97	VAL
1	A	369	VAL
1	B	376	VAL
1	B	418	GLN
1	C	123	ILE
1	C	349	ASP
1	C	387	GLN
2	D	7	THR
2	D	77	LEU
2	D	96	ILE
2	D	117	ILE
2	D	133	ILE
2	D	252	LEU
2	D	354	LYS
2	E	98	VAL
2	E	117	ILE
2	E	152	LYS
2	F	17	ILE
2	F	41	THR
2	F	97	ASN
2	F	117	ILE
2	F	209	LEU
2	F	252	LEU
2	F	258	ILE
3	G	13	ILE
3	G	78	THR
4	H	39	ILE
4	H	102	LYS
4	H	105	LEU
1	J	429	LEU
1	J	495	LEU
1	K	67	ASN
1	K	123	ILE
1	K	132	GLN
1	K	268	ILE
1	K	349	ASP
1	K	376	VAL
1	L	81	ASP
1	L	123	ILE
1	L	268	ILE
1	L	340	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	351	GLN
1	L	387	GLN
2	M	117	ILE
2	M	133	ILE
2	M	200	GLU
2	M	252	LEU
2	M	258	ILE
2	M	459	MET
2	N	17	ILE
2	N	27	GLN
2	N	103	ILE
2	N	117	ILE
2	N	152	LYS
2	N	325	THR
2	N	387	ILE
2	N	463	ILE
2	N	472	LYS
2	O	47	VAL
2	O	117	ILE
2	O	215	VAL
2	O	252	LEU
2	O	293	GLN
3	P	2	THR
3	P	78	THR
3	P	80	ASP
3	P	87	ILE
3	P	131	ASN
3	P	159	TYR
3	P	213	THR
3	P	237	MET
1	S	413	ASP
1	S	441	GLU
1	S	444	VAL
1	T	123	ILE
1	T	268	ILE
1	T	340	ILE
1	T	349	ASP
1	T	418	GLN
1	T	428	GLN
1	T	478	HIS
1	U	159	VAL
1	U	329	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	387	GLN
1	U	441	GLU
2	V	39	ILE
2	V	117	ILE
2	V	252	LEU
2	V	404	VAL
2	V	452	ILE
2	V	463	ILE
2	W	152	LYS
2	W	258	ILE
2	W	387	ILE
2	X	41	THR
2	X	252	LEU
2	X	258	ILE
3	Y	39	ILE
3	Y	124	ASN
3	Y	133	ILE
3	Y	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	454	HIS
1	B	48	ASN
1	B	225	HIS
1	B	304	HIS
1	B	343	ASN
1	B	428	GLN
1	B	454	HIS
1	B	478	HIS
1	B	479	ASN
1	C	48	ASN
1	C	192	ASN
1	C	368	ASN
1	C	381	GLN
1	C	434	GLN
2	D	52	GLN
2	D	118	HIS
2	D	367	HIS
2	D	375	GLN
2	E	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	168	GLN
2	E	263	GLN
2	E	293	GLN
2	E	308	GLN
2	E	328	HIS
2	F	52	GLN
2	F	97	ASN
2	F	168	GLN
2	F	365	GLN
2	F	399	GLN
3	G	15	ASN
3	G	100	ASN
3	G	117	GLN
3	G	122	HIS
3	G	235	ASN
3	G	249	ASN
4	H	31	ASN
4	H	45	HIS
4	H	64	ASN
4	H	126	GLN
5	I	15	ASN
5	I	30	GLN
5	I	46	GLN
1	K	26	ASN
1	K	50	GLN
1	K	67	ASN
1	K	132	GLN
1	K	145	HIS
1	K	210	GLN
1	K	217	GLN
1	K	220	GLN
1	K	454	HIS
1	L	28	ASN
1	L	50	GLN
1	L	304	HIS
1	L	368	ASN
1	L	407	GLN
2	M	53	HIS
2	M	118	HIS
2	M	249	GLN
2	M	367	HIS
2	N	24	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	27	GLN
2	N	53	HIS
2	N	263	GLN
2	N	385	GLN
2	O	118	HIS
2	O	168	GLN
2	O	172	ASN
2	O	328	HIS
2	O	365	GLN
2	O	379	GLN
2	O	399	GLN
3	P	88	HIS
3	P	117	GLN
3	P	122	HIS
3	P	131	ASN
3	P	216	ASN
3	P	224	GLN
1	S	165	GLN
1	S	224	GLN
1	S	304	HIS
1	S	368	ASN
1	T	47	ASN
1	T	48	ASN
1	T	210	GLN
1	T	225	HIS
1	T	304	HIS
1	T	428	GLN
1	T	434	GLN
1	T	454	HIS
1	U	50	GLN
1	U	224	GLN
1	U	381	GLN
1	U	452	ASN
2	V	168	GLN
2	V	293	GLN
2	V	308	GLN
2	V	367	HIS
2	V	375	GLN
2	V	411	GLN
2	V	416	GLN
2	W	35	ASN
2	W	118	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	W	168	GLN
2	W	172	ASN
2	W	328	HIS
2	W	379	GLN
2	W	385	GLN
2	X	27	GLN
2	X	52	GLN
2	X	178	HIS
2	X	195	ASN
2	X	208	ASN
2	X	365	GLN
2	X	379	GLN
3	Y	124	ASN
3	Y	131	ASN
3	Y	216	ASN
3	Y	224	GLN
3	Y	243	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	B	602	-	4,4,4	0.98	0	6,6,6	0.45	0
6	PO4	N	610	-	4,4,4	0.97	0	6,6,6	0.45	0
6	PO4	K	607	-	4,4,4	1.03	0	6,6,6	0.45	0
6	PO4	O	611	-	4,4,4	0.99	0	6,6,6	0.42	0
6	PO4	C	603	-	4,4,4	1.00	0	6,6,6	0.48	0
6	PO4	J	606	-	4,4,4	0.99	0	6,6,6	0.48	0
6	PO4	X	615	-	4,4,4	0.97	0	6,6,6	0.50	0
6	PO4	T	613	-	4,4,4	0.95	0	6,6,6	0.46	0
6	PO4	A	601	-	4,4,4	0.97	0	6,6,6	0.44	0
6	PO4	D	604	-	4,4,4	0.91	0	6,6,6	0.49	0
6	PO4	S	612	-	4,4,4	0.97	0	6,6,6	0.49	0
6	PO4	L	608	-	4,4,4	1.03	0	6,6,6	0.46	0
6	PO4	F	605	-	4,4,4	1.04	0	6,6,6	0.45	0
6	PO4	M	609	-	4,4,4	0.98	0	6,6,6	0.49	0
6	PO4	U	614	-	4,4,4	1.00	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	484/510 (94%)	-0.33	1 (0%) 91 79	70, 104, 128, 143	0
1	B	479/510 (93%)	-0.34	0 100 100	73, 113, 139, 148	0
1	C	484/510 (94%)	-0.35	0 100 100	78, 108, 133, 145	0
1	J	481/510 (94%)	-0.31	0 100 100	83, 111, 134, 143	0
1	K	484/510 (94%)	-0.32	0 100 100	76, 112, 139, 147	0
1	L	484/510 (94%)	-0.39	0 100 100	70, 94, 126, 144	0
1	S	481/510 (94%)	-0.38	0 100 100	81, 112, 130, 141	0
1	T	473/510 (92%)	-0.22	0 100 100	99, 123, 140, 147	0
1	U	477/510 (93%)	-0.24	0 100 100	102, 123, 134, 141	0
2	D	466/484 (96%)	-0.22	1 (0%) 91 79	85, 116, 138, 145	0
2	E	468/484 (96%)	-0.34	0 100 100	68, 111, 136, 149	0
2	F	471/484 (97%)	-0.31	0 100 100	73, 109, 128, 144	0
2	M	469/484 (96%)	-0.36	0 100 100	80, 105, 128, 149	0
2	N	466/484 (96%)	-0.37	0 100 100	71, 113, 132, 143	0
2	O	469/484 (96%)	-0.42	0 100 100	70, 106, 125, 134	0
2	V	455/484 (94%)	0.06	7 (1%) 72 44	99, 129, 146, 154	0
2	W	466/484 (96%)	-0.43	0 100 100	89, 113, 129, 142	0
2	X	469/484 (96%)	-0.31	0 100 100	93, 118, 135, 147	0
3	G	268/278 (96%)	-0.28	0 100 100	72, 110, 128, 138	0
3	P	235/278 (84%)	-0.13	3 (1%) 75 47	65, 127, 143, 150	0
3	Y	187/278 (67%)	-0.26	1 (0%) 87 66	96, 125, 139, 146	0
4	H	116/138 (84%)	-0.13	0 100 100	93, 114, 137, 146	0
4	Q	68/138 (49%)	-0.14	0 100 100	98, 127, 135, 142	0
4	Z	11/138 (7%)	-0.30	0 100 100	129, 134, 140, 142	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	25/61 (40%)	-0.07	0 100 100	112, 131, 137, 138	0
5	I	46/61 (75%)	-0.27	0 100 100	101, 115, 125, 130	0
5	R	25/61 (40%)	-0.23	0 100 100	118, 131, 139, 144	0
All	All	9507/10377 (91%)	-0.30	13 (0%) 92 85	65, 114, 137, 154	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	141	VAL	3.2
2	V	440	SER	3.1
1	A	389	ALA	2.8
3	P	136	ASP	2.5
2	D	387	ILE	2.3
2	V	374	VAL	2.3
3	P	48	GLU	2.2
3	P	118	LEU	2.2
2	V	388	ILE	2.1
2	V	439	ALA	2.1
3	Y	154	MET	2.1
2	V	444	VAL	2.1
2	V	387	ILE	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, 95th 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
6	PO4	D	604	5/5	0.80	0.11	134,136,139,154	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	F	605	5/5	0.87	0.10	92,93,98,101	0
6	PO4	U	614	5/5	0.90	0.07	96,96,100,113	0
6	PO4	A	601	5/5	0.92	0.05	89,90,97,113	0
6	PO4	T	613	5/5	0.93	0.05	101,105,109,116	0
6	PO4	S	612	5/5	0.93	0.04	106,107,112,116	0
6	PO4	X	615	5/5	0.93	0.07	107,125,125,126	0
6	PO4	C	603	5/5	0.94	0.05	86,89,99,99	0
6	PO4	J	606	5/5	0.95	0.06	90,91,94,97	0
6	PO4	O	611	5/5	0.95	0.07	94,96,102,107	0
6	PO4	L	608	5/5	0.96	0.04	82,82,87,96	0
6	PO4	B	602	5/5	0.96	0.06	95,103,112,112	0
6	PO4	K	607	5/5	0.96	0.06	85,94,97,101	0
6	PO4	N	610	5/5	0.97	0.04	89,100,104,116	0
6	PO4	M	609	5/5	0.97	0.06	92,97,106,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.