



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:51 AM UTC

PDB ID : 4QSL / pdb_00004qsl
Title : Crystal Structure of Listeria Monocytogenes Pyruvate Carboxylase
Authors : Choi, P.H.; Tong, L.
Deposited on : 2014-07-04
Resolution : 3.28 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
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

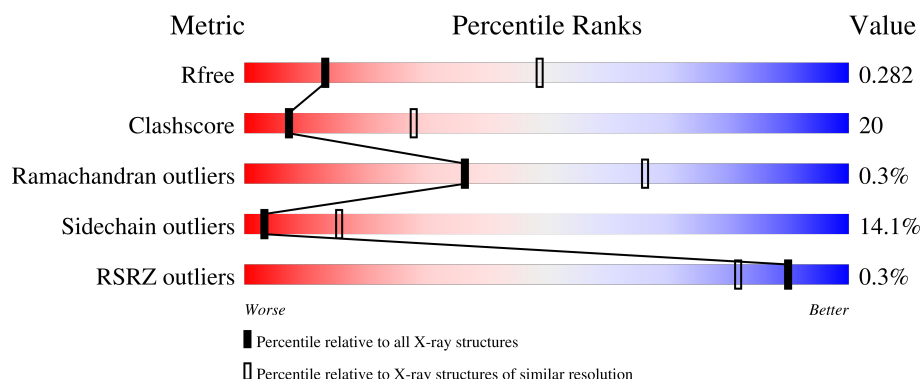
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	1146	
1	B	1146	
1	C	1146	
1	D	1146	
1	E	1146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1146	 57% 29% 5% 8%
1	G	1146	 52% 26% 5% 18%
1	H	1146	 56% 29% 5% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 60495 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.

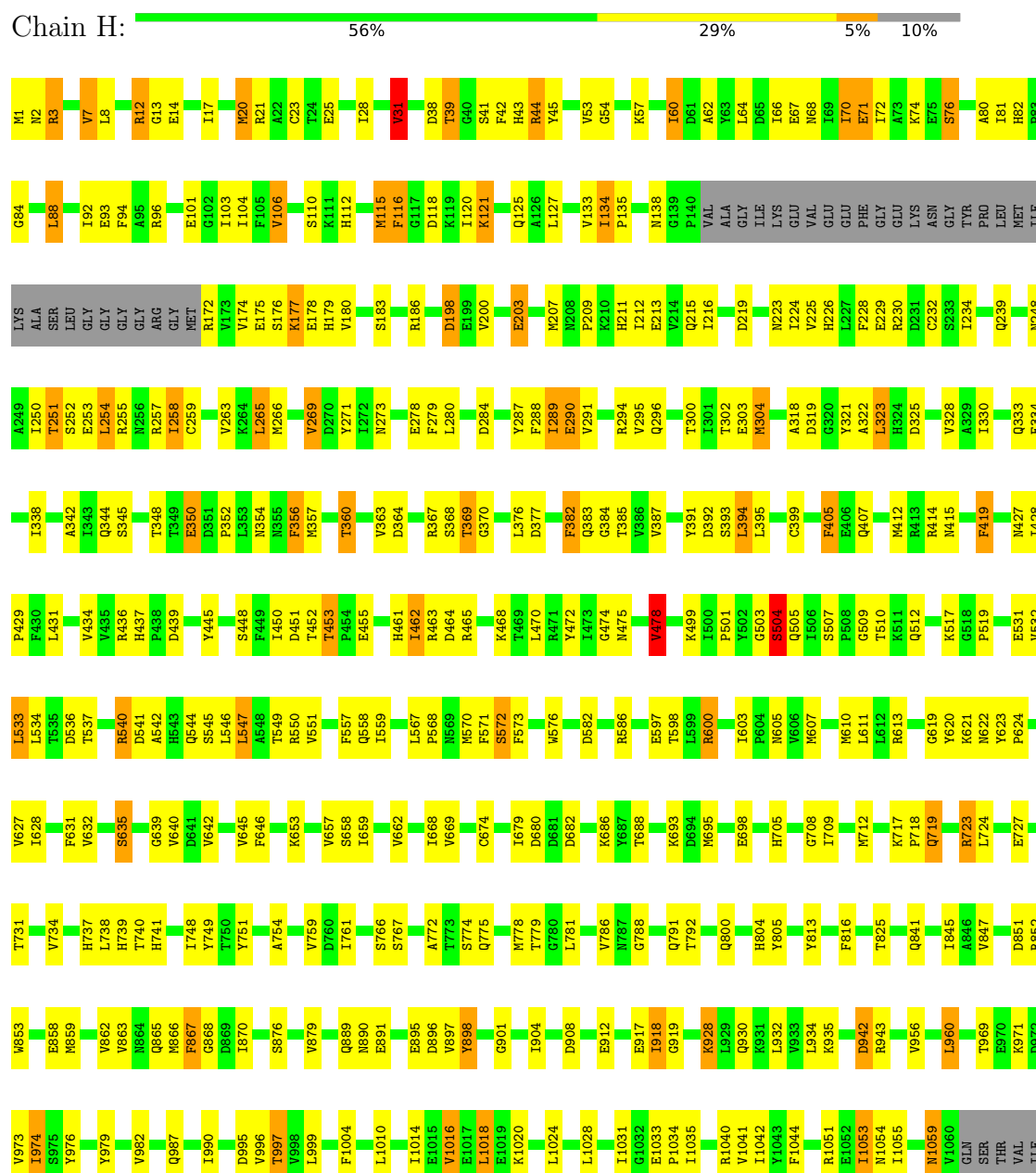
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	F	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	E	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	G	942	Total	C	N	O	S	0	0	0
			6909	4338	1202	1341	28			
1	D	1029	Total	C	N	O	S	0	0	0
			7881	4992	1351	1504	34			
1	A	1052	Total	C	N	O	S	0	0	0
			7969	5063	1353	1518	35			
1	B	1031	Total	C	N	O	S	0	0	0
			7492	4716	1292	1459	25			
1	C	941	Total	C	N	O	S	0	0	0
			6902	4333	1201	1340	28			

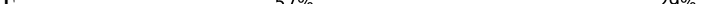
3 Residue-property plots

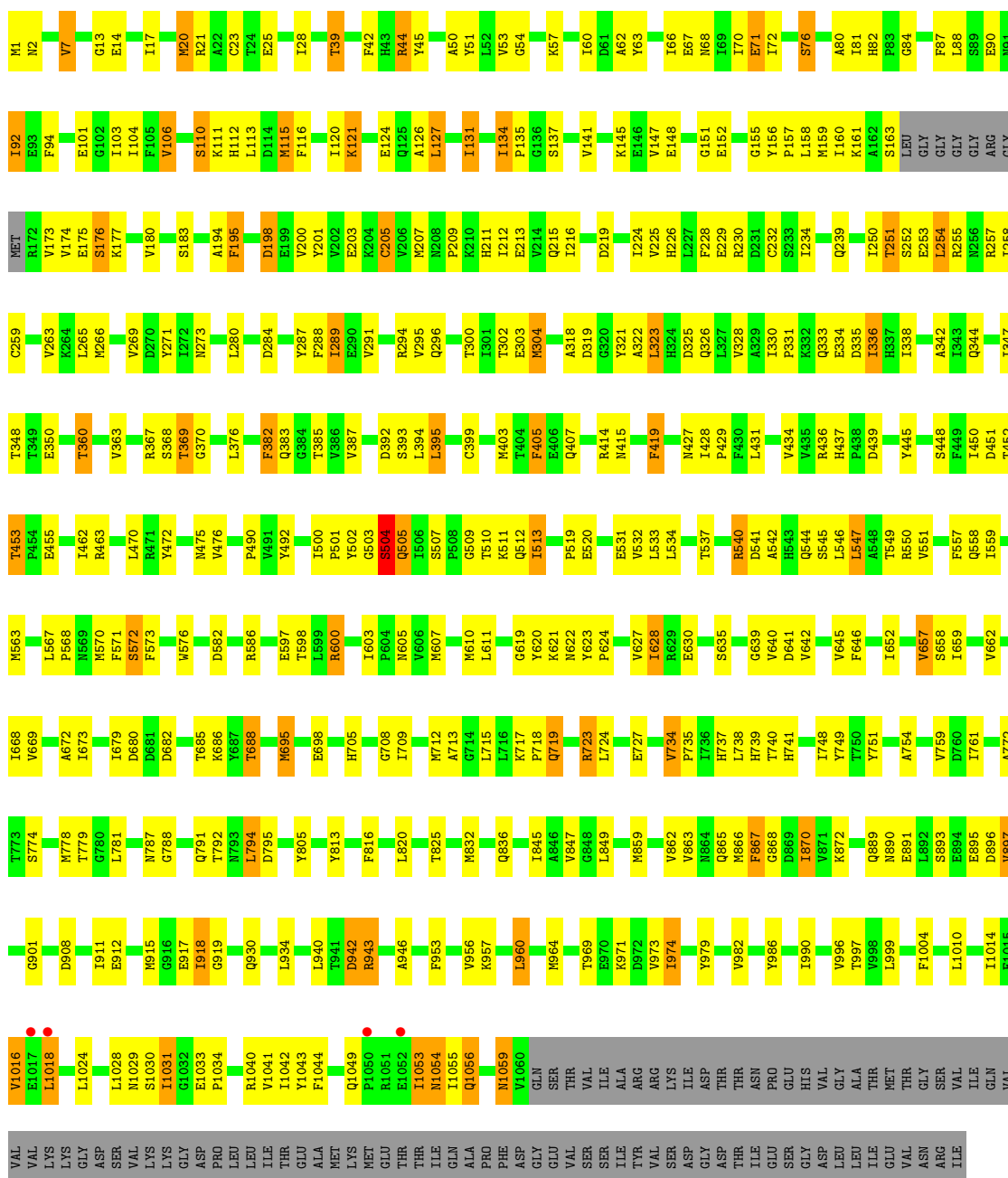
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



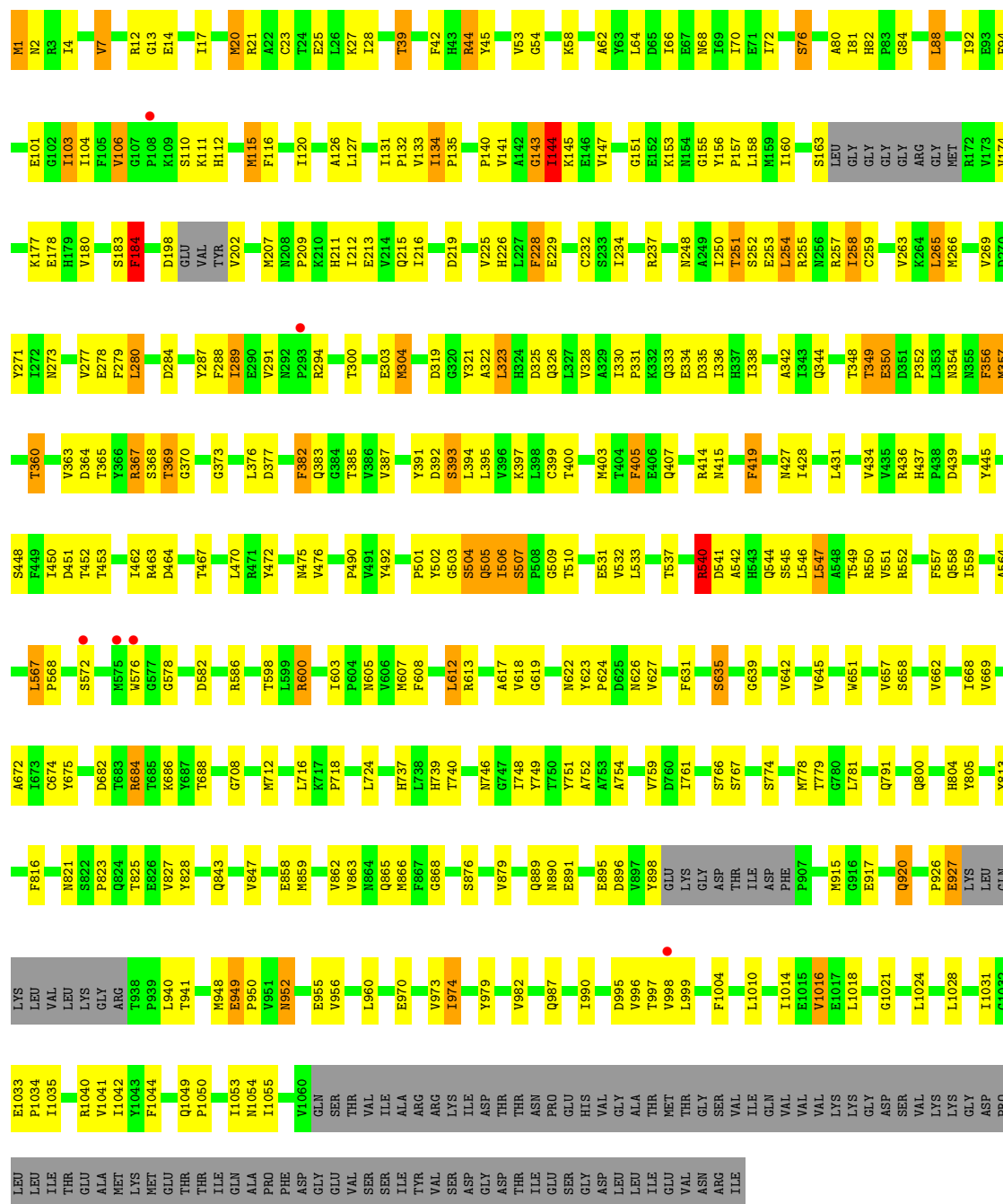
- Molecule 1: Pyruvate carboxylase

Chain F:  57% 29% 5% 8%



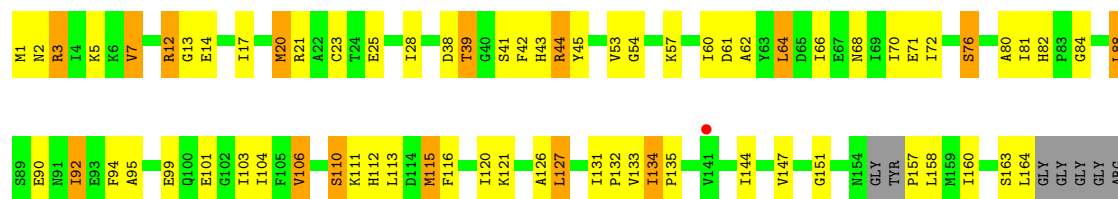
- Molecule 1: Pyruvate carboxylase

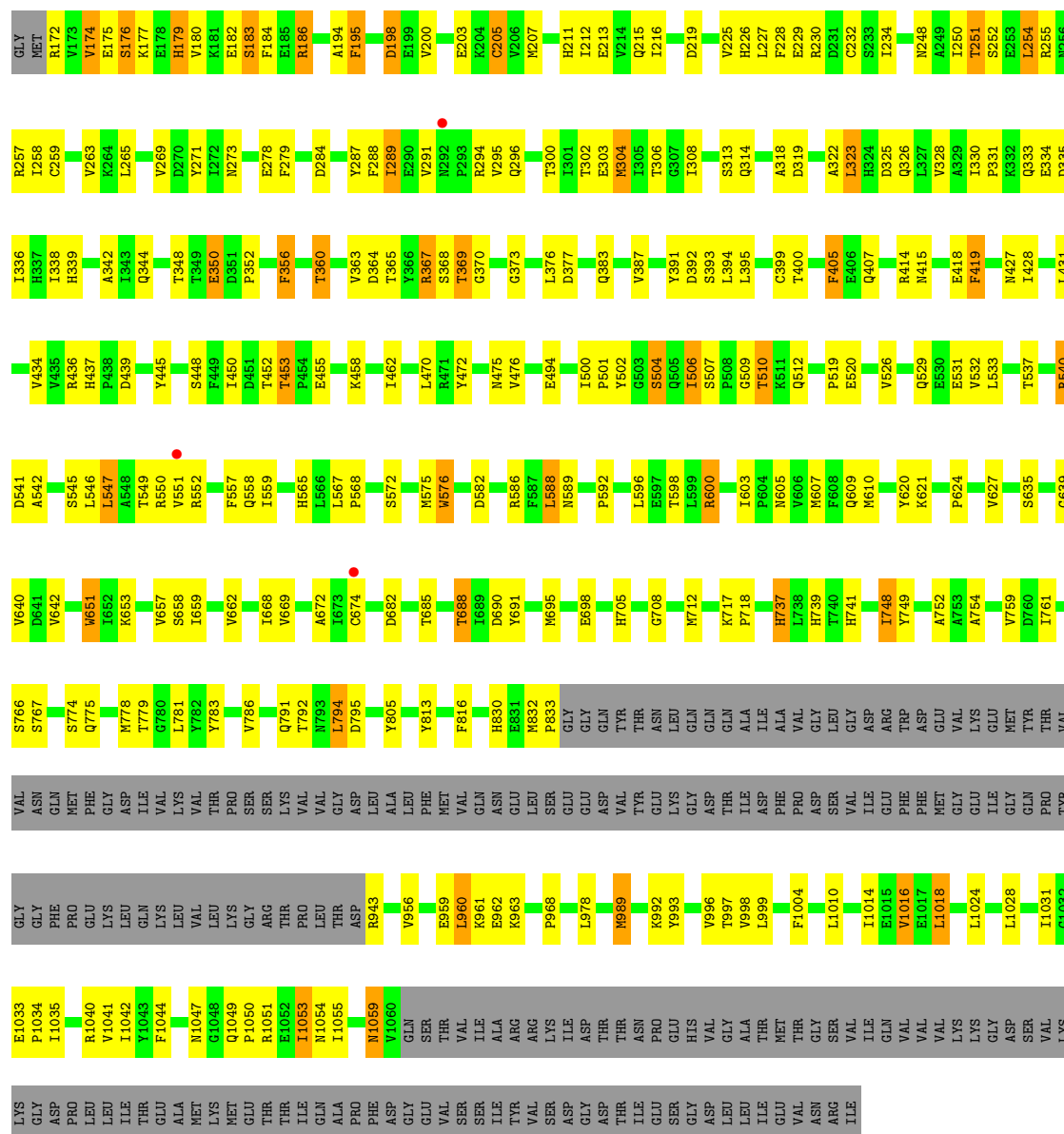




• Molecule 1: Pyruvate carboxylase

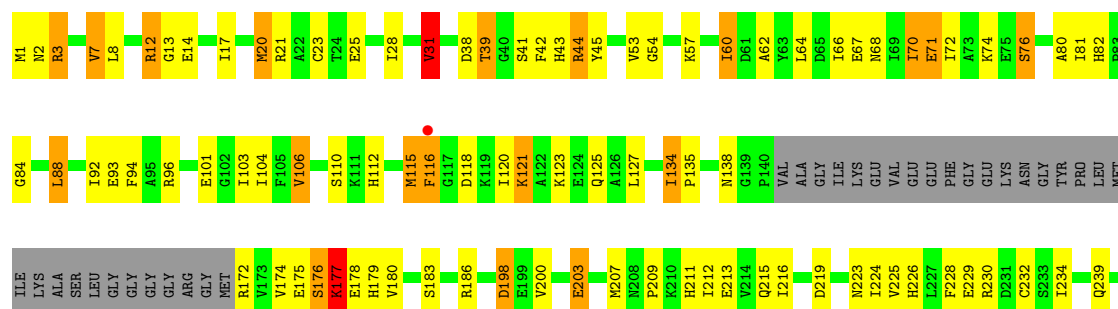
Chain G: 52% 26% 5% 18%





• Molecule 1: Pyruvate carboxylase

Chain D: 56% 29% 5% 10%

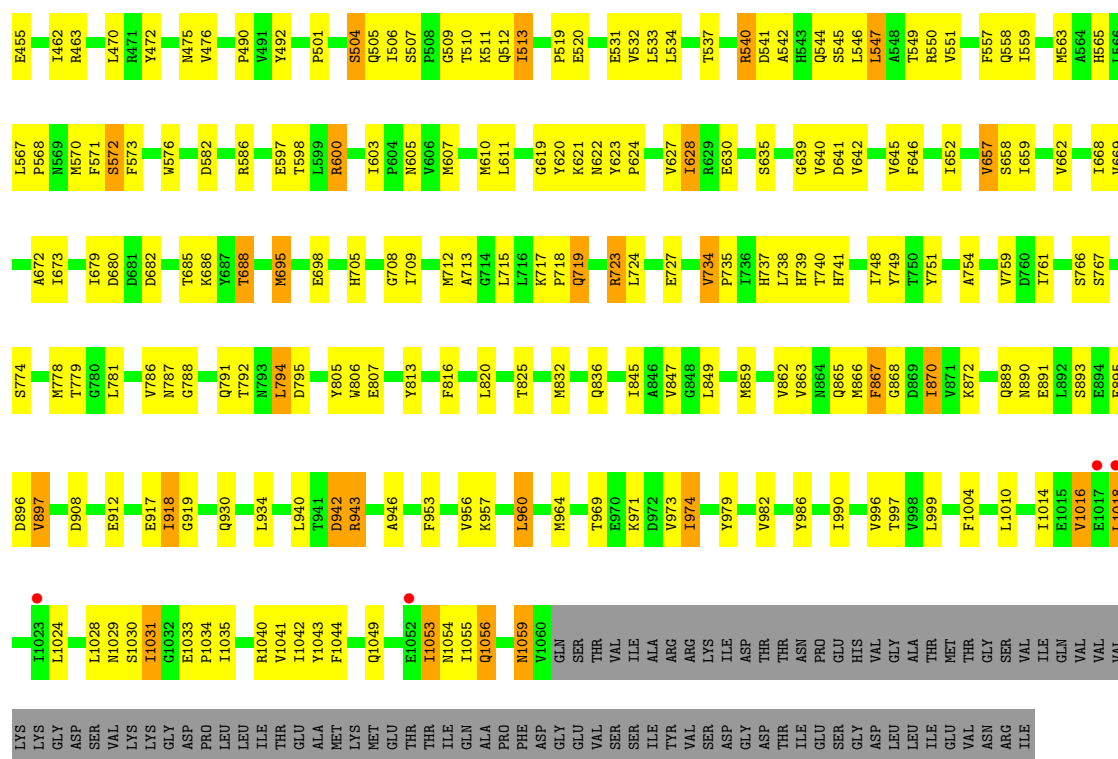


ALA	K971	D851	L724	M622	E520	D335	N248
ARG	D972	R852		Y623			A249
ARG	V973	W853	E727	P624	E531	I336	I250
LYS	I974				V532	I428	T251
ASP	S975	E858	T731	V627	L633	F430	S252
ASP	Y976	M859		I628	L534	H339	E253
THR			V734		T535		L254
THR	Y979	V862		F631	D536	I343	R255
ASN	V982	H863	H737	V632	T537	Q344	I256
GLU		Q864	L738			S345	R257
GLU		Q865	H739			R436	T258
HIS	Q987	M866	T740		R540	H437	C259
VAL		F867	H741		D541	F438	
VAL	I990	C868		G639	A542	D439	
LEU		D869	I748	V640	H543	T349	V263
ALA		I870	V749	V642	Q544	D351	R264
THR	D995		T750		S545	P352	L265
GLU	V996	S876	Y751	V645	L547	I553	M266
VAL	T997			F646	A548	N355	V269
GLY	V998	V879	A754	K653	T549	D451	D270
ASN	L999				R550	M357	Y271
ARG		VAL			V551	T452	I272
ILE	F1004	Q889	V759	V657	F557	T453	N273
GLN	L1010	N890	D760	S658	Q558	P454	
VAL		E891	I761	I659	I559	E455	
VAL							E278
VAL	I1014	E895	S766	V662		H461	F279
LYS	E1015	D896				I462	L280
LYS	V1016	V897			L567	R367	
GLY	E1017	Y898	S774	I668	P568	D464	D284
ASP	L1018		Q775	V669	N569	R465	
SER	E1019	G901			M570	G370	
VAL	K1020	I904	M778	C674	F571	K468	Y287
LYS			T779	I679	S572	T469	F288
LYS	L1024	D908	G780	D680	F573	L376	I289
GLY			L781	D681	W576	D377	E290
ASP	L1028	E912	V786	D682		R471	V291
PRO						Y472	
LEU	I1031	E917	H787	K686	D582	I473	R294
LEU	G1032		G788		G474	G384	V295
ILE	E1033	I918		Y687	R586	M475	Q296
THR	P1034	G919	Q791	T688			
GLU	I1035		T792			V478	T300
ALA		K928			E597		
MET	R1040	L929	Q800	K693	T598	K499	E303
LYS	V1041	Q930		D694	L599	I500	M304
MET	I1042	K931	H804	M695	R600	P501	
GLU	Y1043	L932	Y805	E698		Y502	A318
THR	F1044	V933			I603	G503	D319
THR		L934	Y813	H705	P604	S504	G320
THR		K935			N605	Q505	Y321
ILE	I1053				V606	I506	
GLN	N1054		F816	G708	M607	S507	A322
ALA	I1055			I709		P508	L323
PRO		D942	T825		M610	H324	
PHE		R943			L611	G509	D325
ASP	N1059	V956	Q841	W712		T510	
GLN	V1060			K717	L612	R511	V328
GLY	THR	L960	I845	P718	R613	Q512	A329
GLU							L330
VAL	THR		E846	Q719	G619	K517	
SER	VAL	T969	V847		Y620	R412	Q333
SER	THR	E926			K291	N415	E334
THR	THR						

• Molecule 1: Pyruvate carboxylase

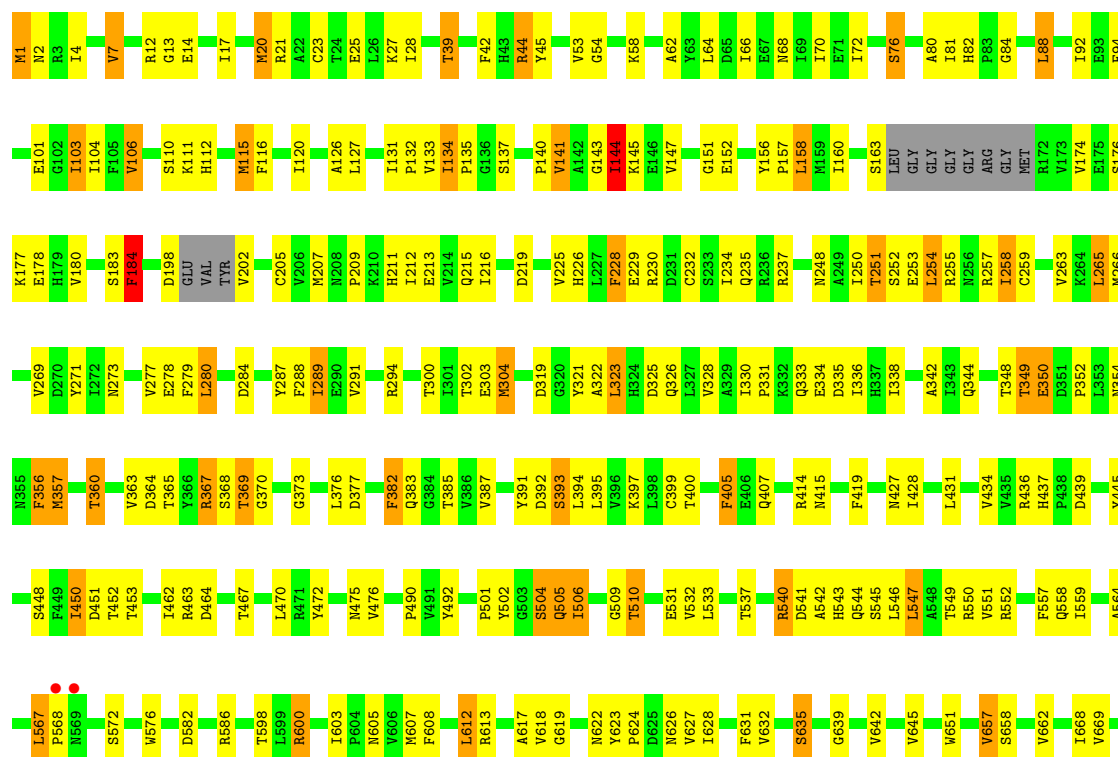
Chain A:  58% 29% 5% 8%

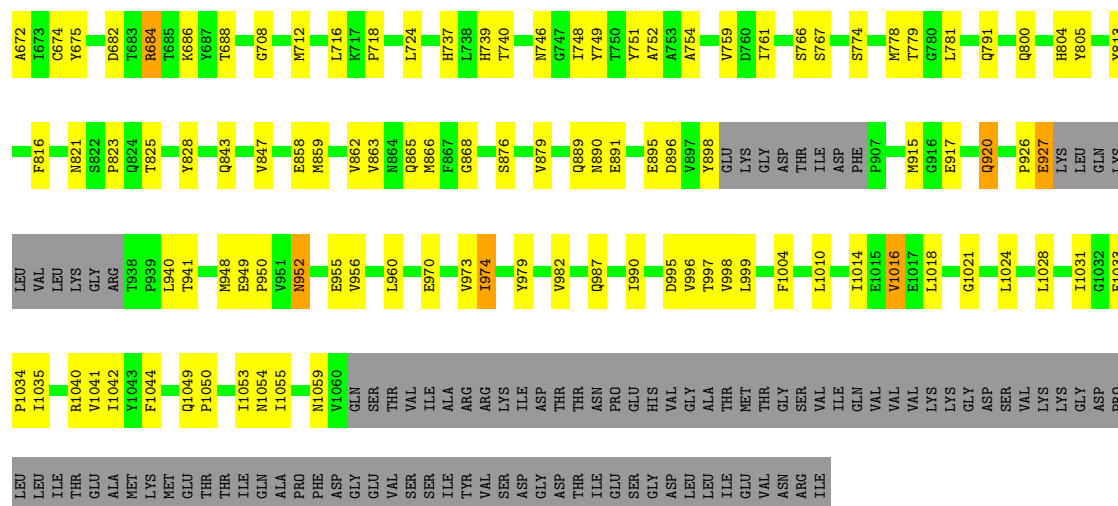
																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							</
--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	----



- Molecule 1: Pyruvate carboxylase

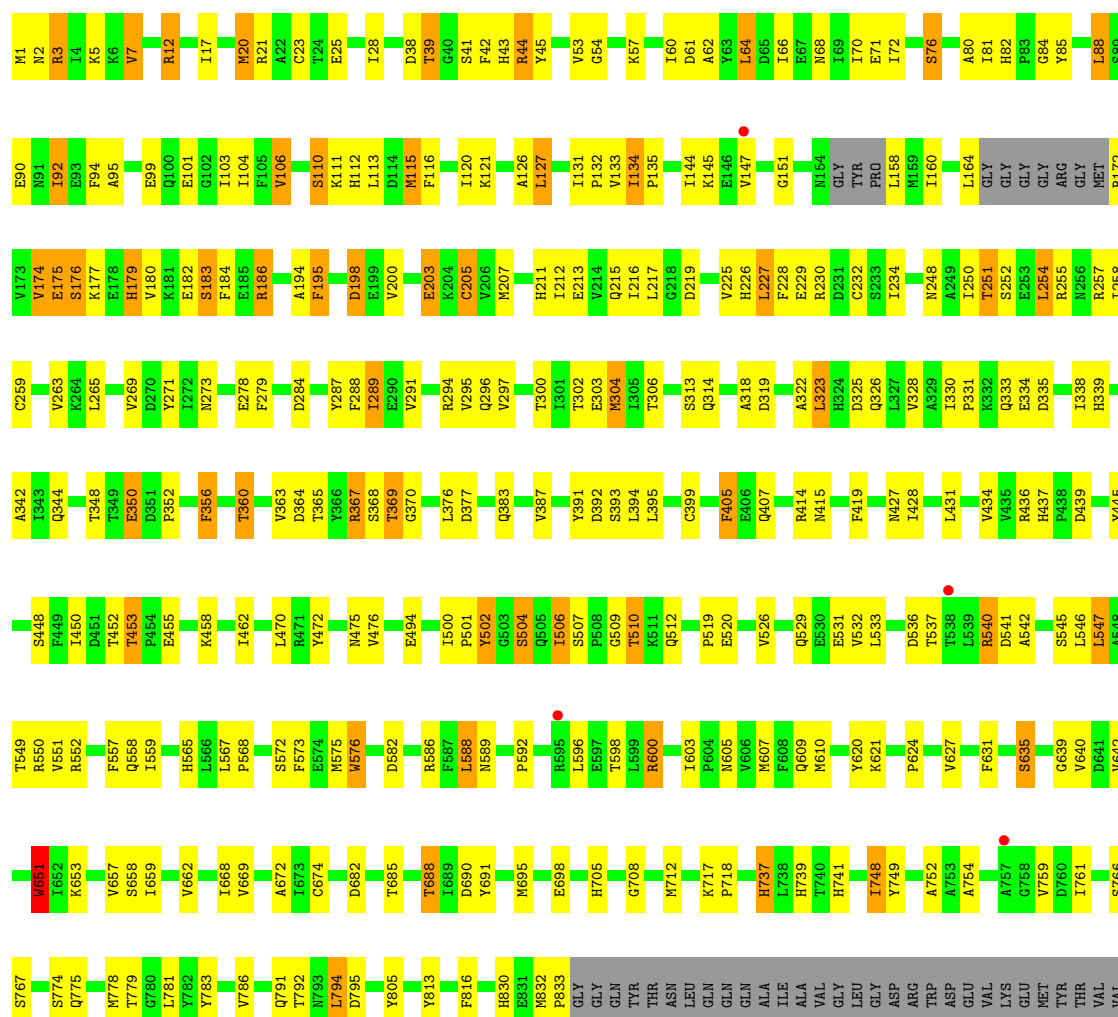
Chain B: 58% 27% 0 10%





• Molecule 1: Pyruvate carboxylase

Chain C: 52% 25% 5% 18%



ASN	GLN	PHE	GLY	ASP	ILE	VAL	LYS	THR	PRO	GLY	SER	SER	LYS	VAL	GLY	ASP	LEU	ALA	LEU	PHE	MET	VAL	GLN	ASN	GLU	LEU	SER	GLU	ASP	VAL	TYR	GLU	LYS	GLY	ASP	THR	ILE	PHE	PHE	MET	GLY	GLU	ILE	GLY	GLN	PRO	TYR	GLY					
I1031	G1032	E1033	P1034	I1035	R1040	V1041	I1042	Y1043	F1044	M1047	G1048	Q1049	P1050	R1051	E1052	I1053	N1054	I1055	N1059	V1060	GLN	SER	THR	VAL	ILE	ALA	ARG	LYS	ILE	ASP	THR	THR	ASN	PRO	GLU	HIS	VAL	GLY	ALA	THR	MET	GLY	SER	VAL	ILE	GLN	VAL	VAL	LYS	LYS	GLY	ASP	SER
VAL	LYS	LYS	GLY	ASP	PRO	LEU	LEU	ILE	THR	GLU	ALA	MET	LYS	MET	GLU	THR	THR	ILE	GLN	ALA	PRO	PHE	ASP	GLY	GLU	VAL	SER	SER	VAL	GLY	ASP	ASP	THR	THR	ILE	GLU	SER	GLY	ASP	LEU	LEU	ILE	GLU	VAL	ASN	ARG	ILE						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 132.62Å 257.54Å 86.65° 79.84° 70.07°	Depositor
Resolution (Å)	47.16 – 3.28 47.16 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.16-3.28) 88.4 (47.16-3.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.284 0.235 , 0.282	Depositor DCC
R_{free} test set	7628 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 138.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.398 for h,h-k,h-l 0.007 for -h,-h+k,-l 0.007 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60495	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

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	0.64	0/8136	0.98	9/11083 (0.1%)
1	B	0.64	0/7639	0.99	19/10443 (0.2%)
1	C	0.66	0/7031	0.97	7/9586 (0.1%)
1	D	0.66	0/8042	1.00	19/10933 (0.2%)
1	E	0.65	0/7639	0.99	19/10443 (0.2%)
1	F	0.64	0/8136	0.98	11/11083 (0.1%)
1	G	0.67	0/7039	0.97	8/9597 (0.1%)
1	H	0.68	1/8042 (0.0%)	1.00	16/10933 (0.1%)
All	All	0.65	1/61704 (0.0%)	0.99	108/84101 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	F	0	1
1	H	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	464	ASP	C-O	-5.00	1.18	1.23

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	478	VAL	CB-CA-C	-12.99	96.61	111.55
1	D	478	VAL	CB-CA-C	-12.14	97.59	111.55
1	E	143	GLY	N-CA-C	9.16	125.77	110.56
1	B	184	PHE	N-CA-CB	8.48	122.31	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	PHE	N-CA-CB	8.47	122.29	110.01
1	H	686	LYS	N-CA-C	8.03	119.66	111.07
1	E	144	ILE	N-CA-C	7.97	121.02	111.05
1	A	686	LYS	N-CA-C	7.85	119.47	111.07
1	B	144	ILE	N-CA-C	7.65	120.62	111.05
1	B	686	LYS	N-CA-C	7.60	119.21	111.07
1	F	686	LYS	N-CA-C	7.59	119.20	111.07
1	E	686	LYS	N-CA-C	7.59	119.19	111.07
1	D	686	LYS	N-CA-C	7.53	119.12	111.07
1	D	505	GLN	N-CA-C	7.40	119.56	108.31
1	D	897	VAL	CB-CA-C	-7.34	102.57	111.97
1	H	897	VAL	CB-CA-C	-7.30	102.62	111.97
1	E	144	ILE	CB-CA-C	-7.23	100.95	112.16
1	A	1029	ASN	N-CA-CB	7.08	121.16	110.19
1	F	1029	ASN	N-CA-CB	7.06	121.13	110.19
1	H	505	GLN	N-CA-C	7.04	119.02	108.31
1	H	31	VAL	CB-CA-C	-6.96	99.79	110.50
1	B	450	ILE	CA-CB-CG1	6.93	122.19	110.40
1	D	31	VAL	CB-CA-C	-6.76	100.09	110.50
1	D	115	MET	CA-CB-CG	6.50	127.09	114.10
1	H	115	MET	CA-CB-CG	6.47	127.04	114.10
1	H	956	VAL	CB-CA-C	-6.46	103.55	112.02
1	C	956	VAL	CB-CA-C	6.46	120.89	112.24
1	G	956	VAL	CB-CA-C	6.44	120.87	112.24
1	B	152	GLU	N-CA-C	6.40	117.92	111.07
1	B	156	TYR	CA-C-N	-6.38	112.58	119.98
1	B	156	TYR	C-N-CA	-6.38	112.58	119.98
1	D	974	ILE	N-CA-CB	6.32	117.94	110.55
1	H	974	ILE	N-CA-CB	6.29	117.91	110.55
1	F	974	ILE	N-CA-CB	6.28	117.90	110.55
1	E	2	ASN	N-CA-C	6.28	124.17	110.80
1	D	956	VAL	CB-CA-C	-6.25	103.84	112.02
1	H	115	MET	N-CA-CB	-6.24	100.61	110.22
1	E	974	ILE	N-CA-CB	6.21	117.81	110.55
1	F	1056	GLN	N-CA-CB	6.20	119.97	109.87
1	D	115	MET	N-CA-CB	-6.19	100.68	110.22
1	B	141	VAL	N-CA-C	6.19	116.16	107.37
1	A	1056	GLN	N-CA-CB	6.18	119.94	109.87
1	B	144	ILE	CB-CA-C	-6.17	102.59	112.16
1	B	450	ILE	N-CA-C	-6.17	103.33	110.05
1	B	974	ILE	N-CA-CB	6.16	117.75	110.55
1	A	974	ILE	N-CA-CB	6.15	117.75	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	956	VAL	CB-CA-C	-6.08	104.06	112.02
1	F	155	GLY	N-CA-C	6.07	120.00	110.96
1	G	651	TRP	CB-CA-C	6.07	120.14	110.19
1	C	690	ASP	N-CA-CB	6.06	118.80	110.01
1	A	956	VAL	CB-CA-C	-6.00	104.15	112.02
1	G	690	ASP	N-CA-CB	6.00	118.71	110.01
1	C	651	TRP	CB-CA-C	5.98	120.00	110.19
1	H	478	VAL	CA-CB-CG2	5.92	120.46	110.40
1	B	2	ASN	N-CA-C	5.89	123.36	110.80
1	E	956	VAL	CB-CA-C	-5.86	104.34	112.02
1	A	155	GLY	N-CA-C	5.83	119.83	110.90
1	D	478	VAL	CA-CB-CG2	5.80	120.26	110.40
1	B	956	VAL	CB-CA-C	-5.79	104.44	112.02
1	D	394	LEU	N-CA-C	5.67	117.92	109.59
1	F	628	ILE	CB-CG1-CD1	5.66	125.69	113.80
1	E	462	ILE	CB-CA-C	5.66	117.81	110.96
1	B	998	VAL	N-CA-C	5.63	118.12	111.09
1	B	336	ILE	CB-CA-C	-5.59	104.54	111.08
1	E	336	ILE	CB-CA-C	-5.57	104.56	111.08
1	C	127	LEU	N-CA-CB	5.57	118.40	110.16
1	B	462	ILE	CB-CA-C	5.57	117.69	110.96
1	E	949	GLU	N-CA-C	-5.55	102.65	110.31
1	G	127	LEU	N-CA-CB	5.52	118.34	110.16
1	A	628	ILE	CB-CG1-CD1	5.51	125.38	113.80
1	E	540	ARG	CG-CD-NE	5.50	124.10	112.00
1	E	998	VAL	N-CA-C	5.49	117.95	111.09
1	D	505	GLN	CB-CA-C	-5.49	110.23	116.54
1	C	998	VAL	N-CA-C	5.46	117.92	111.09
1	G	450	ILE	N-CA-C	-5.46	104.10	110.05
1	H	786	VAL	N-CA-C	5.45	116.83	110.62
1	H	505	GLN	CB-CA-C	-5.44	110.28	116.54
1	D	786	VAL	N-CA-C	5.43	116.81	110.62
1	D	462	ILE	CB-CA-C	-5.36	104.44	111.25
1	C	450	ILE	N-CA-C	-5.35	104.22	110.05
1	H	462	ILE	N-CA-CB	5.32	117.44	111.21
1	D	258	ILE	CB-CG1-CD1	-5.32	102.63	113.80
1	B	450	ILE	CB-CA-C	-5.32	105.74	111.59
1	A	786	VAL	N-CA-C	5.31	116.67	110.62
1	D	177	LYS	N-CA-C	5.30	122.10	110.80
1	H	394	LEU	N-CA-C	5.29	117.37	109.59
1	F	336	ILE	CB-CA-C	-5.27	104.92	111.08
1	E	827	VAL	CB-CA-C	-5.24	105.18	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	998	VAL	N-CA-C	5.23	117.63	111.09
1	E	184	PHE	CB-CA-C	-5.22	102.68	110.88
1	H	258	ILE	CB-CG1-CD1	-5.20	102.88	113.80
1	F	901	GLY	N-CA-C	5.19	118.96	112.73
1	E	153	LYS	N-CA-C	5.19	117.02	111.36
1	E	507	SER	CA-C-N	-5.19	114.61	119.85
1	E	507	SER	C-N-CA	-5.19	114.61	119.85
1	G	786	VAL	N-CA-C	5.18	116.53	110.62
1	B	258	ILE	CB-CA-C	-5.17	105.35	111.97
1	D	336	ILE	CB-CA-C	-5.17	105.03	111.08
1	E	258	ILE	CB-CA-C	-5.13	105.41	111.97
1	A	505	GLN	N-CA-C	5.12	116.10	108.31
1	H	772	ALA	CB-CA-C	-5.10	110.68	116.54
1	F	772	ALA	CB-CA-C	-5.08	110.74	116.63
1	F	1054	ASN	N-CA-CB	5.07	118.52	110.16
1	D	462	ILE	N-CA-CB	5.05	117.52	111.31
1	G	336	ILE	CB-CA-C	-5.03	105.19	111.08
1	D	657	VAL	CB-CA-C	-5.02	105.45	111.88
1	B	657	VAL	CB-CA-C	-5.01	105.47	111.88
1	C	786	VAL	N-CA-C	5.00	116.32	110.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	504	SER	Peptide
1	F	504	SER	Peptide
1	H	504	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7969	0	7573	300	0
1	B	7492	0	6807	339	0
1	C	6902	0	6371	301	0
1	D	7881	0	7579	302	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	7492	0	6807	324	0
1	F	7969	0	7573	309	0
1	G	6909	0	6379	296	0
1	H	7881	0	7579	311	0
All	All	60495	0	56668	2401	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 20.

All (2401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:SER:OG	1:D:412:MET:CE	1.67	1.40
1:H:345:SER:OG	1:H:412:MET:CE	1.68	1.39
1:E:280:LEU:HD12	1:E:289:ILE:CG2	1.54	1.37
1:B:280:LEU:HD12	1:B:289:ILE:CG2	1.55	1.37
1:B:279:PHE:N	1:B:289:ILE:HD11	1.37	1.36
1:E:279:PHE:N	1:E:289:ILE:HD11	1.39	1.35
1:E:180:VAL:HG12	1:E:184:PHE:CZ	1.72	1.23
1:E:144:ILE:HG22	1:E:184:PHE:CE2	1.78	1.19
1:B:279:PHE:CA	1:B:289:ILE:HD11	1.71	1.18
1:E:14:GLU:OE2	1:E:397:LYS:CE	1.91	1.17
1:E:279:PHE:CA	1:E:289:ILE:HD11	1.72	1.17
1:D:345:SER:OG	1:D:412:MET:HE1	1.00	1.17
1:B:180:VAL:HG12	1:B:184:PHE:CZ	1.78	1.17
1:H:345:SER:OG	1:H:412:MET:HE1	1.00	1.17
1:B:14:GLU:OE2	1:B:397:LYS:CE	1.91	1.17
1:B:279:PHE:CA	1:B:289:ILE:CD1	2.22	1.15
1:B:612:LEU:HD11	1:B:617:ALA:HA	1.20	1.15
1:E:612:LEU:HD11	1:E:617:ALA:HA	1.20	1.15
1:E:279:PHE:CA	1:E:289:ILE:CD1	2.23	1.14
1:G:960:LEU:HD12	1:G:968:PRO:HG3	1.25	1.13
1:C:960:LEU:HD12	1:C:968:PRO:HG3	1.25	1.13
1:D:254:LEU:HD22	1:D:258:ILE:HD11	1.32	1.11
1:H:254:LEU:HD22	1:H:258:ILE:HD11	1.32	1.11
1:E:280:LEU:HD12	1:E:289:ILE:HG21	1.13	1.10
1:B:280:LEU:HD12	1:B:289:ILE:HG21	1.13	1.10
1:G:61:ASP:HA	1:G:64:LEU:HD12	1.29	1.09
1:H:8:LEU:HA	1:H:31:VAL:HG23	1.23	1.09
1:D:8:LEU:HA	1:D:31:VAL:HG23	1.24	1.09
1:C:61:ASP:HA	1:C:64:LEU:HD12	1.29	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HG22	1:B:184:PHE:CE2	1.87	1.08
1:B:158:LEU:HD13	1:B:174:VAL:HB	1.30	1.07
1:E:279:PHE:C	1:E:289:ILE:CD1	2.29	1.06
1:B:279:PHE:C	1:B:289:ILE:CD1	2.29	1.06
1:B:612:LEU:CD1	1:B:617:ALA:HA	1.86	1.03
1:E:612:LEU:CD1	1:E:617:ALA:HA	1.87	1.03
1:C:164:LEU:HA	1:C:195:PHE:HE1	1.22	1.02
1:E:219:ASP:HB3	1:E:323:LEU:HD23	1.43	1.01
1:A:219:ASP:HB3	1:A:323:LEU:HD23	1.42	1.01
1:B:219:ASP:HB3	1:B:323:LEU:HD23	1.43	1.01
1:E:144:ILE:HG22	1:E:184:PHE:CZ	1.96	1.00
1:F:369:THR:OG1	1:F:415:ASN:ND2	1.94	1.00
1:A:369:THR:OG1	1:A:415:ASN:ND2	1.94	1.00
1:F:219:ASP:HB3	1:F:323:LEU:HD23	1.44	1.00
1:G:219:ASP:HB3	1:G:323:LEU:HD23	1.42	0.99
1:G:576:TRP:HE1	1:G:596:LEU:HB2	1.27	0.99
1:A:156:TYR:O	1:A:176:SER:HB2	1.61	0.99
1:F:126:ALA:O	1:F:131:ILE:CD1	2.10	0.99
1:E:144:ILE:CG2	1:E:184:PHE:CE2	2.44	0.99
1:C:219:ASP:HB3	1:C:323:LEU:HD23	1.43	0.99
1:C:576:TRP:HE1	1:C:596:LEU:HB2	1.28	0.99
1:G:960:LEU:CD1	1:G:968:PRO:HG3	1.91	0.98
1:C:960:LEU:CD1	1:C:968:PRO:HG3	1.91	0.98
1:H:503:GLY:O	1:C:5:LYS:NZ	1.96	0.98
1:E:915:MET:O	1:E:940:LEU:CB	2.11	0.98
1:A:126:ALA:O	1:A:131:ILE:CD1	2.10	0.98
1:E:280:LEU:CD1	1:E:289:ILE:CG2	2.41	0.98
1:B:280:LEU:CD1	1:B:289:ILE:CG2	2.41	0.98
1:G:367:ARG:HH12	1:G:1049:GLN:CB	1.77	0.97
1:H:219:ASP:HB3	1:H:323:LEU:HD23	1.43	0.97
1:D:369:THR:OG1	1:D:415:ASN:ND2	1.96	0.97
1:C:369:THR:OG1	1:C:415:ASN:ND2	1.98	0.97
1:G:369:THR:OG1	1:G:415:ASN:ND2	1.98	0.97
1:B:158:LEU:HD12	1:B:174:VAL:O	1.64	0.97
1:D:219:ASP:HB3	1:D:323:LEU:HD23	1.44	0.96
1:E:369:THR:OG1	1:E:415:ASN:ND2	1.99	0.96
1:B:369:THR:OG1	1:B:415:ASN:ND2	1.99	0.96
1:H:369:THR:OG1	1:H:415:ASN:ND2	1.98	0.96
1:F:126:ALA:O	1:F:131:ILE:HD13	1.65	0.96
1:A:126:ALA:O	1:A:131:ILE:HD13	1.66	0.96
1:C:367:ARG:HH12	1:C:1049:GLN:CB	1.80	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:OE2	1:B:397:LYS:HE3	1.66	0.95
1:C:164:LEU:HA	1:C:195:PHE:CE1	2.02	0.95
1:C:960:LEU:HD11	1:C:968:PRO:HB3	1.48	0.95
1:G:960:LEU:HD11	1:G:968:PRO:HB3	1.48	0.94
1:E:14:GLU:OE2	1:E:397:LYS:HE3	1.66	0.94
1:E:280:LEU:CD1	1:E:289:ILE:HG21	1.97	0.93
1:E:14:GLU:OE2	1:E:397:LYS:NZ	2.02	0.93
1:B:278:GLU:C	1:B:289:ILE:HD11	1.92	0.93
1:E:564:ALA:HB2	1:E:603:ILE:HG22	1.49	0.93
1:B:280:LEU:CD1	1:B:289:ILE:HG21	1.98	0.93
1:B:564:ALA:HB2	1:B:603:ILE:HG22	1.49	0.93
1:B:14:GLU:OE2	1:B:397:LYS:NZ	2.02	0.92
1:E:278:GLU:C	1:E:289:ILE:HD11	1.94	0.92
1:C:3:ARG:HD2	1:C:104:ILE:HD11	1.51	0.92
1:G:3:ARG:HD2	1:G:104:ILE:HD11	1.53	0.90
1:A:563:MET:HE2	1:A:573:PHE:CE2	2.06	0.90
1:D:3:ARG:HD2	1:D:104:ILE:HD11	1.52	0.90
1:B:279:PHE:HA	1:B:289:ILE:HD13	1.50	0.90
1:H:3:ARG:HD2	1:H:104:ILE:HD11	1.52	0.90
1:G:576:TRP:NE1	1:G:596:LEU:HB2	1.86	0.89
1:F:943:ARG:HD3	1:F:946:ALA:HB2	1.55	0.89
1:F:563:MET:HE2	1:F:573:PHE:CE2	2.07	0.89
1:E:279:PHE:HA	1:E:289:ILE:HD13	1.51	0.89
1:A:943:ARG:HD3	1:A:946:ALA:HB2	1.55	0.89
1:B:279:PHE:CA	1:B:289:ILE:HD13	2.00	0.89
1:B:970:GLU:O	1:B:973:VAL:HG22	1.72	0.89
1:C:576:TRP:NE1	1:C:596:LEU:HB2	1.86	0.89
1:E:970:GLU:O	1:E:973:VAL:HG22	1.73	0.88
1:B:279:PHE:HA	1:B:289:ILE:CD1	2.01	0.88
1:E:279:PHE:CA	1:E:289:ILE:HD13	2.01	0.88
1:E:279:PHE:HA	1:E:289:ILE:CD1	2.01	0.88
1:C:227:LEU:HD23	1:C:306:THR:HG21	1.55	0.88
1:A:347:ILE:O	1:A:395:LEU:HD12	1.74	0.86
1:F:347:ILE:O	1:F:395:LEU:HD12	1.74	0.86
1:D:45:TYR:CE1	1:C:1047:ASN:HB3	2.09	0.86
1:G:61:ASP:HA	1:G:64:LEU:CD1	2.05	0.85
1:C:61:ASP:HA	1:C:64:LEU:CD1	2.06	0.85
1:B:279:PHE:N	1:B:289:ILE:CD1	2.32	0.85
1:D:345:SER:OG	1:D:412:MET:HE3	1.74	0.85
1:H:45:TYR:CE1	1:G:1047:ASN:HB3	2.11	0.84
1:H:345:SER:OG	1:H:412:MET:HE3	1.75	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:VAL:O	1:E:151:GLY:N	2.09	0.84
1:E:180:VAL:HG12	1:E:184:PHE:HZ	1.35	0.83
1:E:279:PHE:N	1:E:289:ILE:CD1	2.33	0.83
1:B:915:MET:O	1:B:940:LEU:CB	2.26	0.83
1:D:172:ARG:HH12	1:D:186:ARG:CB	1.92	0.83
1:E:101:GLU:HB2	1:E:103:ILE:HD13	1.60	0.82
1:B:101:GLU:HB2	1:B:103:ILE:HD13	1.60	0.82
1:B:180:VAL:HG12	1:B:184:PHE:HZ	1.37	0.82
1:B:144:ILE:HG22	1:B:184:PHE:CZ	2.14	0.82
1:C:227:LEU:CD2	1:C:306:THR:HG21	2.10	0.82
1:E:349:THR:HG22	1:E:393:SER:O	1.80	0.82
1:F:51:TYR:CE1	1:E:1021:GLY:HA3	2.15	0.81
1:G:5:LYS:NZ	1:D:503:GLY:O	2.12	0.81
1:C:147:VAL:O	1:C:151:GLY:N	2.11	0.81
1:G:250:ILE:HD11	1:G:255:ARG:HB3	1.62	0.81
1:G:147:VAL:O	1:G:151:GLY:N	2.11	0.81
1:H:172:ARG:HH12	1:H:186:ARG:CB	1.94	0.81
1:H:8:LEU:HA	1:H:31:VAL:CG2	2.08	0.81
1:B:349:THR:HG22	1:B:393:SER:O	1.81	0.81
1:F:673:ILE:HG22	1:F:695:MET:CE	2.11	0.81
1:F:147:VAL:O	1:F:151:GLY:N	2.12	0.80
1:A:147:VAL:O	1:A:151:GLY:N	2.12	0.80
1:C:250:ILE:HD11	1:C:255:ARG:HB3	1.63	0.80
1:A:673:ILE:HG22	1:A:695:MET:CE	2.12	0.80
1:D:8:LEU:HA	1:D:31:VAL:CG2	2.09	0.80
1:H:254:LEU:CD2	1:H:258:ILE:HD11	2.11	0.80
1:G:61:ASP:CA	1:G:64:LEU:HD12	2.12	0.80
1:D:254:LEU:CD2	1:D:258:ILE:HD11	2.11	0.80
1:G:3:ARG:HG3	1:G:319:ASP:OD1	1.82	0.80
1:A:344:GLN:HG3	1:A:399:CYS:SG	2.22	0.80
1:B:144:ILE:CG2	1:B:184:PHE:CE2	2.64	0.80
1:G:219:ASP:HB3	1:G:323:LEU:CD2	2.12	0.80
1:C:61:ASP:CA	1:C:64:LEU:HD12	2.12	0.80
1:E:843:GLN:O	1:E:847:VAL:HG23	1.81	0.80
1:C:3:ARG:HG3	1:C:319:ASP:OD1	1.82	0.80
1:E:979:TYR:HB3	1:E:982:VAL:HG22	1.63	0.79
1:C:344:GLN:HG3	1:C:399:CYS:SG	2.23	0.79
1:H:3:ARG:HG3	1:H:319:ASP:OD1	1.82	0.79
1:B:843:GLN:O	1:B:847:VAL:HG23	1.81	0.79
1:B:876:SER:O	1:B:879:VAL:HG12	1.81	0.79
1:D:3:ARG:HG3	1:D:319:ASP:OD1	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:TYR:HB3	1:A:982:VAL:HG22	1.65	0.79
1:C:66:ILE:O	1:C:70:ILE:HD12	1.83	0.79
1:E:876:SER:O	1:E:879:VAL:HG12	1.82	0.79
1:G:66:ILE:O	1:G:70:ILE:HD12	1.83	0.79
1:G:575:MET:HE1	1:G:576:TRP:HD1	1.46	0.79
1:B:979:TYR:HB3	1:B:982:VAL:HG22	1.64	0.79
1:C:219:ASP:HB3	1:C:323:LEU:CD2	2.13	0.79
1:F:943:ARG:HG2	1:F:943:ARG:O	1.81	0.79
1:D:344:GLN:HG3	1:D:399:CYS:SG	2.23	0.79
1:C:575:MET:HE1	1:C:576:TRP:HD1	1.46	0.79
1:E:72:ILE:O	1:E:76:SER:OG	2.01	0.78
1:A:943:ARG:HG2	1:A:943:ARG:O	1.81	0.78
1:B:72:ILE:O	1:B:76:SER:OG	2.01	0.78
1:C:501:PRO:O	1:C:504:SER:OG	2.01	0.78
1:G:344:GLN:HG3	1:G:399:CYS:SG	2.23	0.78
1:F:979:TYR:HB3	1:F:982:VAL:HG22	1.65	0.78
1:H:344:GLN:HG3	1:H:399:CYS:SG	2.23	0.78
1:H:876:SER:O	1:H:879:VAL:HG12	1.83	0.78
1:F:344:GLN:HG3	1:F:399:CYS:SG	2.24	0.78
1:E:344:GLN:HG3	1:E:399:CYS:SG	2.24	0.78
1:A:219:ASP:HB3	1:A:323:LEU:CD2	2.13	0.78
1:H:510:THR:HG22	1:H:607:MET:SD	2.22	0.78
1:E:66:ILE:O	1:E:70:ILE:HD12	1.82	0.78
1:B:66:ILE:O	1:B:70:ILE:HD12	1.82	0.78
1:E:1:MET:HE1	1:E:4:ILE:HB	1.66	0.78
1:A:66:ILE:O	1:A:70:ILE:HD12	1.82	0.78
1:A:72:ILE:O	1:A:76:SER:OG	2.02	0.78
1:F:72:ILE:O	1:F:76:SER:OG	2.02	0.78
1:F:986:TYR:CE1	1:F:990:ILE:HD12	2.19	0.78
1:B:219:ASP:HB3	1:B:323:LEU:CD2	2.13	0.78
1:B:344:GLN:HG3	1:B:399:CYS:SG	2.24	0.78
1:F:66:ILE:O	1:F:70:ILE:HD12	1.82	0.78
1:E:219:ASP:HB3	1:E:323:LEU:CD2	2.13	0.78
1:D:876:SER:O	1:D:879:VAL:HG12	1.83	0.78
1:H:72:ILE:O	1:H:76:SER:OG	2.01	0.78
1:F:504:SER:HB2	1:F:505:GLN:CG	2.13	0.78
1:D:72:ILE:O	1:D:76:SER:OG	2.01	0.77
1:G:501:PRO:O	1:G:504:SER:OG	2.02	0.77
1:D:219:ASP:HB3	1:D:323:LEU:CD2	2.14	0.77
1:A:986:TYR:CE1	1:A:990:ILE:HD12	2.20	0.77
1:C:540:ARG:NH2	1:C:541:ASP:OD1	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:ASP:HB3	1:H:323:LEU:CD2	2.15	0.77
1:G:72:ILE:O	1:G:76:SER:OG	2.01	0.77
1:D:510:THR:HG22	1:D:607:MET:SD	2.23	0.77
1:B:160:ILE:HD11	1:B:174:VAL:CG2	2.14	0.77
1:E:280:LEU:HD12	1:E:289:ILE:HG23	1.64	0.77
1:F:219:ASP:HB3	1:F:323:LEU:CD2	2.14	0.77
1:B:1:MET:HE1	1:B:4:ILE:HB	1.67	0.77
1:G:540:ARG:NH2	1:G:541:ASP:OD1	2.18	0.77
1:B:280:LEU:HD12	1:B:289:ILE:HG23	1.65	0.77
1:C:72:ILE:O	1:C:76:SER:OG	2.02	0.77
1:E:501:PRO:O	1:E:504:SER:OG	2.03	0.77
1:C:88:LEU:HB3	1:C:94:PHE:HD2	1.50	0.77
1:G:526:VAL:O	1:G:529:GLN:N	2.18	0.76
1:D:979:TYR:HB3	1:D:982:VAL:HG22	1.64	0.76
1:B:160:ILE:HD11	1:B:174:VAL:HG21	1.67	0.76
1:C:526:VAL:O	1:C:529:GLN:N	2.18	0.76
1:G:519:PRO:HB2	1:G:705:HIS:NE2	2.00	0.76
1:B:144:ILE:HG22	1:B:184:PHE:CD2	2.21	0.76
1:G:960:LEU:HD11	1:G:968:PRO:CB	2.15	0.76
1:C:691:TYR:O	1:C:695:MET:HG2	1.85	0.76
1:C:960:LEU:HD11	1:C:968:PRO:CB	2.15	0.76
1:B:228:PHE:HD2	1:B:338:ILE:HD11	1.50	0.76
1:C:519:PRO:HB2	1:C:705:HIS:NE2	2.00	0.76
1:G:691:TYR:O	1:G:695:MET:HG2	1.85	0.76
1:F:51:TYR:CE1	1:E:1021:GLY:CA	2.69	0.76
1:E:279:PHE:C	1:E:289:ILE:HD13	2.08	0.76
1:B:88:LEU:HB3	1:B:94:PHE:HD2	1.50	0.76
1:B:82:HIS:HD2	1:B:84:GLY:H	1.33	0.76
1:E:228:PHE:HD2	1:E:338:ILE:HD11	1.50	0.75
1:G:88:LEU:HB3	1:G:94:PHE:HD2	1.52	0.75
1:B:279:PHE:C	1:B:289:ILE:HD13	2.09	0.75
1:F:124:GLU:O	1:F:127:LEU:HG	1.86	0.75
1:A:501:PRO:O	1:A:504:SER:OG	2.04	0.75
1:H:979:TYR:HB3	1:H:982:VAL:HG22	1.65	0.75
1:E:88:LEU:HB3	1:E:94:PHE:HD2	1.51	0.75
1:B:501:PRO:O	1:B:504:SER:OG	2.04	0.75
1:F:501:PRO:O	1:F:504:SER:OG	2.05	0.75
1:E:82:HIS:HD2	1:E:84:GLY:H	1.34	0.75
1:A:51:TYR:CE1	1:B:1021:GLY:HA3	2.21	0.75
1:H:82:HIS:HD2	1:H:84:GLY:H	1.34	0.75
1:G:685:THR:O	1:G:688:THR:HG23	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:O	1:A:127:LEU:HG	1.86	0.74
1:C:685:THR:O	1:C:688:THR:HG23	1.87	0.74
1:D:82:HIS:HD2	1:D:84:GLY:H	1.35	0.74
1:H:960:LEU:CD1	1:H:976:TYR:CG	2.71	0.74
1:E:88:LEU:HD12	1:E:94:PHE:CD2	2.23	0.74
1:D:45:TYR:CD1	1:C:1047:ASN:HB3	2.22	0.74
1:D:501:PRO:O	1:D:504:SER:OG	2.05	0.74
1:E:800:GLN:O	1:E:804:HIS:ND1	2.20	0.74
1:B:800:GLN:O	1:B:804:HIS:ND1	2.20	0.74
1:D:960:LEU:CD1	1:D:976:TYR:CG	2.71	0.73
1:B:88:LEU:HD12	1:B:94:PHE:CD2	2.23	0.73
1:D:384:GLY:HA3	1:C:1050:PRO:HD3	1.69	0.73
1:H:13:GLY:O	1:H:17:ILE:HD12	1.87	0.73
1:D:13:GLY:O	1:D:17:ILE:HD12	1.87	0.73
1:H:501:PRO:O	1:H:504:SER:OG	2.05	0.73
1:D:800:GLN:O	1:D:804:HIS:ND1	2.20	0.73
1:F:82:HIS:HD2	1:F:84:GLY:H	1.36	0.73
1:G:960:LEU:CD1	1:G:968:PRO:CG	2.65	0.73
1:D:45:TYR:CE1	1:C:1047:ASN:CB	2.71	0.73
1:C:960:LEU:CD1	1:C:968:PRO:CG	2.65	0.73
1:B:141:VAL:HG11	1:B:147:VAL:HG22	1.69	0.73
1:H:960:LEU:HD13	1:H:976:TYR:CG	2.23	0.72
1:F:126:ALA:O	1:F:131:ILE:HD11	1.87	0.72
1:G:227:LEU:HD22	1:G:306:THR:HG21	1.71	0.72
1:D:960:LEU:HD13	1:D:976:TYR:CG	2.24	0.72
1:A:82:HIS:HD2	1:A:84:GLY:H	1.36	0.72
1:F:627:VAL:HG23	1:F:628:ILE:HD12	1.68	0.72
1:G:175:GLU:HG2	1:G:179:HIS:CD2	2.24	0.72
1:A:627:VAL:HG23	1:A:628:ILE:HD12	1.68	0.72
1:B:81:ILE:O	1:B:106:VAL:HG23	1.90	0.72
1:B:160:ILE:CD1	1:B:174:VAL:CG2	2.67	0.72
1:A:156:TYR:O	1:A:176:SER:CB	2.36	0.72
1:H:45:TYR:CD1	1:G:1047:ASN:HB3	2.24	0.72
1:E:234:ILE:HD11	1:E:445:TYR:CZ	2.25	0.72
1:A:126:ALA:O	1:A:131:ILE:HD11	1.88	0.72
1:A:519:PRO:HB2	1:A:705:HIS:NE2	2.05	0.72
1:C:500:ILE:HG21	1:C:565:HIS:CD2	2.24	0.72
1:C:510:THR:OG1	1:C:607:MET:HG3	1.90	0.72
1:E:81:ILE:O	1:E:106:VAL:HG23	1.90	0.72
1:C:228:PHE:CE2	1:C:338:ILE:HG13	2.24	0.72
1:H:519:PRO:HB2	1:H:705:HIS:NE2	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:519:PRO:HB2	1:F:705:HIS:NE2	2.06	0.71
1:G:82:HIS:HD2	1:G:84:GLY:H	1.35	0.71
1:A:234:ILE:HD11	1:A:445:TYR:CZ	2.25	0.71
1:B:990:ILE:HD11	1:B:995:ASP:HA	1.72	0.71
1:E:990:ILE:HD11	1:E:995:ASP:HA	1.72	0.71
1:G:127:LEU:HD22	1:G:133:VAL:HG21	1.71	0.71
1:D:21:ARG:NH1	1:C:370:GLY:C	2.47	0.71
1:C:82:HIS:HD2	1:C:84:GLY:H	1.35	0.71
1:D:279:PHE:CA	1:D:289:ILE:HD11	2.20	0.71
1:B:158:LEU:CD1	1:B:174:VAL:O	2.38	0.71
1:B:234:ILE:HD11	1:B:445:TYR:CZ	2.25	0.71
1:F:234:ILE:HD11	1:F:445:TYR:CZ	2.26	0.71
1:G:88:LEU:HD12	1:G:94:PHE:CD2	2.25	0.71
1:G:510:THR:OG1	1:G:607:MET:HG3	1.91	0.71
1:A:51:TYR:CE1	1:B:1021:GLY:CA	2.74	0.71
1:H:279:PHE:CA	1:H:289:ILE:HD11	2.21	0.71
1:H:45:TYR:CE1	1:G:1047:ASN:CB	2.73	0.71
1:H:21:ARG:NH2	1:G:418:GLU:OE2	2.23	0.71
1:F:504:SER:HB2	1:F:505:GLN:HG3	1.73	0.71
1:B:437:HIS:CD2	1:B:439:ASP:H	2.08	0.71
1:C:226:HIS:ND1	1:C:259:CYS:HB3	2.06	0.71
1:F:414:ARG:HD3	1:E:25:GLU:HG3	1.72	0.71
1:D:175:GLU:N	1:D:175:GLU:OE2	2.23	0.71
1:H:234:ILE:HD11	1:H:445:TYR:CZ	2.25	0.70
1:C:88:LEU:HD12	1:C:94:PHE:CD2	2.26	0.70
1:G:278:GLU:C	1:G:289:ILE:HD11	2.16	0.70
1:E:437:HIS:CD2	1:E:439:ASP:H	2.08	0.70
1:D:60:ILE:H	1:D:60:ILE:HD13	1.53	0.70
1:C:127:LEU:HD22	1:C:133:VAL:HG21	1.72	0.70
1:H:60:ILE:HD13	1:H:60:ILE:H	1.54	0.70
1:H:134:ILE:HD12	1:H:287:TYR:HB3	1.74	0.70
1:E:64:LEU:HD23	1:E:88:LEU:HD23	1.73	0.70
1:E:14:GLU:OE2	1:E:397:LYS:HE2	1.90	0.70
1:D:370:GLY:C	1:C:21:ARG:NH1	2.50	0.70
1:E:157:PRO:O	1:E:158:LEU:HD23	1.92	0.70
1:B:510:THR:OG1	1:B:607:MET:HG3	1.90	0.70
1:C:278:GLU:C	1:C:289:ILE:HD11	2.17	0.70
1:F:1010:LEU:HD21	1:F:1031:ILE:HD11	1.74	0.70
1:B:64:LEU:HD23	1:B:88:LEU:HD23	1.74	0.70
1:F:657:VAL:HG22	1:F:943:ARG:NH2	2.06	0.70
1:D:519:PRO:HB2	1:D:705:HIS:NE2	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:O	1:A:383:GLN:O	2.10	0.70
1:B:14:GLU:OE2	1:B:397:LYS:HE2	1.90	0.70
1:H:64:LEU:HD23	1:H:88:LEU:HD23	1.74	0.70
1:D:234:ILE:HD11	1:D:445:TYR:CZ	2.26	0.70
1:D:370:GLY:O	1:C:21:ARG:NH1	2.25	0.70
1:F:363:VAL:O	1:F:383:GLN:O	2.10	0.69
1:E:82:HIS:HA	1:E:106:VAL:HG23	1.74	0.69
1:A:657:VAL:HG22	1:A:943:ARG:NH2	2.07	0.69
1:B:82:HIS:HA	1:B:106:VAL:HG23	1.74	0.69
1:D:64:LEU:HD23	1:D:88:LEU:HD23	1.75	0.69
1:C:234:ILE:HD11	1:C:445:TYR:CZ	2.28	0.69
1:C:363:VAL:O	1:C:383:GLN:O	2.09	0.69
1:F:134:ILE:HD12	1:F:287:TYR:HB3	1.74	0.69
1:F:657:VAL:HG22	1:F:943:ARG:HH22	1.58	0.69
1:D:363:VAL:O	1:D:383:GLN:O	2.10	0.69
1:G:363:VAL:O	1:G:383:GLN:O	2.10	0.69
1:A:370:GLY:O	1:B:21:ARG:NH1	2.26	0.69
1:A:657:VAL:HG22	1:A:943:ARG:HH22	1.58	0.69
1:H:800:GLN:O	1:H:804:HIS:ND1	2.20	0.68
1:E:180:VAL:HG12	1:E:184:PHE:CE1	2.28	0.68
1:D:134:ILE:HD12	1:D:287:TYR:HB3	1.75	0.68
1:A:863:VAL:HA	1:A:866:MET:HG3	1.74	0.68
1:H:363:VAL:O	1:H:383:GLN:O	2.10	0.68
1:F:157:PRO:O	1:F:158:LEU:HD23	1.93	0.68
1:G:234:ILE:HD11	1:G:445:TYR:CZ	2.28	0.68
1:C:279:PHE:N	1:C:289:ILE:HD11	2.09	0.68
1:H:279:PHE:N	1:H:289:ILE:HD11	2.09	0.68
1:D:21:ARG:NH1	1:C:370:GLY:O	2.27	0.68
1:D:70:ILE:O	1:D:74:LYS:HG2	1.94	0.68
1:C:20:MET:HE1	1:C:43:HIS:O	1.92	0.68
1:C:540:ARG:HH21	1:C:541:ASP:CG	2.01	0.68
1:H:863:VAL:HA	1:H:866:MET:HG3	1.74	0.68
1:F:673:ILE:CG2	1:F:695:MET:CE	2.71	0.68
1:E:363:VAL:O	1:E:383:GLN:O	2.10	0.68
1:G:575:MET:HE1	1:G:576:TRP:CD1	2.26	0.68
1:G:582:ASP:OD2	1:G:586:ARG:NH1	2.26	0.68
1:D:279:PHE:N	1:D:289:ILE:HD11	2.09	0.68
1:A:1010:LEU:HD21	1:A:1031:ILE:HD11	1.75	0.68
1:C:575:MET:HE1	1:C:576:TRP:CD1	2.27	0.68
1:F:679:ILE:HD13	1:F:724:LEU:HD13	1.74	0.68
1:G:20:MET:HE1	1:G:43:HIS:O	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:PHE:N	1:G:289:ILE:HD11	2.09	0.68
1:A:134:ILE:HD12	1:A:287:TYR:HB3	1.75	0.68
1:A:157:PRO:O	1:A:158:LEU:HD23	1.94	0.68
1:B:363:VAL:O	1:B:383:GLN:O	2.10	0.68
1:C:582:ASP:OD2	1:C:586:ARG:NH1	2.26	0.68
1:H:70:ILE:O	1:H:74:LYS:HG2	1.94	0.68
1:F:863:VAL:HA	1:F:866:MET:HG3	1.75	0.68
1:A:370:GLY:C	1:B:21:ARG:NH1	2.51	0.68
1:A:673:ILE:CG2	1:A:695:MET:CE	2.71	0.68
1:H:582:ASP:OD2	1:H:586:ARG:NH1	2.27	0.68
1:B:143:GLY:O	1:B:147:VAL:HG23	1.94	0.68
1:D:990:ILE:HD11	1:D:995:ASP:HA	1.76	0.67
1:D:582:ASP:OD2	1:D:586:ARG:NH1	2.28	0.67
1:E:160:ILE:HD11	1:E:174:VAL:HG21	1.75	0.67
1:D:863:VAL:HA	1:D:866:MET:HG3	1.75	0.67
1:B:158:LEU:HD12	1:B:158:LEU:N	2.09	0.67
1:H:384:GLY:HA3	1:G:1050:PRO:HD3	1.75	0.67
1:G:540:ARG:HH21	1:G:541:ASP:CG	2.03	0.67
1:B:582:ASP:OD2	1:B:586:ARG:NH1	2.27	0.67
1:A:679:ILE:HD13	1:A:724:LEU:HD13	1.75	0.67
1:E:603:ILE:HG13	1:E:608:PHE:CZ	2.30	0.67
1:B:603:ILE:HG13	1:B:608:PHE:CZ	2.30	0.67
1:H:990:ILE:HD11	1:H:995:ASP:HA	1.77	0.67
1:C:66:ILE:HG13	1:C:88:LEU:HD11	1.77	0.67
1:C:198:ASP:O	1:C:200:VAL:HG23	1.95	0.67
1:H:8:LEU:CA	1:H:31:VAL:HG23	2.16	0.67
1:B:603:ILE:HG13	1:B:608:PHE:HZ	1.60	0.67
1:F:198:ASP:O	1:F:200:VAL:HG23	1.95	0.66
1:F:673:ILE:HG22	1:F:695:MET:HE1	1.76	0.66
1:F:550:ARG:HG3	1:F:816:PHE:CD1	2.30	0.66
1:A:582:ASP:OD2	1:A:586:ARG:NH1	2.28	0.66
1:B:437:HIS:HD2	1:B:439:ASP:N	1.91	0.66
1:E:437:HIS:HD2	1:E:439:ASP:N	1.92	0.66
1:E:582:ASP:OD2	1:E:586:ARG:NH1	2.27	0.66
1:G:198:ASP:O	1:G:200:VAL:HG23	1.96	0.66
1:F:370:GLY:C	1:E:21:ARG:NH1	2.53	0.66
1:G:365:THR:HG21	1:G:1051:ARG:HD3	1.77	0.66
1:E:603:ILE:HG13	1:E:608:PHE:HZ	1.60	0.66
1:A:21:ARG:NH1	1:B:370:GLY:O	2.28	0.66
1:A:550:ARG:HG3	1:A:816:PHE:CD1	2.31	0.66
1:A:673:ILE:HG22	1:A:695:MET:HE1	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:THR:HG21	1:C:1051:ARG:HD3	1.78	0.66
1:G:66:ILE:HG13	1:G:88:LEU:HD11	1.78	0.66
1:G:250:ILE:HD11	1:G:255:ARG:CB	2.25	0.66
1:D:679:ILE:HD13	1:D:724:LEU:HD13	1.76	0.66
1:A:414:ARG:HD3	1:B:25:GLU:HG3	1.77	0.66
1:F:250:ILE:HD11	1:F:255:ARG:HB2	1.77	0.66
1:F:582:ASP:OD2	1:F:586:ARG:NH1	2.29	0.66
1:E:250:ILE:HD11	1:E:255:ARG:HB2	1.76	0.66
1:G:227:LEU:CD2	1:G:306:THR:HG21	2.26	0.66
1:A:198:ASP:O	1:A:200:VAL:HG23	1.95	0.66
1:H:250:ILE:HD11	1:H:255:ARG:HB2	1.78	0.66
1:F:120:ILE:HD12	1:F:121:LYS:N	2.11	0.66
1:F:504:SER:HB2	1:F:505:GLN:HG2	1.76	0.66
1:B:147:VAL:O	1:B:151:GLY:N	2.28	0.66
1:B:250:ILE:HD11	1:B:255:ARG:HB2	1.77	0.66
1:D:120:ILE:HD12	1:D:121:LYS:N	2.11	0.65
1:D:250:ILE:HD11	1:D:255:ARG:HB2	1.78	0.65
1:A:250:ILE:HD11	1:A:255:ARG:HB2	1.78	0.65
1:H:176:SER:O	1:H:179:HIS:ND1	2.26	0.65
1:F:126:ALA:C	1:F:131:ILE:HD11	2.21	0.65
1:A:21:ARG:NH1	1:B:370:GLY:C	2.53	0.65
1:H:120:ILE:HD12	1:H:121:LYS:N	2.11	0.65
1:H:659:ILE:HG23	1:H:669:VAL:HG11	1.79	0.65
1:H:679:ILE:HD13	1:H:724:LEU:HD13	1.77	0.65
1:B:158:LEU:HD13	1:B:174:VAL:CB	2.18	0.65
1:F:370:GLY:O	1:E:21:ARG:NH1	2.30	0.65
1:A:151:GLY:HA2	1:A:158:LEU:HD11	1.78	0.65
1:C:120:ILE:HD12	1:C:121:LYS:N	2.11	0.65
1:C:250:ILE:HD11	1:C:255:ARG:CB	2.26	0.65
1:H:66:ILE:HG13	1:H:88:LEU:HD11	1.79	0.65
1:F:21:ARG:NH1	1:E:370:GLY:O	2.29	0.65
1:G:127:LEU:CD2	1:G:133:VAL:HG21	2.26	0.65
1:H:352:PRO:HA	1:H:356:PHE:CD1	2.32	0.65
1:D:66:ILE:HG13	1:D:88:LEU:HD11	1.79	0.65
1:A:120:ILE:HD12	1:A:121:LYS:N	2.12	0.65
1:D:659:ILE:HG23	1:D:669:VAL:HG11	1.79	0.65
1:B:141:VAL:CG1	1:B:147:VAL:HG22	2.27	0.65
1:B:603:ILE:HD12	1:B:608:PHE:CE1	2.32	0.65
1:E:14:GLU:CD	1:E:397:LYS:CE	2.70	0.64
1:A:470:LEU:HD22	1:A:1044:PHE:CD2	2.32	0.64
1:G:960:LEU:HD13	1:G:961:LYS:N	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:ARG:HG3	1:D:816:PHE:CD1	2.33	0.64
1:B:464:ASP:OD2	1:B:467:THR:OG1	2.15	0.64
1:C:127:LEU:CD2	1:C:133:VAL:HG21	2.27	0.64
1:H:901:GLY:HA3	1:H:932:LEU:HD22	1.79	0.64
1:F:943:ARG:HD3	1:F:946:ALA:CB	2.27	0.64
1:E:464:ASP:OD2	1:E:467:THR:OG1	2.15	0.64
1:E:603:ILE:HD12	1:E:608:PHE:CE1	2.33	0.64
1:E:952:ASN:OD1	1:E:955:GLU:N	2.19	0.64
1:E:66:ILE:HG13	1:E:88:LEU:HD11	1.78	0.64
1:A:25:GLU:HG3	1:B:414:ARG:HD3	1.80	0.64
1:B:952:ASN:OD1	1:B:955:GLU:N	2.19	0.64
1:C:960:LEU:HD13	1:C:961:LYS:N	2.12	0.64
1:H:550:ARG:HG3	1:H:816:PHE:CD1	2.33	0.64
1:F:21:ARG:NH1	1:E:370:GLY:C	2.55	0.64
1:B:66:ILE:HG13	1:B:88:LEU:HD11	1.78	0.64
1:F:511:LYS:HZ3	1:F:641:ASP:CG	2.06	0.64
1:A:943:ARG:HD3	1:A:946:ALA:CB	2.27	0.64
1:B:144:ILE:CG2	1:B:184:PHE:CD2	2.81	0.64
1:F:504:SER:CB	1:F:505:GLN:HG2	2.28	0.64
1:D:901:GLY:HA3	1:D:932:LEU:HD22	1.79	0.64
1:A:126:ALA:C	1:A:131:ILE:HD11	2.22	0.64
1:H:328:VAL:HG12	1:H:330:ILE:HG13	1.80	0.64
1:H:546:LEU:HB3	1:H:547:LEU:HD13	1.80	0.64
1:D:328:VAL:HG12	1:D:330:ILE:HG13	1.80	0.64
1:H:198:ASP:O	1:H:200:VAL:HG23	1.97	0.64
1:G:174:VAL:HG12	1:G:176:SER:H	1.63	0.64
1:G:500:ILE:HG21	1:G:565:HIS:CD2	2.33	0.64
1:D:198:ASP:O	1:D:200:VAL:HG23	1.98	0.64
1:H:116:PHE:HE2	1:H:266:MET:HE1	1.63	0.64
1:E:14:GLU:CD	1:E:397:LYS:HE3	2.22	0.64
1:H:116:PHE:CE2	1:H:266:MET:HE1	2.33	0.63
1:E:550:ARG:HG3	1:E:816:PHE:CD1	2.34	0.63
1:G:120:ILE:HD12	1:G:121:LYS:N	2.12	0.63
1:A:659:ILE:HG23	1:A:669:VAL:HG11	1.80	0.63
1:B:228:PHE:CE2	1:B:338:ILE:HG13	2.33	0.63
1:B:740:THR:HG22	1:B:751:TYR:CE1	2.33	0.63
1:D:546:LEU:HB3	1:D:547:LEU:HD13	1.81	0.63
1:A:563:MET:HE2	1:A:573:PHE:CD2	2.32	0.63
1:F:659:ILE:HG23	1:F:669:VAL:HG11	1.80	0.63
1:E:740:THR:HG22	1:E:751:TYR:CE1	2.33	0.63
1:B:254:LEU:HD22	1:B:258:ILE:HD11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:PHE:CE2	1:D:266:MET:HE1	2.34	0.63
1:H:541:ASP:OD2	1:H:739:HIS:CE1	2.52	0.63
1:E:228:PHE:CE2	1:E:338:ILE:HG13	2.34	0.63
1:D:116:PHE:HE2	1:D:266:MET:HE1	1.63	0.63
1:B:14:GLU:CD	1:B:397:LYS:HE3	2.23	0.63
1:B:550:ARG:HG3	1:B:816:PHE:CD1	2.34	0.63
1:C:227:LEU:HD23	1:C:306:THR:CG2	2.29	0.63
1:E:254:LEU:HD22	1:E:258:ILE:HD11	1.81	0.63
1:G:659:ILE:HG23	1:G:669:VAL:HG11	1.79	0.63
1:C:254:LEU:HD22	1:C:258:ILE:HD11	1.81	0.63
1:F:328:VAL:HG12	1:F:330:ILE:HG13	1.81	0.63
1:F:673:ILE:CG2	1:F:695:MET:HE3	2.28	0.63
1:G:550:ARG:HG3	1:G:816:PHE:CD1	2.33	0.63
1:D:680:ASP:OD1	1:D:723:ARG:NH1	2.31	0.63
1:B:328:VAL:HG12	1:B:330:ILE:HG13	1.81	0.63
1:H:290:GLU:OE2	1:H:291:VAL:N	2.31	0.63
1:F:470:LEU:HD22	1:F:1044:PHE:CD2	2.34	0.63
1:E:352:PRO:HA	1:E:356:PHE:CD1	2.33	0.63
1:C:174:VAL:HG12	1:C:176:SER:H	1.64	0.63
1:C:328:VAL:HG12	1:C:330:ILE:HG13	1.81	0.63
1:H:942:ASP:N	1:H:942:ASP:OD1	2.32	0.62
1:E:328:VAL:HG12	1:E:330:ILE:HG13	1.81	0.62
1:G:254:LEU:HD22	1:G:258:ILE:HD11	1.81	0.62
1:D:740:THR:HG22	1:D:751:TYR:CE1	2.34	0.62
1:A:511:LYS:HZ3	1:A:641:ASP:CG	2.07	0.62
1:A:740:THR:HG22	1:A:751:TYR:CE1	2.35	0.62
1:H:740:THR:HG22	1:H:751:TYR:CE1	2.34	0.62
1:D:352:PRO:HA	1:D:356:PHE:CD1	2.34	0.62
1:B:141:VAL:HG21	1:B:202:VAL:CB	2.28	0.62
1:B:278:GLU:C	1:B:289:ILE:CD1	2.69	0.62
1:H:680:ASP:OD1	1:H:723:ARG:NH1	2.32	0.62
1:D:541:ASP:OD2	1:D:739:HIS:CE1	2.52	0.62
1:C:659:ILE:HG23	1:C:669:VAL:HG11	1.80	0.62
1:F:563:MET:HE2	1:F:573:PHE:CD2	2.33	0.62
1:G:546:LEU:HB3	1:G:547:LEU:HD13	1.81	0.62
1:D:174:VAL:C	1:D:175:GLU:OE2	2.42	0.62
1:A:254:LEU:HD22	1:A:258:ILE:HD11	1.80	0.62
1:A:673:ILE:CG2	1:A:695:MET:HE3	2.28	0.62
1:B:437:HIS:HD2	1:B:439:ASP:H	1.46	0.62
1:B:940:LEU:O	1:B:941:THR:HG22	1.99	0.62
1:B:952:ASN:OD1	1:B:952:ASN:C	2.42	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:VAL:O	1:C:529:GLN:CB	2.47	0.62
1:F:740:THR:HG22	1:F:751:TYR:CE1	2.35	0.62
1:E:952:ASN:OD1	1:E:952:ASN:C	2.42	0.62
1:D:624:PRO:O	1:D:627:VAL:HG22	1.99	0.62
1:C:832:MET:HG3	1:C:833:PRO:CD	2.30	0.62
1:D:942:ASP:OD1	1:D:942:ASP:N	2.33	0.62
1:F:624:PRO:O	1:F:627:VAL:HG22	2.00	0.62
1:A:541:ASP:OD2	1:A:739:HIS:CE1	2.52	0.62
1:G:624:PRO:O	1:G:627:VAL:HG22	2.00	0.62
1:C:624:PRO:O	1:C:627:VAL:HG22	2.00	0.62
1:G:328:VAL:HG12	1:G:330:ILE:HG13	1.82	0.62
1:A:624:PRO:O	1:A:627:VAL:HG22	2.00	0.62
1:B:352:PRO:HA	1:B:356:PHE:CD1	2.34	0.62
1:C:546:LEU:HB3	1:C:547:LEU:HD13	1.82	0.62
1:H:17:ILE:HD11	1:H:43:HIS:HB3	1.82	0.61
1:F:254:LEU:HD22	1:F:258:ILE:HD11	1.81	0.61
1:A:219:ASP:CB	1:A:323:LEU:HD23	2.27	0.61
1:G:526:VAL:O	1:G:529:GLN:CB	2.48	0.61
1:C:550:ARG:HG3	1:C:816:PHE:CD1	2.35	0.61
1:H:624:PRO:O	1:H:627:VAL:HG22	2.00	0.61
1:F:25:GLU:HG3	1:E:414:ARG:HD3	1.83	0.61
1:F:546:LEU:HB3	1:F:547:LEU:HD13	1.82	0.61
1:E:278:GLU:C	1:E:289:ILE:CD1	2.70	0.61
1:G:352:PRO:HA	1:G:356:PHE:CD1	2.35	0.61
1:D:177:LYS:HG3	1:D:178:GLU:H	1.64	0.61
1:H:537:THR:O	1:H:540:ARG:O	2.19	0.61
1:E:180:VAL:CG1	1:E:184:PHE:CZ	2.66	0.61
1:G:832:MET:HG3	1:G:833:PRO:CD	2.31	0.61
1:B:624:PRO:O	1:B:627:VAL:HG22	2.00	0.61
1:C:537:THR:O	1:C:540:ARG:O	2.18	0.61
1:H:360:THR:HA	1:H:387:VAL:CG2	2.31	0.61
1:F:151:GLY:HA2	1:F:158:LEU:HD11	1.81	0.61
1:F:174:VAL:HG12	1:F:176:SER:H	1.64	0.61
1:F:541:ASP:OD2	1:F:739:HIS:CE1	2.53	0.61
1:E:624:PRO:O	1:E:627:VAL:HG22	2.00	0.61
1:G:537:THR:O	1:G:540:ARG:O	2.18	0.61
1:A:328:VAL:HG12	1:A:330:ILE:HG13	1.82	0.61
1:B:546:LEU:HB3	1:B:547:LEU:HD13	1.83	0.61
1:C:352:PRO:HA	1:C:356:PHE:CD1	2.35	0.61
1:E:749:TYR:CZ	1:G:752:ALA:HB1	2.36	0.61
1:D:537:THR:O	1:D:540:ARG:O	2.19	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:GLU:N	1:F:175:GLU:OE2	2.33	0.61
1:E:219:ASP:CB	1:E:323:LEU:HD23	2.27	0.61
1:E:234:ILE:HD11	1:E:445:TYR:CE1	2.36	0.61
1:G:360:THR:HA	1:G:387:VAL:CG2	2.31	0.61
1:A:832:MET:HG2	1:A:836:GLN:HG2	1.81	0.61
1:C:360:THR:HA	1:C:387:VAL:CG2	2.31	0.61
1:H:360:THR:HA	1:H:387:VAL:HG23	1.83	0.61
1:A:942:ASP:N	1:A:942:ASP:OD1	2.33	0.61
1:H:254:LEU:O	1:H:258:ILE:HD12	2.01	0.60
1:B:219:ASP:CB	1:B:323:LEU:HD23	2.27	0.60
1:F:942:ASP:N	1:F:942:ASP:OD1	2.33	0.60
1:E:213:GLU:OE2	1:E:232:CYS:SG	2.54	0.60
1:A:175:GLU:N	1:A:175:GLU:OE2	2.34	0.60
1:B:14:GLU:CD	1:B:397:LYS:CE	2.71	0.60
1:B:234:ILE:HD11	1:B:445:TYR:CE1	2.36	0.60
1:G:110:SER:HA	1:G:113:LEU:HD12	1.82	0.60
1:D:254:LEU:O	1:D:258:ILE:HD12	2.01	0.60
1:A:546:LEU:HB3	1:A:547:LEU:HD13	1.83	0.60
1:B:537:THR:O	1:B:540:ARG:O	2.19	0.60
1:E:537:THR:O	1:E:540:ARG:O	2.19	0.60
1:G:278:GLU:C	1:G:289:ILE:CD1	2.74	0.60
1:G:576:TRP:CD1	1:G:596:LEU:HB2	2.37	0.60
1:C:278:GLU:C	1:C:289:ILE:CD1	2.74	0.60
1:F:1031:ILE:HG22	1:F:1042:ILE:HG13	1.84	0.60
1:D:17:ILE:HD11	1:D:43:HIS:HB3	1.84	0.60
1:D:360:THR:HA	1:D:387:VAL:CG2	2.31	0.60
1:C:110:SER:HA	1:C:113:LEU:HD12	1.82	0.60
1:C:576:TRP:CD1	1:C:596:LEU:HB2	2.37	0.60
1:F:537:THR:O	1:F:540:ARG:O	2.19	0.60
1:F:680:ASP:OD1	1:F:723:ARG:NH1	2.33	0.60
1:E:546:LEU:HB3	1:E:547:LEU:HD13	1.84	0.60
1:A:174:VAL:HG12	1:A:176:SER:H	1.66	0.60
1:A:537:THR:O	1:A:540:ARG:O	2.19	0.60
1:C:541:ASP:OD2	1:C:739:HIS:CE1	2.55	0.60
1:H:611:LEU:HD11	1:H:646:PHE:CE1	2.37	0.60
1:F:611:LEU:HD11	1:F:646:PHE:CE1	2.37	0.60
1:F:832:MET:HG2	1:F:836:GLN:HG2	1.81	0.60
1:E:979:TYR:HB3	1:E:982:VAL:CG2	2.31	0.60
1:D:25:GLU:HG3	1:C:414:ARG:HD3	1.83	0.60
1:A:1031:ILE:HG22	1:A:1042:ILE:HG13	1.84	0.60
1:H:12:ARG:NH2	1:H:38:ASP:OD1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:ASP:CB	1:H:323:LEU:HD23	2.27	0.60
1:E:382:PHE:CE1	1:E:385:THR:HB	2.36	0.60
1:G:552:ARG:HA	1:G:588:LEU:HD11	1.83	0.60
1:B:160:ILE:HD12	1:B:174:VAL:HG23	1.84	0.60
1:F:126:ALA:CA	1:F:131:ILE:HD11	2.31	0.60
1:G:541:ASP:OD2	1:G:739:HIS:CE1	2.55	0.60
1:D:12:ARG:NH2	1:D:38:ASP:OD1	2.34	0.60
1:H:134:ILE:HD12	1:H:287:TYR:CB	2.32	0.60
1:E:360:THR:HA	1:E:387:VAL:CG2	2.31	0.60
1:E:940:LEU:O	1:E:941:THR:HG22	2.02	0.60
1:D:360:THR:HA	1:D:387:VAL:HG23	1.84	0.60
1:A:234:ILE:HD11	1:A:445:TYR:CE1	2.36	0.60
1:A:680:ASP:OD1	1:A:723:ARG:NH1	2.33	0.60
1:A:979:TYR:HB3	1:A:982:VAL:CG2	2.32	0.60
1:E:437:HIS:HD2	1:E:439:ASP:H	1.47	0.59
1:D:219:ASP:CB	1:D:323:LEU:HD23	2.28	0.59
1:D:290:GLU:OE2	1:D:291:VAL:N	2.32	0.59
1:B:360:THR:HA	1:B:387:VAL:CG2	2.32	0.59
1:C:470:LEU:HD22	1:C:1044:PHE:CD2	2.37	0.59
1:H:370:GLY:O	1:G:21:ARG:NH1	2.36	0.59
1:H:414:ARG:HD3	1:G:25:GLU:HG3	1.82	0.59
1:F:979:TYR:HB3	1:F:982:VAL:CG2	2.32	0.59
1:E:541:ASP:OD2	1:E:739:HIS:CE1	2.55	0.59
1:F:234:ILE:HD11	1:F:445:TYR:CE1	2.37	0.59
1:E:280:LEU:N	1:E:289:ILE:HD13	2.18	0.59
1:G:470:LEU:HD22	1:G:1044:PHE:CD2	2.38	0.59
1:D:45:TYR:CE2	1:C:1047:ASN:O	2.55	0.59
1:D:611:LEU:HD11	1:D:646:PHE:CE1	2.37	0.59
1:D:979:TYR:HB3	1:D:982:VAL:CG2	2.33	0.59
1:A:110:SER:HA	1:A:113:LEU:HD12	1.83	0.59
1:F:110:SER:HA	1:F:113:LEU:HD12	1.83	0.59
1:F:134:ILE:HD12	1:F:287:TYR:CB	2.32	0.59
1:E:470:LEU:HD22	1:E:1044:PHE:CD2	2.38	0.59
1:C:552:ARG:HA	1:C:588:LEU:HD11	1.84	0.59
1:G:360:THR:HA	1:G:387:VAL:HG23	1.83	0.59
1:A:866:MET:HE1	1:A:897:VAL:HG21	1.85	0.59
1:B:541:ASP:OD2	1:B:739:HIS:CE1	2.56	0.59
1:B:979:TYR:HB3	1:B:982:VAL:CG2	2.32	0.59
1:H:234:ILE:HD11	1:H:445:TYR:CE1	2.37	0.59
1:F:866:MET:HE1	1:F:897:VAL:HG21	1.85	0.59
1:A:134:ILE:HD12	1:A:287:TYR:CB	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:GLN:HA	1:A:868:GLY:O	2.03	0.59
1:C:360:THR:HA	1:C:387:VAL:HG23	1.83	0.59
1:D:45:TYR:CZ	1:C:1047:ASN:HB3	2.38	0.59
1:A:126:ALA:CA	1:A:131:ILE:HD11	2.32	0.59
1:H:64:LEU:CD2	1:H:88:LEU:HD23	2.33	0.59
1:H:134:ILE:CD1	1:H:287:TYR:CB	2.81	0.59
1:F:511:LYS:NZ	1:F:641:ASP:OD1	2.35	0.59
1:D:213:GLU:OE2	1:D:232:CYS:SG	2.55	0.59
1:A:611:LEU:HD11	1:A:646:PHE:CE1	2.38	0.59
1:B:382:PHE:CE1	1:B:385:THR:HB	2.38	0.59
1:D:21:ARG:HH12	1:C:370:GLY:C	2.11	0.58
1:D:322:ALA:N	1:D:325:ASP:OD2	2.36	0.58
1:A:511:LYS:NZ	1:A:641:ASP:OD1	2.35	0.58
1:B:280:LEU:N	1:B:289:ILE:HD13	2.18	0.58
1:H:470:LEU:HD22	1:H:1044:PHE:CD2	2.38	0.58
1:H:979:TYR:HB3	1:H:982:VAL:CG2	2.34	0.58
1:E:141:VAL:HG21	1:E:202:VAL:CB	2.33	0.58
1:D:134:ILE:HD12	1:D:287:TYR:CB	2.33	0.58
1:B:64:LEU:CD2	1:B:88:LEU:HD23	2.32	0.58
1:F:134:ILE:CD1	1:F:287:TYR:CB	2.81	0.58
1:E:64:LEU:CD2	1:E:88:LEU:HD23	2.32	0.58
1:E:360:THR:HA	1:E:387:VAL:HG23	1.84	0.58
1:E:228:PHE:CD2	1:E:338:ILE:HD11	2.37	0.58
1:G:653:LYS:O	1:G:943:ARG:HD3	2.03	0.58
1:D:64:LEU:CD2	1:D:88:LEU:HD23	2.34	0.58
1:D:470:LEU:HD22	1:D:1044:PHE:CD2	2.38	0.58
1:B:360:THR:HA	1:B:387:VAL:HG23	1.84	0.58
1:C:653:LYS:O	1:C:943:ARG:HD3	2.03	0.58
1:H:45:TYR:CE2	1:G:1047:ASN:O	2.57	0.58
1:H:322:ALA:N	1:H:325:ASP:OD2	2.36	0.58
1:D:234:ILE:HD11	1:D:445:TYR:CE1	2.38	0.58
1:B:348:THR:OG1	1:B:350:GLU:HG3	2.04	0.58
1:D:898:TYR:HD1	1:D:928:LYS:CE	2.16	0.58
1:B:470:LEU:HD22	1:B:1044:PHE:CD2	2.39	0.58
1:H:550:ARG:HG3	1:H:816:PHE:CE1	2.39	0.58
1:F:92:ILE:HD13	1:F:113:LEU:HB2	1.86	0.58
1:E:823:PRO:O	1:G:767:SER:HB3	2.04	0.58
1:A:134:ILE:CD1	1:A:287:TYR:CB	2.81	0.58
1:B:213:GLU:OE2	1:B:232:CYS:SG	2.55	0.58
1:F:322:ALA:N	1:F:325:ASP:OD2	2.36	0.58
1:E:322:ALA:N	1:E:325:ASP:OD2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:MET:HE3	1:A:342:ALA:HB1	1.84	0.58
1:C:304:MET:HE3	1:C:342:ALA:HB1	1.85	0.58
1:H:304:MET:HE3	1:H:342:ALA:HB1	1.86	0.58
1:H:898:TYR:HD1	1:H:928:LYS:CE	2.16	0.58
1:E:278:GLU:HB2	1:E:289:ILE:HG13	1.84	0.58
1:D:134:ILE:CD1	1:D:287:TYR:CB	2.82	0.58
1:D:304:MET:HE3	1:D:342:ALA:HB1	1.86	0.58
1:A:360:THR:HA	1:A:387:VAL:CG2	2.33	0.58
1:B:603:ILE:CD1	1:B:608:PHE:CE1	2.86	0.58
1:H:177:LYS:HG3	1:H:178:GLU:H	1.68	0.58
1:F:304:MET:HE3	1:F:342:ALA:HB1	1.84	0.58
1:F:382:PHE:CE1	1:F:385:THR:HB	2.38	0.58
1:E:603:ILE:CD1	1:E:608:PHE:CE1	2.86	0.58
1:G:53:VAL:HG13	1:G:54:GLY:N	2.18	0.58
1:A:322:ALA:N	1:A:325:ASP:OD2	2.37	0.58
1:B:101:GLU:CB	1:B:103:ILE:HD13	2.32	0.58
1:H:175:GLU:HB2	1:H:179:HIS:CG	2.39	0.57
1:F:213:GLU:OE2	1:F:232:CYS:SG	2.54	0.57
1:F:360:THR:HA	1:F:387:VAL:CG2	2.34	0.57
1:F:865:GLN:HA	1:F:868:GLY:O	2.04	0.57
1:B:749:TYR:CZ	1:C:752:ALA:HB1	2.39	0.57
1:B:823:PRO:O	1:C:767:SER:HB3	2.04	0.57
1:C:234:ILE:HD11	1:C:445:TYR:CE1	2.38	0.57
1:E:101:GLU:CB	1:E:103:ILE:HD13	2.32	0.57
1:G:164:LEU:HA	1:G:195:PHE:HE1	1.68	0.57
1:A:213:GLU:OE2	1:A:232:CYS:SG	2.54	0.57
1:B:278:GLU:HB2	1:B:289:ILE:HG13	1.85	0.57
1:C:53:VAL:HG13	1:C:54:GLY:H	1.70	0.57
1:C:228:PHE:HE2	1:C:338:ILE:HG13	1.70	0.57
1:G:53:VAL:HG13	1:G:54:GLY:H	1.70	0.57
1:G:367:ARG:NH1	1:G:1049:GLN:CB	2.60	0.57
1:G:520:GLU:OE1	1:G:705:HIS:CD2	2.57	0.57
1:C:53:VAL:HG13	1:C:54:GLY:N	2.18	0.57
1:F:360:THR:HA	1:F:387:VAL:HG23	1.86	0.57
1:A:92:ILE:HD13	1:A:113:LEU:HB2	1.87	0.57
1:B:322:ALA:N	1:B:325:ASP:OD2	2.37	0.57
1:F:80:ALA:HB2	1:F:104:ILE:HB	1.87	0.57
1:D:550:ARG:HG3	1:D:816:PHE:CE1	2.40	0.57
1:D:551:VAL:HA	1:D:813:TYR:CE2	2.40	0.57
1:D:865:GLN:HA	1:D:868:GLY:O	2.04	0.57
1:A:360:THR:HA	1:A:387:VAL:HG23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:MET:HE3	1:B:342:ALA:HB1	1.86	0.57
1:C:674:CYS:HB3	1:C:712:MET:HE1	1.86	0.57
1:E:348:THR:OG1	1:E:350:GLU:HG3	2.05	0.57
1:E:926:PRO:O	1:E:927:GLU:HB2	2.03	0.57
1:C:160:ILE:HG22	1:C:200:VAL:CG1	2.34	0.57
1:C:520:GLU:OE1	1:C:705:HIS:CD2	2.57	0.57
1:F:986:TYR:CZ	1:F:990:ILE:HD12	2.38	0.57
1:G:160:ILE:HG22	1:G:200:VAL:CG1	2.34	0.57
1:A:550:ARG:HG3	1:A:816:PHE:CE1	2.40	0.57
1:B:603:ILE:HD12	1:B:608:PHE:HE1	1.69	0.57
1:F:673:ILE:HG21	1:F:695:MET:HE3	1.85	0.57
1:E:304:MET:HE3	1:E:342:ALA:HB1	1.86	0.57
1:E:349:THR:HG23	1:E:393:SER:CB	2.35	0.57
1:E:651:TRP:CZ2	1:E:920:GLN:HG3	2.40	0.57
1:G:234:ILE:HD11	1:G:445:TYR:CE1	2.39	0.57
1:C:589:ASN:OD1	1:C:989:MET:HE1	2.05	0.57
1:G:304:MET:HE3	1:G:342:ALA:HB1	1.86	0.57
1:G:550:ARG:HG3	1:G:816:PHE:CE1	2.40	0.57
1:G:589:ASN:OD1	1:G:989:MET:HE1	2.05	0.57
1:G:674:CYS:HB3	1:G:712:MET:HE1	1.87	0.57
1:A:382:PHE:CE1	1:A:385:THR:HB	2.39	0.57
1:A:557:PHE:CE1	1:A:598:THR:HB	2.40	0.57
1:A:986:TYR:CZ	1:A:990:ILE:HD12	2.39	0.57
1:B:394:LEU:HD12	1:B:395:LEU:N	2.20	0.57
1:B:504:SER:O	1:B:506:ILE:HG12	2.05	0.57
1:C:540:ARG:HH21	1:C:541:ASP:CB	2.18	0.57
1:H:557:PHE:CE1	1:H:598:THR:HB	2.40	0.57
1:H:623:TYR:HB3	1:H:627:VAL:HG21	1.87	0.57
1:F:713:ALA:HB3	1:F:715:LEU:CD1	2.34	0.57
1:G:126:ALA:HB1	1:G:131:ILE:HD11	1.87	0.57
1:B:651:TRP:CZ2	1:B:920:GLN:HG3	2.40	0.57
1:B:926:PRO:O	1:B:927:GLU:HB2	2.04	0.57
1:F:859:MET:O	1:F:863:VAL:HG23	2.05	0.56
1:G:322:ALA:N	1:G:325:ASP:OD2	2.38	0.56
1:G:540:ARG:HH21	1:G:541:ASP:HA	1.69	0.56
1:B:859:MET:O	1:B:863:VAL:HG23	2.05	0.56
1:H:382:PHE:CE1	1:H:385:THR:HB	2.40	0.56
1:E:394:LEU:HD12	1:E:395:LEU:N	2.20	0.56
1:E:859:MET:O	1:E:863:VAL:HG23	2.05	0.56
1:E:865:GLN:HA	1:E:868:GLY:O	2.05	0.56
1:D:623:TYR:HB3	1:D:627:VAL:HG21	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ILE:HG21	1:A:695:MET:HE3	1.86	0.56
1:B:53:VAL:HG13	1:B:54:GLY:N	2.20	0.56
1:B:865:GLN:HA	1:B:868:GLY:O	2.05	0.56
1:H:45:TYR:CZ	1:G:1047:ASN:HB3	2.41	0.56
1:H:551:VAL:HA	1:H:813:TYR:CE2	2.40	0.56
1:H:859:MET:O	1:H:863:VAL:HG23	2.05	0.56
1:F:348:THR:OG1	1:F:350:GLU:HG3	2.05	0.56
1:E:603:ILE:HD12	1:E:608:PHE:HE1	1.70	0.56
1:G:92:ILE:HD13	1:G:113:LEU:HB2	1.87	0.56
1:G:540:ARG:HH21	1:G:541:ASP:CB	2.19	0.56
1:G:576:TRP:CZ2	1:G:592:PRO:HB2	2.40	0.56
1:D:8:LEU:CA	1:D:31:VAL:HG23	2.16	0.56
1:D:382:PHE:CE1	1:D:385:THR:HB	2.40	0.56
1:A:348:THR:OG1	1:A:350:GLU:HG3	2.05	0.56
1:C:92:ILE:HD13	1:C:113:LEU:HB2	1.87	0.56
1:C:126:ALA:HB1	1:C:131:ILE:HD11	1.88	0.56
1:E:550:ARG:HG3	1:E:816:PHE:CE1	2.41	0.56
1:D:859:MET:O	1:D:863:VAL:HG23	2.05	0.56
1:A:859:MET:O	1:A:863:VAL:HG23	2.06	0.56
1:C:322:ALA:N	1:C:325:ASP:OD2	2.38	0.56
1:C:576:TRP:CZ2	1:C:592:PRO:HB2	2.40	0.56
1:H:278:GLU:C	1:H:289:ILE:CD1	2.79	0.56
1:F:321:TYR:HB3	1:F:325:ASP:OD2	2.05	0.56
1:E:80:ALA:HB2	1:E:104:ILE:HB	1.88	0.56
1:A:80:ALA:HB2	1:A:104:ILE:HB	1.88	0.56
1:A:321:TYR:HB3	1:A:325:ASP:OD2	2.05	0.56
1:B:158:LEU:HD12	1:B:158:LEU:H	1.67	0.56
1:H:1031:ILE:HG23	1:H:1042:ILE:HG13	1.88	0.56
1:F:1041:VAL:HG12	1:F:1043:TYR:CE1	2.40	0.56
1:E:209:PRO:HB2	1:E:280:LEU:HD23	1.87	0.56
1:E:987:GLN:O	1:E:990:ILE:HG22	2.05	0.56
1:D:1031:ILE:HG23	1:D:1042:ILE:HG13	1.88	0.56
1:B:88:LEU:HB3	1:B:94:PHE:CD2	2.37	0.56
1:B:450:ILE:HG22	1:B:451:ASP:N	2.21	0.56
1:B:987:GLN:O	1:B:990:ILE:HG22	2.05	0.56
1:H:134:ILE:HD11	1:H:287:TYR:HB2	1.87	0.56
1:F:160:ILE:HG22	1:F:200:VAL:CG1	2.35	0.56
1:G:164:LEU:HA	1:G:195:PHE:CE1	2.40	0.56
1:D:134:ILE:HD11	1:D:287:TYR:HB2	1.87	0.56
1:D:321:TYR:HB3	1:D:325:ASP:OD2	2.06	0.56
1:A:506:ILE:HD11	1:A:565:HIS:CE1	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:PRO:HB2	1:B:280:LEU:HD23	1.87	0.56
1:B:367:ARG:HH12	1:B:1049:GLN:HB2	1.70	0.56
1:C:194:ALA:C	1:C:195:PHE:HD2	2.14	0.56
1:D:557:PHE:CE1	1:D:598:THR:HB	2.41	0.56
1:D:898:TYR:CD1	1:D:928:LYS:HE2	2.40	0.56
1:B:288:PHE:CD1	1:B:288:PHE:C	2.84	0.56
1:H:321:TYR:HB3	1:H:325:ASP:OD2	2.06	0.56
1:H:908:ASP:O	1:H:912:GLU:HG3	2.06	0.56
1:F:550:ARG:HG3	1:F:816:PHE:CE1	2.41	0.56
1:F:557:PHE:CE1	1:F:598:THR:HB	2.41	0.56
1:E:53:VAL:HG13	1:E:54:GLY:N	2.20	0.56
1:D:908:ASP:O	1:D:912:GLU:HG3	2.06	0.56
1:A:630:GLU:HG2	1:A:953:PHE:HE1	1.70	0.56
1:H:600:ARG:NH1	1:H:603:ILE:O	2.39	0.56
1:H:865:GLN:HA	1:H:868:GLY:O	2.06	0.56
1:H:898:TYR:CD1	1:H:928:LYS:HE2	2.40	0.56
1:F:511:LYS:NZ	1:F:641:ASP:CG	2.64	0.56
1:E:505:GLN:OE1	1:E:505:GLN:HA	2.05	0.56
1:H:175:GLU:OE2	1:H:175:GLU:N	2.39	0.55
1:H:541:ASP:OD2	1:H:741:HIS:HE1	1.89	0.55
1:E:266:MET:HE3	1:E:277:VAL:CG2	2.35	0.55
1:G:348:THR:OG1	1:G:350:GLU:HG3	2.05	0.55
1:D:278:GLU:C	1:D:289:ILE:CD1	2.79	0.55
1:A:160:ILE:HG22	1:A:200:VAL:CG1	2.36	0.55
1:B:349:THR:HG23	1:B:393:SER:CB	2.36	0.55
1:H:80:ALA:HB2	1:H:104:ILE:HB	1.88	0.55
1:E:147:VAL:HG21	1:E:184:PHE:CE1	2.40	0.55
1:D:80:ALA:HB2	1:D:104:ILE:HB	1.88	0.55
1:H:510:THR:CG2	1:H:607:MET:SD	2.92	0.55
1:F:986:TYR:CE1	1:F:990:ILE:CD1	2.89	0.55
1:F:1031:ILE:CG2	1:F:1042:ILE:HG13	2.36	0.55
1:E:367:ARG:HH12	1:E:1049:GLN:HB2	1.71	0.55
1:G:557:PHE:CE1	1:G:598:THR:HB	2.41	0.55
1:A:511:LYS:NZ	1:A:641:ASP:CG	2.64	0.55
1:B:80:ALA:HB2	1:B:104:ILE:HB	1.88	0.55
1:C:348:THR:OG1	1:C:350:GLU:HG3	2.05	0.55
1:C:832:MET:HG3	1:C:833:PRO:HD2	1.88	0.55
1:H:348:THR:OG1	1:H:350:GLU:HG3	2.06	0.55
1:H:394:LEU:HD12	1:H:395:LEU:N	2.21	0.55
1:F:53:VAL:HG13	1:F:54:GLY:N	2.21	0.55
1:E:88:LEU:HB3	1:E:94:PHE:CD2	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:HB1	1:B:131:ILE:HD11	1.88	0.55
1:H:960:LEU:CD1	1:H:976:TYR:CD1	2.89	0.55
1:E:82:HIS:HA	1:E:106:VAL:CG2	2.37	0.55
1:E:626:ASN:CG	1:E:950:PRO:HB3	2.31	0.55
1:G:620:TYR:CD2	1:G:621:LYS:N	2.74	0.55
1:D:960:LEU:CD1	1:D:976:TYR:CD1	2.89	0.55
1:A:215:GLN:C	1:A:216:ILE:HD12	2.32	0.55
1:A:713:ALA:HB3	1:A:715:LEU:CD1	2.35	0.55
1:B:82:HIS:HA	1:B:106:VAL:CG2	2.37	0.55
1:B:266:MET:HE3	1:B:277:VAL:CG2	2.36	0.55
1:B:623:TYR:HB3	1:B:627:VAL:HG21	1.89	0.55
1:B:626:ASN:CG	1:B:950:PRO:HB3	2.31	0.55
1:C:557:PHE:CE1	1:C:598:THR:HB	2.42	0.55
1:H:53:VAL:HG13	1:H:54:GLY:N	2.20	0.55
1:H:987:GLN:O	1:H:990:ILE:HG22	2.07	0.55
1:F:134:ILE:HD11	1:F:287:TYR:HB2	1.87	0.55
1:E:279:PHE:C	1:E:289:ILE:HD12	2.26	0.55
1:E:540:ARG:HH21	1:E:541:ASP:CG	2.15	0.55
1:D:345:SER:CB	1:D:412:MET:CE	2.81	0.55
1:A:394:LEU:HD12	1:A:395:LEU:N	2.22	0.55
1:A:986:TYR:CE1	1:A:990:ILE:CD1	2.90	0.55
1:A:1031:ILE:CG2	1:A:1042:ILE:HG13	2.37	0.55
1:A:1041:VAL:HG12	1:A:1043:TYR:CE1	2.41	0.55
1:B:279:PHE:C	1:B:289:ILE:HD12	2.26	0.55
1:C:550:ARG:HG3	1:C:816:PHE:CE1	2.42	0.55
1:F:630:GLU:HG2	1:F:953:PHE:HE1	1.71	0.55
1:G:194:ALA:C	1:G:195:PHE:HD2	2.15	0.55
1:G:1031:ILE:HG23	1:G:1042:ILE:HG13	1.89	0.55
1:D:348:THR:OG1	1:D:350:GLU:HG3	2.06	0.55
1:A:134:ILE:HD11	1:A:287:TYR:HB2	1.87	0.55
1:A:740:THR:HG22	1:A:751:TYR:CZ	2.42	0.55
1:C:1031:ILE:HG23	1:C:1042:ILE:HG13	1.89	0.55
1:D:177:LYS:O	1:D:180:VAL:HG23	2.07	0.55
1:D:465:ARG:HG2	1:D:465:ARG:O	2.07	0.55
1:A:53:VAL:HG13	1:A:54:GLY:N	2.21	0.55
1:H:465:ARG:O	1:H:465:ARG:HG2	2.07	0.55
1:E:160:ILE:CD1	1:E:174:VAL:CG2	2.85	0.55
1:D:987:GLN:O	1:D:990:ILE:HG22	2.07	0.55
1:B:550:ARG:HG3	1:B:816:PHE:CE1	2.42	0.55
1:H:259:CYS:O	1:H:263:VAL:HG23	2.07	0.55
1:H:622:ASN:ND2	1:H:917:GLU:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:674:CYS:HB3	1:H:712:MET:HE1	1.88	0.55
1:E:126:ALA:HB1	1:E:131:ILE:HD11	1.89	0.55
1:E:1031:ILE:HG23	1:E:1042:ILE:HG13	1.89	0.55
1:D:674:CYS:HB3	1:D:712:MET:HE1	1.88	0.55
1:D:928:LYS:O	1:D:932:LEU:HD12	2.07	0.55
1:A:63:TYR:HB2	1:A:87:PHE:CD2	2.42	0.55
1:B:551:VAL:HA	1:B:813:TYR:CE2	2.42	0.55
1:C:215:GLN:C	1:C:216:ILE:HD12	2.32	0.55
1:C:394:LEU:HD12	1:C:395:LEU:N	2.21	0.55
1:C:540:ARG:HH21	1:C:541:ASP:HA	1.71	0.55
1:H:228:PHE:CE2	1:H:338:ILE:HG13	2.42	0.54
1:H:345:SER:CB	1:H:412:MET:CE	2.81	0.54
1:D:44:ARG:HD3	1:D:45:TYR:CD1	2.42	0.54
1:D:259:CYS:O	1:D:263:VAL:HG23	2.08	0.54
1:B:235:GLN:O	1:B:450:ILE:HG13	2.07	0.54
1:B:1031:ILE:HG23	1:B:1042:ILE:HG13	1.89	0.54
1:H:928:LYS:O	1:H:932:LEU:HD12	2.07	0.54
1:F:394:LEU:HD12	1:F:395:LEU:N	2.23	0.54
1:E:259:CYS:O	1:E:263:VAL:HG23	2.07	0.54
1:G:80:ALA:HB2	1:G:104:ILE:HB	1.88	0.54
1:D:53:VAL:HG13	1:D:54:GLY:N	2.21	0.54
1:D:394:LEU:HD12	1:D:395:LEU:N	2.22	0.54
1:D:510:THR:CG2	1:D:607:MET:SD	2.93	0.54
1:B:472:TYR:OH	1:B:1004:PHE:CD2	2.59	0.54
1:F:600:ARG:NH1	1:F:603:ILE:O	2.40	0.54
1:A:600:ARG:NH1	1:A:603:ILE:O	2.40	0.54
1:A:908:ASP:O	1:A:912:GLU:HG3	2.06	0.54
1:B:740:THR:HG22	1:B:751:TYR:CZ	2.41	0.54
1:C:620:TYR:CD2	1:C:621:LYS:N	2.75	0.54
1:H:44:ARG:HD3	1:H:45:TYR:CD1	2.42	0.54
1:F:134:ILE:CD1	1:F:287:TYR:HB3	2.36	0.54
1:F:160:ILE:CG2	1:F:200:VAL:HG11	2.37	0.54
1:G:160:ILE:CG2	1:G:200:VAL:HG11	2.37	0.54
1:G:394:LEU:HD12	1:G:395:LEU:N	2.22	0.54
1:G:620:TYR:HD2	1:G:621:LYS:N	2.05	0.54
1:G:832:MET:HG3	1:G:833:PRO:HD2	1.89	0.54
1:F:623:TYR:HB3	1:F:627:VAL:HG21	1.88	0.54
1:G:20:MET:CE	1:G:43:HIS:O	2.55	0.54
1:D:600:ARG:NH1	1:D:603:ILE:O	2.41	0.54
1:B:120:ILE:HD12	1:B:140:PRO:HG3	1.88	0.54
1:C:177:LYS:O	1:C:180:VAL:HG23	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:N	1:C:195:PHE:CD2	2.75	0.54
1:F:567:LEU:N	1:F:568:PRO:CD	2.70	0.54
1:F:740:THR:HG22	1:F:751:TYR:CZ	2.43	0.54
1:E:209:PRO:CB	1:E:280:LEU:HD23	2.38	0.54
1:E:551:VAL:HA	1:E:813:TYR:CE2	2.43	0.54
1:B:259:CYS:O	1:B:263:VAL:HG23	2.07	0.54
1:C:259:CYS:O	1:C:263:VAL:HG23	2.07	0.54
1:F:259:CYS:O	1:F:263:VAL:HG23	2.07	0.54
1:F:395:LEU:HD12	1:F:395:LEU:H	1.71	0.54
1:E:740:THR:HG22	1:E:751:TYR:CZ	2.42	0.54
1:G:215:GLN:C	1:G:216:ILE:HD12	2.33	0.54
1:D:541:ASP:OD2	1:D:741:HIS:HE1	1.91	0.54
1:B:228:PHE:HD2	1:B:338:ILE:CD1	2.21	0.54
1:C:80:ALA:HB2	1:C:104:ILE:HB	1.88	0.54
1:C:600:ARG:NH1	1:C:603:ILE:O	2.41	0.54
1:H:25:GLU:HG3	1:G:414:ARG:HD3	1.89	0.54
1:F:120:ILE:HD12	1:F:121:LYS:HG2	1.90	0.54
1:E:623:TYR:HB3	1:E:627:VAL:HG21	1.90	0.54
1:G:177:LYS:O	1:G:180:VAL:HG23	2.08	0.54
1:D:597:GLU:OE1	1:D:971:LYS:NZ	2.26	0.54
1:A:160:ILE:CG2	1:A:200:VAL:HG11	2.38	0.54
1:A:370:GLY:C	1:B:21:ARG:HH12	2.16	0.54
1:H:509:GLY:N	1:H:512:GLN:OE1	2.39	0.54
1:H:597:GLU:OE1	1:H:971:LYS:NZ	2.26	0.54
1:H:862:VAL:O	1:H:866:MET:HG2	2.08	0.54
1:F:502:TYR:CD1	1:F:503:GLY:N	2.76	0.54
1:F:870:ILE:O	1:F:872:LYS:NZ	2.39	0.54
1:E:472:TYR:OH	1:E:1004:PHE:CD2	2.60	0.54
1:G:259:CYS:O	1:G:263:VAL:HG23	2.08	0.54
1:A:126:ALA:HB1	1:A:131:ILE:HD11	1.90	0.54
1:B:600:ARG:NH1	1:B:603:ILE:O	2.41	0.54
1:C:20:MET:CE	1:C:43:HIS:O	2.56	0.54
1:C:160:ILE:CG2	1:C:200:VAL:HG11	2.38	0.54
1:F:63:TYR:HB2	1:F:87:PHE:CD2	2.43	0.54
1:E:278:GLU:CB	1:E:289:ILE:HG13	2.38	0.54
1:A:571:PHE:CD2	1:A:572:SER:HB3	2.44	0.54
1:B:209:PRO:CB	1:B:280:LEU:HD23	2.38	0.54
1:E:147:VAL:HG11	1:E:180:VAL:CG1	2.38	0.53
1:E:160:ILE:HD11	1:E:174:VAL:CG2	2.38	0.53
1:E:215:GLN:C	1:E:216:ILE:HD12	2.33	0.53
1:E:228:PHE:HD2	1:E:338:ILE:CD1	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:TYR:HB3	1:E:325:ASP:OD2	2.08	0.53
1:D:862:VAL:O	1:D:866:MET:HG2	2.08	0.53
1:A:259:CYS:O	1:A:263:VAL:HG23	2.08	0.53
1:B:278:GLU:CB	1:B:289:ILE:HG13	2.38	0.53
1:F:66:ILE:HG23	1:F:94:PHE:CD1	2.43	0.53
1:F:908:ASP:O	1:F:912:GLU:HG3	2.07	0.53
1:E:674:CYS:HB3	1:E:712:MET:HE1	1.89	0.53
1:G:609:GLN:HE22	1:G:737:HIS:HE1	1.54	0.53
1:A:134:ILE:CD1	1:A:287:TYR:HB3	2.37	0.53
1:A:623:TYR:HB3	1:A:627:VAL:HG21	1.88	0.53
1:B:53:VAL:HG13	1:B:54:GLY:H	1.72	0.53
1:B:160:ILE:HD12	1:B:174:VAL:CG2	2.37	0.53
1:H:53:VAL:HG13	1:H:54:GLY:H	1.73	0.53
1:F:215:GLN:C	1:F:216:ILE:HD12	2.34	0.53
1:F:849:LEU:HD12	1:F:849:LEU:N	2.22	0.53
1:E:120:ILE:HD12	1:E:140:PRO:HG3	1.89	0.53
1:E:600:ARG:NH1	1:E:603:ILE:O	2.41	0.53
1:G:600:ARG:NH1	1:G:603:ILE:O	2.41	0.53
1:A:849:LEU:N	1:A:849:LEU:HD12	2.22	0.53
1:A:870:ILE:O	1:A:872:LYS:NZ	2.40	0.53
1:B:321:TYR:HB3	1:B:325:ASP:OD2	2.09	0.53
1:F:571:PHE:CD2	1:F:572:SER:HB3	2.44	0.53
1:E:288:PHE:CD1	1:E:288:PHE:C	2.87	0.53
1:D:414:ARG:HD3	1:C:25:GLU:HG3	1.89	0.53
1:D:622:ASN:ND2	1:D:917:GLU:O	2.41	0.53
1:A:21:ARG:HH12	1:B:370:GLY:C	2.17	0.53
1:A:225:VAL:HG13	1:A:333:GLN:NE2	2.23	0.53
1:B:81:ILE:O	1:B:106:VAL:CG2	2.57	0.53
1:F:597:GLU:OE1	1:F:971:LYS:NZ	2.26	0.53
1:G:195:PHE:CD2	1:G:195:PHE:N	2.76	0.53
1:D:225:VAL:HG13	1:D:333:GLN:NE2	2.23	0.53
1:D:509:GLY:N	1:D:512:GLN:OE1	2.40	0.53
1:D:571:PHE:CD2	1:D:572:SER:HB3	2.44	0.53
1:A:120:ILE:HD12	1:A:121:LYS:HG2	1.91	0.53
1:A:134:ILE:HG22	1:A:203:GLU:HB3	1.89	0.53
1:A:597:GLU:OE1	1:A:971:LYS:NZ	2.26	0.53
1:C:228:PHE:CD2	1:C:338:ILE:CG1	2.92	0.53
1:C:620:TYR:HD2	1:C:621:LYS:N	2.06	0.53
1:F:54:GLY:HA3	1:F:62:ALA:HB1	1.91	0.53
1:F:126:ALA:HB1	1:F:131:ILE:HD11	1.90	0.53
1:G:219:ASP:CB	1:G:323:LEU:HD23	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLY:C	1:C:21:ARG:HH12	2.14	0.53
1:B:674:CYS:HB3	1:B:712:MET:HE1	1.89	0.53
1:F:134:ILE:CD1	1:F:287:TYR:HB2	2.39	0.53
1:F:177:LYS:O	1:F:180:VAL:HG23	2.09	0.53
1:E:81:ILE:O	1:E:106:VAL:CG2	2.57	0.53
1:D:1:MET:HE1	1:D:319:ASP:HB2	1.91	0.53
1:D:53:VAL:HG13	1:D:54:GLY:H	1.73	0.53
1:D:788:GLY:N	1:A:719:GLN:HG2	2.24	0.53
1:A:134:ILE:CD1	1:A:287:TYR:HB2	2.38	0.53
1:G:960:LEU:HD13	1:G:960:LEU:C	2.33	0.53
1:D:740:THR:HG22	1:D:751:TYR:CZ	2.44	0.53
1:A:395:LEU:HD12	1:A:395:LEU:H	1.73	0.53
1:A:567:LEU:N	1:A:568:PRO:CD	2.71	0.53
1:C:960:LEU:HD13	1:C:960:LEU:C	2.33	0.53
1:H:120:ILE:HD12	1:H:121:LYS:HG2	1.90	0.53
1:H:740:THR:HG22	1:H:751:TYR:CZ	2.44	0.53
1:H:1059:ASN:OD1	1:H:1059:ASN:N	2.42	0.53
1:F:134:ILE:HG22	1:F:203:GLU:HB3	1.90	0.53
1:F:225:VAL:HG13	1:F:333:GLN:NE2	2.24	0.53
1:F:541:ASP:OD2	1:F:741:HIS:HE1	1.92	0.53
1:E:752:ALA:HB1	1:G:749:TYR:CZ	2.43	0.53
1:D:251:THR:HG23	1:D:254:LEU:HB2	1.91	0.53
1:D:1059:ASN:N	1:D:1059:ASN:OD1	2.42	0.53
1:H:213:GLU:OE2	1:H:232:CYS:SG	2.55	0.53
1:H:251:THR:HG23	1:H:254:LEU:HB2	1.91	0.53
1:F:251:THR:HG23	1:F:254:LEU:HB2	1.90	0.53
1:E:280:LEU:CD1	1:E:289:ILE:HG22	2.37	0.53
1:G:509:GLY:N	1:G:512:GLN:OE1	2.39	0.53
1:D:215:GLN:C	1:D:216:ILE:HD12	2.34	0.53
1:H:1:MET:HE1	1:H:319:ASP:HB2	1.91	0.52
1:F:195:PHE:N	1:F:195:PHE:CD2	2.77	0.52
1:E:53:VAL:HG13	1:E:54:GLY:H	1.73	0.52
1:G:540:ARG:NH2	1:G:541:ASP:HA	2.25	0.52
1:D:228:PHE:CE2	1:D:338:ILE:HG13	2.44	0.52
1:A:66:ILE:HG23	1:A:94:PHE:CD1	2.44	0.52
1:F:475:ASN:HA	1:F:1055:ILE:HG21	1.92	0.52
1:F:551:VAL:HA	1:F:813:TYR:CE2	2.44	0.52
1:G:213:GLU:OE2	1:G:232:CYS:SG	2.55	0.52
1:G:227:LEU:HD21	1:G:308:ILE:HD12	1.91	0.52
1:A:1:MET:HE1	1:A:319:ASP:HB2	1.90	0.52
1:A:1010:LEU:HA	1:A:1028:LEU:HD23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:609:GLN:HE22	1:C:737:HIS:HE1	1.55	0.52
1:F:2:ASN:HB2	1:F:321:TYR:OH	2.10	0.52
1:F:370:GLY:C	1:E:21:ARG:HH12	2.18	0.52
1:D:1010:LEU:HA	1:D:1028:LEU:HD23	1.91	0.52
1:A:54:GLY:HA3	1:A:62:ALA:HB1	1.91	0.52
1:A:251:THR:HG23	1:A:254:LEU:HB2	1.90	0.52
1:A:551:VAL:HA	1:A:813:TYR:CE2	2.44	0.52
1:H:370:GLY:C	1:G:21:ARG:NH1	2.68	0.52
1:F:1:MET:HE1	1:F:319:ASP:HB2	1.90	0.52
1:F:509:GLY:N	1:F:512:GLN:OE1	2.40	0.52
1:E:251:THR:HG23	1:E:254:LEU:HB2	1.90	0.52
1:A:53:VAL:HG13	1:A:54:GLY:H	1.74	0.52
1:A:541:ASP:OD2	1:A:741:HIS:HE1	1.92	0.52
1:H:134:ILE:CD1	1:H:287:TYR:HB2	2.39	0.52
1:H:134:ILE:CD1	1:H:287:TYR:HB3	2.36	0.52
1:F:230:ARG:NH2	1:F:296:GLN:OE1	2.43	0.52
1:E:143:GLY:O	1:E:147:VAL:HG23	2.10	0.52
1:E:472:TYR:OH	1:E:1004:PHE:O	2.27	0.52
1:G:160:ILE:CG2	1:G:200:VAL:CG1	2.87	0.52
1:D:996:VAL:O	1:D:999:LEU:HD12	2.09	0.52
1:A:195:PHE:CD2	1:A:195:PHE:N	2.78	0.52
1:B:226:HIS:ND1	1:B:259:CYS:HB3	2.24	0.52
1:B:280:LEU:CD1	1:B:289:ILE:HG22	2.38	0.52
1:F:53:VAL:HG13	1:F:54:GLY:H	1.74	0.52
1:D:230:ARG:NH2	1:D:296:GLN:OE1	2.42	0.52
1:A:177:LYS:O	1:A:180:VAL:HG23	2.09	0.52
1:A:230:ARG:NH2	1:A:296:GLN:OE1	2.43	0.52
1:F:1041:VAL:CG1	1:F:1043:TYR:CE1	2.92	0.52
1:E:54:GLY:HA3	1:E:62:ALA:HB1	1.90	0.52
1:D:54:GLY:HA3	1:D:62:ALA:HB1	1.91	0.52
1:D:120:ILE:HD12	1:D:121:LYS:HG2	1.91	0.52
1:D:134:ILE:CD1	1:D:287:TYR:HB2	2.39	0.52
1:C:1:MET:HE1	1:C:319:ASP:HB2	1.91	0.52
1:C:213:GLU:OE2	1:C:232:CYS:SG	2.54	0.52
1:C:219:ASP:CB	1:C:323:LEU:HD23	2.28	0.52
1:C:251:THR:HG23	1:C:254:LEU:HB2	1.90	0.52
1:H:631:PHE:C	1:H:631:PHE:CD2	2.88	0.52
1:H:996:VAL:O	1:H:999:LEU:HD12	2.10	0.52
1:F:996:VAL:O	1:F:997:THR:C	2.53	0.52
1:G:251:THR:HG23	1:G:254:LEU:HB2	1.90	0.52
1:D:405:PHE:C	1:D:405:PHE:CD2	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:CD1	1:B:174:VAL:HG23	2.39	0.52
1:B:215:GLN:C	1:B:216:ILE:HD12	2.35	0.52
1:C:996:VAL:O	1:C:999:LEU:HD12	2.09	0.52
1:H:225:VAL:HG13	1:H:333:GLN:NE2	2.25	0.52
1:G:164:LEU:HD22	1:G:195:PHE:CZ	2.44	0.52
1:A:2:ASN:HB2	1:A:321:TYR:OH	2.10	0.52
1:A:996:VAL:O	1:A:999:LEU:HD12	2.09	0.52
1:B:472:TYR:OH	1:B:1004:PHE:O	2.28	0.52
1:C:160:ILE:CG2	1:C:200:VAL:CG1	2.88	0.52
1:H:177:LYS:O	1:H:180:VAL:HG23	2.10	0.52
1:E:180:VAL:CG1	1:E:184:PHE:HZ	2.14	0.52
1:E:557:PHE:CE1	1:E:598:THR:HB	2.45	0.52
1:G:250:ILE:CD1	1:G:255:ARG:HB3	2.37	0.52
1:D:2:ASN:HB2	1:D:321:TYR:OH	2.10	0.52
1:D:226:HIS:H	1:D:333:GLN:HE22	1.58	0.52
1:A:475:ASN:HA	1:A:1055:ILE:HG21	1.92	0.52
1:C:23:CYS:HB3	1:C:28:ILE:HB	1.92	0.52
1:C:54:GLY:HA3	1:C:62:ALA:HB1	1.92	0.52
1:H:115:MET:HG2	1:H:125:GLN:HG3	1.92	0.51
1:H:541:ASP:OD2	1:H:741:HIS:CE1	2.63	0.51
1:F:996:VAL:O	1:F:999:LEU:HD12	2.09	0.51
1:E:266:MET:CE	1:E:277:VAL:HG22	2.39	0.51
1:G:1:MET:HE1	1:G:319:ASP:HB2	1.91	0.51
1:G:54:GLY:HA3	1:G:62:ALA:HB1	1.93	0.51
1:G:1059:ASN:OD1	1:G:1059:ASN:N	2.41	0.51
1:D:177:LYS:CG	1:D:178:GLU:H	2.22	0.51
1:D:465:ARG:O	1:D:465:ARG:CG	2.58	0.51
1:D:475:ASN:HA	1:D:1055:ILE:HG21	1.92	0.51
1:B:54:GLY:HA3	1:B:62:ALA:HB1	1.91	0.51
1:C:367:ARG:NH1	1:C:1049:GLN:CB	2.63	0.51
1:C:509:GLY:N	1:C:512:GLN:OE1	2.40	0.51
1:H:54:GLY:HA3	1:H:62:ALA:HB1	1.92	0.51
1:H:226:HIS:H	1:H:333:GLN:HE22	1.58	0.51
1:F:1010:LEU:HA	1:F:1028:LEU:HD23	1.92	0.51
1:E:147:VAL:HG21	1:E:184:PHE:HE1	1.74	0.51
1:G:17:ILE:HA	1:G:20:MET:HG3	1.91	0.51
1:G:23:CYS:HB3	1:G:28:ILE:HB	1.92	0.51
1:A:734:VAL:HG12	1:A:735:PRO:HD2	1.92	0.51
1:B:557:PHE:CE1	1:B:598:THR:HB	2.45	0.51
1:H:66:ILE:HG23	1:H:94:PHE:HD1	1.75	0.51
1:H:475:ASN:HA	1:H:1055:ILE:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:ARG:NH2	1:E:541:ASP:OD1	2.44	0.51
1:E:996:VAL:O	1:E:999:LEU:HD12	2.10	0.51
1:G:225:VAL:HG13	1:G:333:GLN:NE2	2.26	0.51
1:G:228:PHE:CE2	1:G:338:ILE:HG13	2.45	0.51
1:G:996:VAL:O	1:G:999:LEU:HD12	2.09	0.51
1:D:120:ILE:HD12	1:D:121:LYS:H	1.76	0.51
1:B:356:PHE:CD1	1:B:356:PHE:N	2.79	0.51
1:B:996:VAL:O	1:B:999:LEU:HD12	2.10	0.51
1:C:88:LEU:HB3	1:C:94:PHE:CD2	2.38	0.51
1:H:93:GLU:O	1:H:96:ARG:HG2	2.11	0.51
1:H:465:ARG:O	1:H:465:ARG:CG	2.58	0.51
1:H:571:PHE:CD2	1:H:572:SER:HB3	2.45	0.51
1:H:1010:LEU:HA	1:H:1028:LEU:HD23	1.92	0.51
1:F:2:ASN:HB3	1:F:319:ASP:OD2	2.11	0.51
1:F:21:ARG:HH12	1:E:370:GLY:C	2.19	0.51
1:F:734:VAL:HG12	1:F:735:PRO:HD2	1.93	0.51
1:E:131:ILE:HD12	1:E:132:PRO:O	2.10	0.51
1:G:540:ARG:HH21	1:G:541:ASP:CA	2.23	0.51
1:B:131:ILE:HD12	1:B:132:PRO:O	2.10	0.51
1:B:158:LEU:CD1	1:B:174:VAL:HB	2.22	0.51
1:H:2:ASN:HB2	1:H:321:TYR:OH	2.10	0.51
1:F:160:ILE:CG2	1:F:200:VAL:CG1	2.88	0.51
1:F:862:VAL:O	1:F:866:MET:HG2	2.09	0.51
1:B:251:THR:HG23	1:B:254:LEU:HB2	1.91	0.51
1:B:266:MET:CE	1:B:277:VAL:HG22	2.40	0.51
1:B:475:ASN:HA	1:B:1055:ILE:HG21	1.92	0.51
1:C:225:VAL:HG13	1:C:333:GLN:NE2	2.26	0.51
1:H:21:ARG:NH1	1:G:370:GLY:C	2.68	0.51
1:E:475:ASN:HA	1:E:1055:ILE:HG21	1.92	0.51
1:E:749:TYR:CZ	1:G:752:ALA:CB	2.94	0.51
1:G:183:SER:HA	1:G:186:ARG:HD2	1.92	0.51
1:D:754:ALA:HB1	1:D:759:VAL:HG11	1.92	0.51
1:A:2:ASN:HB3	1:A:319:ASP:OD2	2.11	0.51
1:A:1041:VAL:CG1	1:A:1043:TYR:CE1	2.93	0.51
1:C:183:SER:HA	1:C:186:ARG:HD2	1.92	0.51
1:C:228:PHE:CD2	1:C:338:ILE:HG13	2.46	0.51
1:H:120:ILE:HD12	1:H:121:LYS:H	1.76	0.51
1:H:405:PHE:C	1:H:405:PHE:CD2	2.89	0.51
1:E:675:TYR:CE2	1:E:716:LEU:CD1	2.93	0.51
1:D:93:GLU:O	1:D:96:ARG:HG2	2.11	0.51
1:D:631:PHE:C	1:D:631:PHE:CD2	2.89	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:CD1	1:A:565:HIS:CE1	2.93	0.51
1:A:509:GLY:N	1:A:512:GLN:OE1	2.41	0.51
1:C:1059:ASN:N	1:C:1059:ASN:OD1	2.42	0.51
1:H:230:ARG:NH2	1:H:296:GLN:OE1	2.43	0.51
1:F:44:ARG:HD3	1:F:45:TYR:CD1	2.46	0.51
1:E:12:ARG:CZ	1:E:391:TYR:CD1	2.94	0.51
1:E:180:VAL:O	1:E:184:PHE:CE2	2.64	0.51
1:D:112:HIS:CE1	1:D:271:TYR:HA	2.46	0.51
1:B:552:ARG:HD2	1:B:1004:PHE:CD1	2.46	0.51
1:C:250:ILE:CD1	1:C:255:ARG:HB3	2.37	0.51
1:H:354:ASN:HD22	1:H:357:MET:CB	2.23	0.51
1:H:754:ALA:HB1	1:H:759:VAL:HG11	1.93	0.51
1:G:131:ILE:HD12	1:G:132:PRO:O	2.11	0.51
1:G:134:ILE:HG22	1:G:203:GLU:HB3	1.93	0.51
1:D:134:ILE:CD1	1:D:287:TYR:HB3	2.38	0.51
1:A:754:ALA:HB1	1:A:759:VAL:HG11	1.93	0.51
1:C:2:ASN:HB3	1:C:319:ASP:OD2	2.11	0.51
1:C:131:ILE:HD12	1:C:132:PRO:O	2.11	0.51
1:H:737:HIS:HA	1:H:761:ILE:O	2.11	0.51
1:H:788:GLY:N	1:F:719:GLN:HG2	2.25	0.51
1:E:226:HIS:H	1:E:333:GLN:HE22	1.58	0.51
1:G:2:ASN:HB3	1:G:319:ASP:OD2	2.12	0.51
1:A:44:ARG:HD3	1:A:45:TYR:CD1	2.46	0.51
1:A:862:VAL:O	1:A:866:MET:HG2	2.10	0.51
1:A:1059:ASN:N	1:A:1059:ASN:OD1	2.42	0.51
1:B:12:ARG:CZ	1:B:391:TYR:CD1	2.94	0.51
1:C:832:MET:HG3	1:C:833:PRO:HD3	1.93	0.51
1:H:112:HIS:CE1	1:H:271:TYR:HA	2.46	0.50
1:H:960:LEU:HD13	1:H:976:TYR:CD2	2.46	0.50
1:F:737:HIS:HA	1:F:761:ILE:O	2.12	0.50
1:E:502:TYR:HD1	1:E:503:GLY:N	2.08	0.50
1:E:752:ALA:CB	1:G:749:TYR:CZ	2.94	0.50
1:D:115:MET:HG2	1:D:125:GLN:HG3	1.93	0.50
1:D:541:ASP:OD2	1:D:741:HIS:CE1	2.64	0.50
1:D:662:VAL:HB	1:D:669:VAL:HG22	1.93	0.50
1:D:719:GLN:HG2	1:A:788:GLY:N	2.26	0.50
1:A:160:ILE:CG2	1:A:200:VAL:CG1	2.89	0.50
1:C:475:ASN:HA	1:C:1055:ILE:HG21	1.92	0.50
1:H:453:THR:HG22	1:H:455:GLU:OE1	2.11	0.50
1:G:475:ASN:HA	1:G:1055:ILE:HG21	1.92	0.50
1:A:996:VAL:O	1:A:997:THR:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:H	1:B:333:GLN:HE22	1.58	0.50
1:B:228:PHE:CD2	1:B:338:ILE:HD11	2.37	0.50
1:B:675:TYR:CE2	1:B:716:LEU:CD1	2.94	0.50
1:C:44:ARG:HD3	1:C:45:TYR:CD1	2.46	0.50
1:C:510:THR:OG1	1:C:607:MET:CG	2.58	0.50
1:C:651:TRP:NE1	1:C:653:LYS:CB	2.75	0.50
1:H:116:PHE:N	1:H:116:PHE:CD1	2.77	0.50
1:H:356:PHE:N	1:H:356:PHE:HD1	2.10	0.50
1:F:1059:ASN:N	1:F:1059:ASN:OD1	2.43	0.50
1:E:23:CYS:HB3	1:E:28:ILE:HB	1.92	0.50
1:E:541:ASP:HA	1:E:544:GLN:HB3	1.94	0.50
1:G:127:LEU:HD22	1:G:133:VAL:CG2	2.41	0.50
1:G:1010:LEU:HA	1:G:1028:LEU:HD23	1.93	0.50
1:D:44:ARG:HD3	1:D:45:TYR:CE1	2.46	0.50
1:D:453:THR:HG22	1:D:455:GLU:OE1	2.12	0.50
1:A:737:HIS:HA	1:A:761:ILE:O	2.12	0.50
1:C:120:ILE:HD12	1:C:121:LYS:H	1.76	0.50
1:H:42:PHE:HA	1:H:45:TYR:CD2	2.46	0.50
1:H:428:ILE:HA	1:H:431:LEU:HD12	1.93	0.50
1:H:662:VAL:HB	1:H:669:VAL:HG22	1.94	0.50
1:F:570:MET:HG3	1:F:573:PHE:HE1	1.76	0.50
1:B:180:VAL:CG1	1:B:184:PHE:CZ	2.72	0.50
1:H:215:GLN:C	1:H:216:ILE:HD12	2.36	0.50
1:G:112:HIS:O	1:G:116:PHE:HD2	1.95	0.50
1:G:662:VAL:HB	1:G:669:VAL:HG22	1.93	0.50
1:G:737:HIS:HA	1:G:761:ILE:O	2.11	0.50
1:D:7:VAL:HG11	1:D:23:CYS:SG	2.52	0.50
1:C:453:THR:HG22	1:C:455:GLU:OE1	2.12	0.50
1:C:610:MET:HG2	1:C:640:VAL:HG11	1.94	0.50
1:H:2:ASN:HB3	1:H:319:ASP:OD2	2.11	0.50
1:H:766:SER:O	1:H:767:SER:C	2.55	0.50
1:F:219:ASP:CB	1:F:323:LEU:HD23	2.28	0.50
1:F:754:ALA:HB1	1:F:759:VAL:HG11	1.94	0.50
1:E:112:HIS:CE1	1:E:271:TYR:HA	2.47	0.50
1:E:552:ARG:HD2	1:E:1004:PHE:CD1	2.46	0.50
1:G:610:MET:HG2	1:G:640:VAL:HG11	1.94	0.50
1:D:66:ILE:HG23	1:D:94:PHE:HD1	1.76	0.50
1:C:134:ILE:HG22	1:C:203:GLU:HB3	1.94	0.50
1:C:540:ARG:HH21	1:C:541:ASP:CA	2.24	0.50
1:H:44:ARG:HD3	1:H:45:TYR:CE1	2.47	0.50
1:H:356:PHE:CD1	1:H:356:PHE:N	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:567:LEU:N	1:H:568:PRO:CD	2.73	0.50
1:F:112:HIS:CE1	1:F:271:TYR:HA	2.47	0.50
1:G:7:VAL:HG11	1:G:23:CYS:SG	2.52	0.50
1:G:453:THR:HG22	1:G:455:GLU:OE1	2.12	0.50
1:G:832:MET:HG3	1:G:833:PRO:HD3	1.94	0.50
1:B:23:CYS:HB3	1:B:28:ILE:HB	1.93	0.50
1:C:551:VAL:HA	1:C:813:TYR:CE2	2.46	0.50
1:C:589:ASN:OD1	1:C:989:MET:CE	2.60	0.50
1:C:1010:LEU:HA	1:C:1028:LEU:HD23	1.93	0.50
1:G:589:ASN:OD1	1:G:989:MET:CE	2.60	0.50
1:G:996:VAL:O	1:G:997:THR:C	2.54	0.50
1:D:12:ARG:NH1	1:D:391:TYR:CB	2.74	0.50
1:D:42:PHE:HA	1:D:45:TYR:CD2	2.46	0.50
1:D:532:VAL:HG12	1:D:791:GLN:O	2.12	0.50
1:C:230:ARG:NH2	1:C:296:GLN:OE1	2.45	0.50
1:H:17:ILE:HA	1:H:20:MET:HG3	1.93	0.50
1:H:21:ARG:NH1	1:G:370:GLY:O	2.44	0.50
1:H:532:VAL:HG12	1:H:791:GLN:O	2.12	0.50
1:H:719:GLN:HG2	1:F:788:GLY:N	2.27	0.50
1:F:288:PHE:C	1:F:288:PHE:CD1	2.90	0.50
1:F:405:PHE:C	1:F:405:PHE:CD2	2.89	0.50
1:F:622:ASN:ND2	1:F:917:GLU:O	2.45	0.50
1:E:228:PHE:CD2	1:E:338:ILE:CG1	2.95	0.50
1:G:44:ARG:HD3	1:G:45:TYR:CD1	2.47	0.50
1:G:510:THR:OG1	1:G:607:MET:CG	2.58	0.50
1:D:2:ASN:HB3	1:D:319:ASP:OD2	2.11	0.50
1:D:176:SER:OG	1:D:177:LYS:HE2	2.12	0.50
1:D:737:HIS:HA	1:D:761:ILE:O	2.12	0.50
1:A:112:HIS:CE1	1:A:271:TYR:HA	2.47	0.50
1:A:134:ILE:CG2	1:A:203:GLU:HB3	2.42	0.50
1:B:180:VAL:HG12	1:B:184:PHE:CE1	2.38	0.50
1:B:228:PHE:CD2	1:B:338:ILE:CG1	2.95	0.50
1:C:737:HIS:HA	1:C:761:ILE:O	2.12	0.50
1:F:541:ASP:OD2	1:F:741:HIS:CE1	2.65	0.49
1:E:428:ILE:HA	1:E:431:LEU:HD12	1.94	0.49
1:D:116:PHE:N	1:D:116:PHE:CD1	2.77	0.49
1:D:996:VAL:O	1:D:997:THR:C	2.54	0.49
1:A:226:HIS:H	1:A:333:GLN:HE22	1.58	0.49
1:B:134:ILE:HD12	1:B:287:TYR:CB	2.42	0.49
1:C:7:VAL:HG11	1:C:23:CYS:SG	2.52	0.49
1:F:532:VAL:HG12	1:F:791:GLN:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:PHE:CD1	1:E:356:PHE:N	2.81	0.49
1:G:111:LYS:O	1:G:115:MET:HG2	2.12	0.49
1:G:213:GLU:O	1:G:229:GLU:HA	2.12	0.49
1:G:428:ILE:HA	1:G:431:LEU:HD12	1.93	0.49
1:D:546:LEU:CD1	1:D:774:SER:HB2	2.42	0.49
1:A:570:MET:HG3	1:A:573:PHE:HE1	1.77	0.49
1:B:177:LYS:O	1:B:178:GLU:CB	2.60	0.49
1:H:7:VAL:HG11	1:H:23:CYS:SG	2.52	0.49
1:F:42:PHE:HA	1:F:45:TYR:CD2	2.47	0.49
1:F:134:ILE:CG2	1:F:203:GLU:HB3	2.43	0.49
1:F:428:ILE:HA	1:F:431:LEU:HD12	1.94	0.49
1:F:712:MET:O	1:F:741:HIS:HD2	1.95	0.49
1:E:546:LEU:CD1	1:E:774:SER:HB2	2.43	0.49
1:E:754:ALA:HB1	1:E:759:VAL:HG11	1.94	0.49
1:E:1010:LEU:HA	1:E:1028:LEU:HD23	1.94	0.49
1:D:356:PHE:CD1	1:D:356:PHE:N	2.80	0.49
1:B:754:ALA:HB1	1:B:759:VAL:HG11	1.94	0.49
1:C:356:PHE:CD1	1:C:356:PHE:N	2.81	0.49
1:C:546:LEU:CD1	1:C:774:SER:HB2	2.43	0.49
1:C:662:VAL:HB	1:C:669:VAL:HG22	1.94	0.49
1:H:474:GLY:O	1:H:478:VAL:HG23	2.12	0.49
1:H:708:GLY:HA2	1:H:737:HIS:O	2.12	0.49
1:H:851:ASP:OD2	1:H:852:ARG:N	2.45	0.49
1:F:226:HIS:H	1:F:333:GLN:HE22	1.59	0.49
1:F:534:LEU:O	1:F:570:MET:HE3	2.13	0.49
1:G:754:ALA:HB1	1:G:759:VAL:HG11	1.94	0.49
1:D:17:ILE:HA	1:D:20:MET:HG3	1.94	0.49
1:D:213:GLU:O	1:D:229:GLU:HA	2.12	0.49
1:D:428:ILE:HA	1:D:431:LEU:HD12	1.94	0.49
1:B:356:PHE:N	1:B:356:PHE:HD1	2.09	0.49
1:B:1010:LEU:HA	1:B:1028:LEU:HD23	1.94	0.49
1:C:112:HIS:O	1:C:116:PHE:HD2	1.96	0.49
1:C:226:HIS:H	1:C:333:GLN:HE22	1.58	0.49
1:H:12:ARG:NH1	1:H:391:TYR:CB	2.75	0.49
1:H:546:LEU:CD1	1:H:774:SER:HB2	2.42	0.49
1:F:111:LYS:O	1:F:115:MET:HG2	2.12	0.49
1:G:88:LEU:HB3	1:G:94:PHE:CD2	2.39	0.49
1:G:230:ARG:NH2	1:G:296:GLN:OE1	2.46	0.49
1:G:520:GLU:OE1	1:G:705:HIS:NE2	2.45	0.49
1:A:42:PHE:HA	1:A:45:TYR:CD2	2.47	0.49
1:A:541:ASP:OD2	1:A:741:HIS:CE1	2.66	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:MET:HB3	1:A:573:PHE:HE2	1.75	0.49
1:A:622:ASN:ND2	1:A:917:GLU:O	2.46	0.49
1:B:112:HIS:CE1	1:B:271:TYR:HA	2.47	0.49
1:B:567:LEU:N	1:B:568:PRO:CD	2.75	0.49
1:B:996:VAL:O	1:B:997:THR:C	2.56	0.49
1:C:17:ILE:HA	1:C:20:MET:HG3	1.94	0.49
1:C:127:LEU:HD22	1:C:133:VAL:CG2	2.42	0.49
1:C:540:ARG:NH2	1:C:541:ASP:HA	2.26	0.49
1:H:176:SER:OG	1:H:177:LYS:HE2	2.12	0.49
1:E:226:HIS:ND1	1:E:259:CYS:HB3	2.27	0.49
1:G:176:SER:O	1:G:179:HIS:CD2	2.65	0.49
1:G:356:PHE:CD1	1:G:356:PHE:N	2.81	0.49
1:G:546:LEU:CD1	1:G:774:SER:HB2	2.43	0.49
1:G:551:VAL:HA	1:G:813:TYR:CE2	2.47	0.49
1:D:356:PHE:N	1:D:356:PHE:HD1	2.11	0.49
1:A:453:THR:HG22	1:A:455:GLU:OE1	2.12	0.49
1:B:368:SER:HA	1:B:419:PHE:CE1	2.48	0.49
1:B:541:ASP:HA	1:B:544:GLN:HB3	1.95	0.49
1:B:603:ILE:CD1	1:B:608:PHE:CZ	2.95	0.49
1:H:23:CYS:HB3	1:H:28:ILE:HB	1.95	0.49
1:H:540:ARG:O	1:H:542:ALA:N	2.43	0.49
1:H:996:VAL:O	1:H:997:THR:C	2.54	0.49
1:F:708:GLY:HA2	1:F:737:HIS:O	2.13	0.49
1:E:228:PHE:CD2	1:E:338:ILE:HG13	2.48	0.49
1:E:567:LEU:N	1:E:568:PRO:CD	2.75	0.49
1:G:182:GLU:O	1:G:186:ARG:HD2	2.13	0.49
1:G:437:HIS:CE1	1:G:439:ASP:HB2	2.48	0.49
1:G:519:PRO:HB2	1:G:705:HIS:HE2	1.76	0.49
1:G:532:VAL:HG12	1:G:791:GLN:O	2.13	0.49
1:D:851:ASP:OD2	1:D:852:ARG:N	2.45	0.49
1:A:226:HIS:ND1	1:A:259:CYS:HB3	2.28	0.49
1:B:112:HIS:O	1:B:116:PHE:HD2	1.95	0.49
1:B:428:ILE:HA	1:B:431:LEU:HD12	1.95	0.49
1:B:546:LEU:CD1	1:B:774:SER:HB2	2.43	0.49
1:C:520:GLU:OE1	1:C:705:HIS:NE2	2.46	0.49
1:C:754:ALA:HB1	1:C:759:VAL:HG11	1.94	0.49
1:C:996:VAL:O	1:C:997:THR:C	2.55	0.49
1:F:453:THR:HG22	1:F:455:GLU:OE1	2.12	0.49
1:E:7:VAL:HG11	1:E:23:CYS:SG	2.53	0.49
1:E:112:HIS:O	1:E:116:PHE:HD2	1.95	0.49
1:G:112:HIS:CE1	1:G:271:TYR:HA	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:405:PHE:C	1:G:405:PHE:CD2	2.90	0.49
1:D:567:LEU:N	1:D:568:PRO:CD	2.74	0.49
1:A:111:LYS:O	1:A:115:MET:HG2	2.13	0.49
1:A:511:LYS:NZ	1:A:641:ASP:OD2	2.46	0.49
1:A:532:VAL:HG12	1:A:791:GLN:O	2.12	0.49
1:A:534:LEU:O	1:A:570:MET:HE3	2.13	0.49
1:B:510:THR:OG1	1:B:607:MET:CG	2.59	0.49
1:E:225:VAL:HG13	1:E:333:GLN:NE2	2.28	0.49
1:E:708:GLY:HA2	1:E:737:HIS:O	2.13	0.49
1:D:23:CYS:HB3	1:D:28:ILE:HB	1.95	0.49
1:D:534:LEU:O	1:D:570:MET:HE3	2.12	0.49
1:D:540:ARG:O	1:D:542:ALA:N	2.43	0.49
1:D:960:LEU:HD13	1:D:976:TYR:CD2	2.47	0.49
1:A:708:GLY:HA2	1:A:737:HIS:O	2.13	0.49
1:B:1:MET:HE3	1:B:319:ASP:OD2	2.13	0.49
1:C:519:PRO:HB2	1:C:705:HIS:HE2	1.75	0.49
1:C:532:VAL:HG12	1:C:791:GLN:O	2.13	0.49
1:H:918:ILE:HD12	1:H:919:GLY:H	1.77	0.49
1:F:23:CYS:HB3	1:F:28:ILE:HB	1.94	0.49
1:F:213:GLU:O	1:F:229:GLU:HA	2.12	0.49
1:F:918:ILE:HD12	1:F:919:GLY:H	1.78	0.49
1:E:64:LEU:CD2	1:E:88:LEU:CD2	2.91	0.49
1:G:226:HIS:H	1:G:333:GLN:HE22	1.58	0.49
1:D:708:GLY:HA2	1:D:737:HIS:O	2.13	0.49
1:A:7:VAL:HG11	1:A:23:CYS:SG	2.53	0.49
1:A:712:MET:O	1:A:741:HIS:HD2	1.96	0.49
1:B:708:GLY:HA2	1:B:737:HIS:O	2.13	0.49
1:C:111:LYS:O	1:C:115:MET:HG2	2.13	0.49
1:C:112:HIS:CE1	1:C:271:TYR:HA	2.47	0.49
1:C:182:GLU:O	1:C:186:ARG:HD2	2.13	0.49
1:H:42:PHE:HA	1:H:45:TYR:HD2	1.78	0.48
1:F:563:MET:HB3	1:F:573:PHE:HE2	1.76	0.48
1:D:620:TYR:CE2	1:D:621:LYS:HE3	2.47	0.48
1:A:709:ILE:HB	1:A:738:LEU:CD1	2.43	0.48
1:B:44:ARG:HD3	1:B:45:TYR:CD1	2.47	0.48
1:B:631:PHE:C	1:B:631:PHE:CD2	2.91	0.48
1:C:213:GLU:O	1:C:229:GLU:HA	2.13	0.48
1:H:226:HIS:ND1	1:H:259:CYS:HB3	2.28	0.48
1:F:226:HIS:ND1	1:F:259:CYS:HB3	2.28	0.48
1:F:662:VAL:HB	1:F:669:VAL:HG22	1.95	0.48
1:F:709:ILE:HB	1:F:738:LEU:CD1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:948:MET:HE2	1:E:948:MET:HA	1.94	0.48
1:E:996:VAL:O	1:E:997:THR:C	2.56	0.48
1:D:42:PHE:HA	1:D:45:TYR:HD2	1.78	0.48
1:D:541:ASP:HA	1:D:544:GLN:HB3	1.94	0.48
1:A:546:LEU:CD1	1:A:774:SER:HB2	2.42	0.48
1:A:918:ILE:HD12	1:A:919:GLY:H	1.78	0.48
1:B:7:VAL:HG11	1:B:23:CYS:SG	2.53	0.48
1:C:12:ARG:NH1	1:C:38:ASP:OD2	2.46	0.48
1:C:356:PHE:N	1:C:356:PHE:HD1	2.12	0.48
1:H:611:LEU:HD11	1:H:646:PHE:CD1	2.48	0.48
1:H:712:MET:O	1:H:741:HIS:HD2	1.96	0.48
1:F:511:LYS:NZ	1:F:641:ASP:OD2	2.47	0.48
1:E:532:VAL:HG12	1:E:791:GLN:O	2.12	0.48
1:G:42:PHE:HA	1:G:45:TYR:CD2	2.47	0.48
1:G:589:ASN:CG	1:G:989:MET:HE2	2.37	0.48
1:D:279:PHE:C	1:D:289:ILE:HD11	2.38	0.48
1:D:766:SER:O	1:D:767:SER:C	2.57	0.48
1:A:213:GLU:O	1:A:229:GLU:HA	2.12	0.48
1:A:228:PHE:CE2	1:A:338:ILE:HG13	2.48	0.48
1:B:12:ARG:CZ	1:B:391:TYR:HD1	2.25	0.48
1:B:532:VAL:HG12	1:B:791:GLN:O	2.12	0.48
1:C:960:LEU:HD11	1:C:968:PRO:CG	2.36	0.48
1:F:228:PHE:CE2	1:F:338:ILE:HG13	2.48	0.48
1:F:546:LEU:CD1	1:F:774:SER:HB2	2.42	0.48
1:E:44:ARG:HD3	1:E:45:TYR:CD1	2.48	0.48
1:G:356:PHE:N	1:G:356:PHE:HD1	2.12	0.48
1:G:960:LEU:HD11	1:G:968:PRO:CG	2.36	0.48
1:D:611:LEU:HD11	1:D:646:PHE:CD1	2.48	0.48
1:A:23:CYS:HB3	1:A:28:ILE:HB	1.95	0.48
1:A:156:TYR:CB	1:A:157:PRO:HD3	2.43	0.48
1:F:611:LEU:HD11	1:F:646:PHE:CD1	2.48	0.48
1:E:12:ARG:CZ	1:E:391:TYR:HD1	2.25	0.48
1:E:344:GLN:HG3	1:E:399:CYS:HG	1.78	0.48
1:G:12:ARG:NH1	1:G:38:ASP:OD2	2.47	0.48
1:G:182:GLU:O	1:G:186:ARG:NE	2.45	0.48
1:G:288:PHE:CD1	1:G:288:PHE:C	2.91	0.48
1:G:567:LEU:N	1:G:568:PRO:CD	2.76	0.48
1:G:992:LYS:HE3	1:G:993:TYR:CZ	2.47	0.48
1:D:474:GLY:O	1:D:478:VAL:HG23	2.13	0.48
1:A:533:LEU:O	1:A:761:ILE:HA	2.14	0.48
1:B:662:VAL:HB	1:B:669:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:PHE:C	1:C:288:PHE:CD1	2.91	0.48
1:C:589:ASN:CG	1:C:989:MET:HE2	2.38	0.48
1:H:213:GLU:O	1:H:229:GLU:HA	2.14	0.48
1:H:279:PHE:C	1:H:289:ILE:HD11	2.38	0.48
1:H:534:LEU:O	1:H:570:MET:HE3	2.13	0.48
1:F:7:VAL:HG11	1:F:23:CYS:SG	2.54	0.48
1:E:603:ILE:CD1	1:E:608:PHE:CZ	2.96	0.48
1:G:830:HIS:O	1:G:832:MET:HE2	2.13	0.48
1:A:266:MET:HE1	1:A:271:TYR:CE1	2.47	0.48
1:A:611:LEU:HD11	1:A:646:PHE:CD1	2.48	0.48
1:B:64:LEU:CD2	1:B:88:LEU:CD2	2.91	0.48
1:B:82:HIS:CD2	1:B:84:GLY:H	2.23	0.48
1:B:228:PHE:CD2	1:B:338:ILE:HG13	2.48	0.48
1:B:626:ASN:ND2	1:B:950:PRO:HB3	2.28	0.48
1:C:992:LYS:HE3	1:C:993:TYR:CZ	2.48	0.48
1:E:626:ASN:ND2	1:E:950:PRO:HB3	2.28	0.48
1:E:737:HIS:HA	1:E:761:ILE:O	2.13	0.48
1:G:144:ILE:HG23	1:G:184:PHE:CD2	2.49	0.48
1:D:437:HIS:CE1	1:D:439:ASP:HB2	2.49	0.48
1:D:712:MET:O	1:D:741:HIS:HD2	1.96	0.48
1:B:180:VAL:O	1:B:184:PHE:CE2	2.67	0.48
1:B:737:HIS:HA	1:B:761:ILE:O	2.13	0.48
1:F:42:PHE:HA	1:F:45:TYR:HD2	1.78	0.48
1:F:533:LEU:O	1:F:761:ILE:HA	2.14	0.48
1:G:472:TYR:OH	1:G:1004:PHE:O	2.28	0.48
1:D:918:ILE:HD12	1:D:919:GLY:H	1.78	0.48
1:C:176:SER:O	1:C:179:HIS:CD2	2.66	0.48
1:C:963:LYS:HA	1:C:963:LYS:HE3	1.96	0.48
1:F:120:ILE:HD12	1:F:121:LYS:H	1.76	0.48
1:F:541:ASP:HA	1:F:544:GLN:HB3	1.95	0.48
1:E:662:VAL:HB	1:E:669:VAL:HG22	1.94	0.48
1:D:354:ASN:HD22	1:D:357:MET:CB	2.26	0.48
1:B:144:ILE:HD12	1:B:145:LYS:H	1.79	0.48
1:B:749:TYR:CZ	1:C:752:ALA:CB	2.97	0.48
1:C:158:LEU:C	1:C:205:CYS:SG	2.97	0.48
1:C:175:GLU:HG3	1:C:179:HIS:CD2	2.48	0.48
1:C:428:ILE:HA	1:C:431:LEU:HD12	1.94	0.48
1:C:437:HIS:CE1	1:C:439:ASP:HB2	2.49	0.48
1:H:437:HIS:CE1	1:H:439:ASP:HB2	2.49	0.48
1:H:709:ILE:HB	1:H:738:LEU:CD1	2.44	0.48
1:F:1041:VAL:HG11	1:F:1043:TYR:HE1	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:631:PHE:C	1:E:631:PHE:CD2	2.92	0.48
1:A:112:HIS:O	1:A:116:PHE:HD2	1.95	0.48
1:A:428:ILE:HA	1:A:431:LEU:HD12	1.96	0.48
1:A:541:ASP:HA	1:A:544:GLN:HB3	1.95	0.48
1:C:42:PHE:HA	1:C:45:TYR:CD2	2.48	0.48
1:H:472:TYR:OH	1:H:1004:PHE:O	2.27	0.47
1:H:559:ILE:HD13	1:H:805:TYR:CG	2.49	0.47
1:F:347:ILE:O	1:F:395:LEU:CD1	2.55	0.47
1:G:120:ILE:HD12	1:G:121:LYS:H	1.79	0.47
1:G:533:LEU:O	1:G:761:ILE:HA	2.14	0.47
1:G:651:TRP:NE1	1:G:653:LYS:CB	2.77	0.47
1:D:226:HIS:ND1	1:D:259:CYS:HB3	2.29	0.47
1:C:510:THR:OG1	1:C:607:MET:SD	2.71	0.47
1:E:675:TYR:CE2	1:E:716:LEU:HD12	2.49	0.47
1:G:42:PHE:HA	1:G:45:TYR:HD2	1.79	0.47
1:D:472:TYR:OH	1:D:1004:PHE:O	2.28	0.47
1:A:662:VAL:HB	1:A:669:VAL:HG22	1.95	0.47
1:B:180:VAL:CG1	1:B:184:PHE:HZ	2.17	0.47
1:C:533:LEU:O	1:C:761:ILE:HA	2.15	0.47
1:H:82:HIS:CD2	1:H:84:GLY:H	2.24	0.47
1:H:610:MET:HG2	1:H:640:VAL:HG11	1.95	0.47
1:E:64:LEU:HD23	1:E:88:LEU:CD2	2.44	0.47
1:E:368:SER:HA	1:E:419:PHE:CE1	2.49	0.47
1:E:509:GLY:HA3	1:E:605:ASN:O	2.14	0.47
1:G:144:ILE:HA	1:G:184:PHE:CE2	2.50	0.47
1:A:194:ALA:HB1	1:A:195:PHE:CE2	2.49	0.47
1:A:405:PHE:C	1:A:405:PHE:CD2	2.91	0.47
1:B:752:ALA:HB1	1:C:749:TYR:CZ	2.48	0.47
1:C:182:GLU:O	1:C:186:ARG:NE	2.46	0.47
1:H:64:LEU:CD2	1:H:88:LEU:CD2	2.92	0.47
1:H:898:TYR:HD1	1:H:928:LYS:HE2	1.77	0.47
1:F:112:HIS:O	1:F:116:PHE:HD2	1.96	0.47
1:F:437:HIS:CE1	1:F:439:ASP:HB2	2.49	0.47
1:G:510:THR:OG1	1:G:607:MET:SD	2.71	0.47
1:D:176:SER:O	1:D:179:HIS:ND1	2.26	0.47
1:A:288:PHE:C	1:A:288:PHE:CD1	2.92	0.47
1:B:405:PHE:C	1:B:405:PHE:CD2	2.92	0.47
1:B:464:ASP:CG	1:B:467:THR:OG1	2.58	0.47
1:H:278:GLU:C	1:H:289:ILE:HD11	2.40	0.47
1:F:509:GLY:HA3	1:F:605:ASN:O	2.14	0.47
1:E:134:ILE:HD12	1:E:287:TYR:CB	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ASN:ND2	1:E:357:MET:HB3	2.29	0.47
1:E:356:PHE:N	1:E:356:PHE:HD1	2.11	0.47
1:E:464:ASP:CG	1:E:467:THR:OG1	2.58	0.47
1:D:709:ILE:HB	1:D:738:LEU:CD1	2.45	0.47
1:B:540:ARG:HH21	1:B:541:ASP:CG	2.23	0.47
1:C:509:GLY:HA3	1:C:605:ASN:O	2.14	0.47
1:C:567:LEU:N	1:C:568:PRO:CD	2.77	0.47
1:H:352:PRO:HA	1:H:356:PHE:CE1	2.49	0.47
1:H:620:TYR:CE2	1:H:621:LYS:HE3	2.48	0.47
1:E:540:ARG:O	1:E:542:ALA:N	2.45	0.47
1:D:278:GLU:C	1:D:289:ILE:HD11	2.40	0.47
1:A:42:PHE:HA	1:A:45:TYR:HD2	1.79	0.47
1:A:509:GLY:HA3	1:A:605:ASN:O	2.14	0.47
1:B:225:VAL:HG13	1:B:333:GLN:NE2	2.30	0.47
1:B:540:ARG:O	1:B:542:ALA:N	2.46	0.47
1:C:830:HIS:O	1:C:832:MET:HE2	2.14	0.47
1:H:450:ILE:HG22	1:H:451:ASP:N	2.29	0.47
1:H:546:LEU:HD11	1:H:774:SER:HB2	1.97	0.47
1:E:111:LYS:O	1:E:115:MET:HG2	2.14	0.47
1:E:450:ILE:HG22	1:E:451:ASP:N	2.29	0.47
1:E:533:LEU:O	1:E:761:ILE:HA	2.15	0.47
1:E:1018:LEU:HD11	1:E:1024:LEU:HD11	1.95	0.47
1:G:157:PRO:O	1:G:205:CYS:HB2	2.15	0.47
1:G:509:GLY:HA3	1:G:605:ASN:O	2.14	0.47
1:G:963:LYS:HA	1:G:963:LYS:HE3	1.96	0.47
1:D:369:THR:O	1:D:376:LEU:HD11	2.15	0.47
1:D:559:ILE:HD13	1:D:805:TYR:CG	2.49	0.47
1:A:120:ILE:HD12	1:A:121:LYS:H	1.78	0.47
1:A:347:ILE:O	1:A:395:LEU:CD1	2.55	0.47
1:A:437:HIS:CE1	1:A:439:ASP:HB2	2.50	0.47
1:A:559:ILE:HD13	1:A:805:TYR:CG	2.50	0.47
1:B:64:LEU:HD23	1:B:88:LEU:CD2	2.44	0.47
1:B:533:LEU:O	1:B:761:ILE:HA	2.15	0.47
1:B:559:ILE:HD13	1:B:805:TYR:CG	2.50	0.47
1:B:675:TYR:CE2	1:B:716:LEU:HD12	2.50	0.47
1:C:3:ARG:CD	1:C:104:ILE:HD11	2.35	0.47
1:C:90:GLU:HA	1:C:113:LEU:HD22	1.97	0.47
1:C:226:HIS:CE1	1:C:259:CYS:HB3	2.49	0.47
1:C:227:LEU:HD22	1:C:306:THR:HG21	1.93	0.47
1:C:708:GLY:HA2	1:C:737:HIS:O	2.14	0.47
1:C:778:MET:HG3	1:C:779:THR:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:541:ASP:HA	1:H:544:GLN:HB3	1.96	0.47
1:F:540:ARG:O	1:F:542:ALA:N	2.45	0.47
1:E:213:GLU:O	1:E:229:GLU:HA	2.14	0.47
1:D:64:LEU:CD2	1:D:88:LEU:CD2	2.93	0.47
1:B:17:ILE:HA	1:B:20:MET:HG3	1.96	0.47
1:B:111:LYS:O	1:B:115:MET:HG2	2.14	0.47
1:B:651:TRP:CE2	1:B:920:GLN:HG3	2.50	0.47
1:H:619:GLY:HA3	1:H:623:TYR:HE2	1.80	0.47
1:F:194:ALA:HB1	1:F:195:PHE:CE2	2.50	0.47
1:E:4:ILE:HD12	1:E:319:ASP:OD1	2.14	0.47
1:E:17:ILE:HA	1:E:20:MET:HG3	1.97	0.47
1:E:559:ILE:HD13	1:E:805:TYR:CG	2.50	0.47
1:G:300:THR:O	1:G:303:GLU:HB2	2.14	0.47
1:G:708:GLY:HA2	1:G:737:HIS:O	2.14	0.47
1:G:778:MET:HG3	1:G:779:THR:N	2.29	0.47
1:D:70:ILE:HG21	1:D:101:GLU:HG3	1.96	0.47
1:D:610:MET:HG2	1:D:640:VAL:HG11	1.96	0.47
1:A:1041:VAL:HG11	1:A:1043:TYR:HE1	1.78	0.47
1:E:1041:VAL:HG22	1:E:1054:ASN:OD1	2.15	0.47
1:D:116:PHE:N	1:D:116:PHE:HD1	2.13	0.47
1:D:546:LEU:HD11	1:D:774:SER:HB2	1.97	0.47
1:B:510:THR:OG1	1:B:607:MET:SD	2.73	0.47
1:B:622:ASN:ND2	1:B:917:GLU:O	2.47	0.47
1:B:1018:LEU:HD11	1:B:1024:LEU:HD11	1.96	0.47
1:B:1041:VAL:HG22	1:B:1054:ASN:OD1	2.15	0.47
1:H:116:PHE:N	1:H:116:PHE:HD1	2.13	0.46
1:H:369:THR:O	1:H:376:LEU:HD11	2.15	0.46
1:F:106:VAL:HG13	1:F:318:ALA:HB2	1.97	0.46
1:E:651:TRP:CE2	1:E:920:GLN:HG3	2.50	0.46
1:G:81:ILE:HG13	1:G:103:ILE:HG21	1.97	0.46
1:G:90:GLU:HA	1:G:113:LEU:HD22	1.97	0.46
1:G:1041:VAL:HG22	1:G:1054:ASN:OD1	2.15	0.46
1:B:213:GLU:O	1:B:229:GLU:HA	2.14	0.46
1:B:718:PRO:HG2	1:B:749:TYR:CD2	2.50	0.46
1:G:134:ILE:HD12	1:G:287:TYR:CB	2.45	0.46
1:D:300:THR:O	1:D:303:GLU:HB2	2.15	0.46
1:D:369:THR:HG1	1:D:415:ASN:ND2	2.07	0.46
1:A:148:GLU:O	1:A:152:GLU:N	2.46	0.46
1:B:278:GLU:C	1:B:289:ILE:CG1	2.89	0.46
1:C:81:ILE:HG13	1:C:103:ILE:HG21	1.97	0.46
1:C:106:VAL:HG13	1:C:318:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HD12	1:C:287:TYR:CB	2.45	0.46
1:C:300:THR:O	1:C:303:GLU:HB2	2.14	0.46
1:H:288:PHE:CD1	1:H:288:PHE:C	2.92	0.46
1:H:509:GLY:HA3	1:H:605:ASN:O	2.16	0.46
1:F:369:THR:O	1:F:376:LEU:HD11	2.14	0.46
1:D:82:HIS:CD2	1:D:84:GLY:H	2.25	0.46
1:D:123:LYS:NZ	1:D:134:ILE:O	2.41	0.46
1:D:607:MET:HE2	1:D:642:VAL:HG23	1.97	0.46
1:A:513:ILE:N	1:A:513:ILE:HD12	2.30	0.46
1:A:847:VAL:HG11	1:A:889:GLN:OE1	2.15	0.46
1:C:42:PHE:HA	1:C:45:TYR:HD2	1.80	0.46
1:C:1041:VAL:HG22	1:C:1054:ASN:OD1	2.15	0.46
1:F:194:ALA:C	1:F:195:PHE:CD2	2.94	0.46
1:F:1041:VAL:CG1	1:F:1043:TYR:HE1	2.29	0.46
1:E:70:ILE:HG21	1:E:101:GLU:HG3	1.98	0.46
1:G:3:ARG:CD	1:G:104:ILE:HD11	2.35	0.46
1:G:106:VAL:HG13	1:G:318:ALA:HB2	1.97	0.46
1:A:157:PRO:C	1:A:205:CYS:HB2	2.40	0.46
1:A:331:PRO:HB2	1:A:335:ASP:HB2	1.97	0.46
1:B:70:ILE:HG21	1:B:101:GLU:HG3	1.98	0.46
1:B:300:THR:O	1:B:303:GLU:HB2	2.15	0.46
1:B:509:GLY:HA3	1:B:605:ASN:O	2.15	0.46
1:H:106:VAL:HG13	1:H:318:ALA:HB2	1.97	0.46
1:H:319:ASP:OD2	1:H:321:TYR:HE2	1.99	0.46
1:F:513:ILE:N	1:F:513:ILE:HD12	2.30	0.46
1:F:559:ILE:HD13	1:F:805:TYR:CG	2.51	0.46
1:F:620:TYR:CD2	1:F:621:LYS:HB3	2.51	0.46
1:F:847:VAL:HG11	1:F:889:GLN:OE1	2.16	0.46
1:F:1010:LEU:HD21	1:F:1031:ILE:CD1	2.42	0.46
1:A:194:ALA:C	1:A:195:PHE:CD2	2.94	0.46
1:B:540:ARG:HA	1:B:543:HIS:NE2	2.31	0.46
1:H:70:ILE:HG21	1:H:101:GLU:HG3	1.97	0.46
1:E:369:THR:O	1:E:376:LEU:HD11	2.16	0.46
1:E:718:PRO:HG2	1:E:749:TYR:CD2	2.50	0.46
1:D:847:VAL:HG11	1:D:889:GLN:OE1	2.15	0.46
1:B:81:ILE:HG13	1:B:103:ILE:HG21	1.96	0.46
1:B:344:GLN:HG3	1:B:399:CYS:HG	1.80	0.46
1:F:331:PRO:HB2	1:F:335:ASP:HB2	1.98	0.46
1:E:82:HIS:CD2	1:E:84:GLY:H	2.24	0.46
1:E:177:LYS:O	1:E:178:GLU:CB	2.62	0.46
1:E:300:THR:O	1:E:303:GLU:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:LEU:C	1:G:205:CYS:SG	2.99	0.46
1:D:319:ASP:OD2	1:D:321:TYR:HE2	1.99	0.46
1:D:509:GLY:HA3	1:D:605:ASN:O	2.16	0.46
1:A:540:ARG:O	1:A:542:ALA:N	2.45	0.46
1:B:778:MET:HG3	1:B:779:THR:N	2.30	0.46
1:C:405:PHE:C	1:C:405:PHE:CD2	2.93	0.46
1:C:546:LEU:HD11	1:C:774:SER:HB2	1.97	0.46
1:F:68:ASN:O	1:F:72:ILE:HG13	2.16	0.46
1:F:266:MET:HE1	1:F:271:TYR:CE1	2.50	0.46
1:F:546:LEU:HD11	1:F:774:SER:HB2	1.98	0.46
1:D:81:ILE:HG13	1:D:103:ILE:HG21	1.98	0.46
1:A:68:ASN:O	1:A:72:ILE:HG13	2.16	0.46
1:A:106:VAL:HG13	1:A:318:ALA:HB2	1.98	0.46
1:A:369:THR:O	1:A:376:LEU:HD11	2.15	0.46
1:A:546:LEU:HD11	1:A:774:SER:HB2	1.98	0.46
1:H:81:ILE:HG13	1:H:103:ILE:HG21	1.98	0.46
1:H:541:ASP:OD2	1:H:739:HIS:HE1	1.99	0.46
1:F:794:LEU:HD12	1:F:795:ASP:O	2.16	0.46
1:E:266:MET:CE	1:E:277:VAL:CG2	2.94	0.46
1:E:546:LEU:HD11	1:E:774:SER:HB2	1.97	0.46
1:E:622:ASN:ND2	1:E:917:GLU:O	2.48	0.46
1:G:576:TRP:CD1	1:G:596:LEU:HD22	2.51	0.46
1:D:619:GLY:HA3	1:D:623:TYR:HE2	1.81	0.46
1:A:794:LEU:HD12	1:A:795:ASP:O	2.16	0.46
1:A:893:SER:O	1:A:897:VAL:HG13	2.16	0.46
1:A:1018:LEU:HD11	1:A:1024:LEU:HD11	1.97	0.46
1:B:369:THR:O	1:B:376:LEU:HD11	2.16	0.46
1:H:177:LYS:CG	1:H:178:GLU:H	2.25	0.46
1:H:280:LEU:HG	1:H:289:ILE:HG12	1.98	0.46
1:H:607:MET:HE2	1:H:642:VAL:HG23	1.98	0.46
1:F:1018:LEU:HD11	1:F:1024:LEU:HD11	1.97	0.46
1:G:766:SER:O	1:G:767:SER:C	2.59	0.46
1:D:257:ARG:NH2	1:D:284:ASP:O	2.49	0.46
1:D:533:LEU:O	1:D:761:ILE:HA	2.15	0.46
1:D:541:ASP:OD2	1:D:739:HIS:HE1	1.99	0.46
1:D:898:TYR:HD1	1:D:928:LYS:HE2	1.77	0.46
1:A:620:TYR:CD2	1:A:621:LYS:HB3	2.51	0.46
1:F:156:TYR:CB	1:F:157:PRO:HD3	2.46	0.45
1:E:778:MET:HG3	1:E:779:THR:N	2.31	0.45
1:G:226:HIS:ND1	1:G:259:CYS:HB3	2.31	0.45
1:G:546:LEU:HD11	1:G:774:SER:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ARG:HH12	1:D:391:TYR:HB2	1.81	0.45
1:D:106:VAL:HG13	1:D:318:ALA:HB2	1.97	0.45
1:A:541:ASP:OD2	1:A:739:HIS:HE1	1.98	0.45
1:B:266:MET:CE	1:B:277:VAL:CG2	2.94	0.45
1:B:288:PHE:CD1	1:B:289:ILE:N	2.84	0.45
1:C:369:THR:O	1:C:376:LEU:HD11	2.16	0.45
1:H:3:ARG:CD	1:H:104:ILE:HD11	2.35	0.45
1:H:12:ARG:HH12	1:H:391:TYR:HB2	1.82	0.45
1:H:847:VAL:HG11	1:H:889:GLN:OE1	2.15	0.45
1:F:148:GLU:O	1:F:152:GLU:N	2.47	0.45
1:E:155:GLY:O	1:E:158:LEU:HD21	2.15	0.45
1:E:209:PRO:CG	1:E:280:LEU:HD23	2.47	0.45
1:G:160:ILE:HG22	1:G:200:VAL:HG11	1.97	0.45
1:G:369:THR:O	1:G:376:LEU:HD11	2.16	0.45
1:A:610:MET:HG2	1:A:640:VAL:HG11	1.97	0.45
1:B:68:ASN:O	1:B:72:ILE:HG13	2.16	0.45
1:B:134:ILE:CD1	1:B:287:TYR:CB	2.95	0.45
1:B:278:GLU:O	1:B:289:ILE:HG12	2.16	0.45
1:C:559:ILE:HD13	1:C:805:TYR:CG	2.51	0.45
1:H:64:LEU:HD23	1:H:88:LEU:CD2	2.45	0.45
1:H:904:ILE:O	1:H:935:LYS:NZ	2.40	0.45
1:F:17:ILE:HA	1:F:20:MET:HG3	1.98	0.45
1:F:610:MET:HG2	1:F:640:VAL:HG11	1.97	0.45
1:E:257:ARG:NH2	1:E:284:ASP:O	2.49	0.45
1:E:437:HIS:CD2	1:E:439:ASP:N	2.73	0.45
1:G:365:THR:HG21	1:G:1051:ARG:CD	2.43	0.45
1:G:559:ILE:HD13	1:G:805:TYR:CG	2.51	0.45
1:D:450:ILE:HG22	1:D:451:ASP:N	2.31	0.45
1:B:448:SER:O	1:B:452:THR:HG23	2.16	0.45
1:C:1018:LEU:HD11	1:C:1024:LEU:HD11	1.97	0.45
1:H:257:ARG:NH2	1:H:284:ASP:O	2.49	0.45
1:H:847:VAL:HG12	1:H:847:VAL:O	2.17	0.45
1:F:70:ILE:HG21	1:F:101:GLU:HG3	1.99	0.45
1:F:893:SER:O	1:F:897:VAL:HG13	2.17	0.45
1:E:253:GLU:OE2	1:E:257:ARG:NH1	2.50	0.45
1:E:278:GLU:O	1:E:289:ILE:HG12	2.16	0.45
1:G:68:ASN:O	1:G:72:ILE:HG13	2.16	0.45
1:G:164:LEU:HD22	1:G:195:PHE:CE1	2.50	0.45
1:G:331:PRO:HB2	1:G:335:ASP:HB2	1.98	0.45
1:A:448:SER:O	1:A:452:THR:HG23	2.16	0.45
1:B:354:ASN:ND2	1:B:357:MET:HB3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:HG22	1:C:200:VAL:HG11	1.98	0.45
1:C:331:PRO:HB2	1:C:335:ASP:HB2	1.98	0.45
1:H:778:MET:HG3	1:H:779:THR:N	2.32	0.45
1:H:930:GLN:O	1:H:934:LEU:HG	2.16	0.45
1:H:1018:LEU:HD11	1:H:1024:LEU:HD11	1.97	0.45
1:E:68:ASN:O	1:E:72:ILE:HG13	2.16	0.45
1:E:81:ILE:HG13	1:E:103:ILE:HG21	1.97	0.45
1:E:684:ARG:HA	1:E:684:ARG:HH11	1.82	0.45
1:D:13:GLY:C	1:D:17:ILE:HD12	2.41	0.45
1:D:68:ASN:O	1:D:72:ILE:HG13	2.16	0.45
1:D:280:LEU:HG	1:D:289:ILE:HG12	1.99	0.45
1:B:257:ARG:NH2	1:B:284:ASP:O	2.49	0.45
1:B:505:GLN:C	1:B:506:ILE:HG12	2.41	0.45
1:B:752:ALA:CB	1:C:749:TYR:CZ	3.00	0.45
1:H:17:ILE:O	1:H:21:ARG:HG3	2.17	0.45
1:H:68:ASN:O	1:H:72:ILE:HG13	2.16	0.45
1:H:533:LEU:O	1:H:761:ILE:HA	2.15	0.45
1:H:653:LYS:O	1:H:943:ARG:HD3	2.15	0.45
1:F:541:ASP:OD2	1:F:739:HIS:HE1	1.99	0.45
1:E:278:GLU:C	1:E:289:ILE:CG1	2.90	0.45
1:G:134:ILE:CG2	1:G:203:GLU:HB3	2.47	0.45
1:G:144:ILE:HG23	1:G:184:PHE:HD2	1.80	0.45
1:D:3:ARG:CD	1:D:104:ILE:HD11	2.35	0.45
1:A:657:VAL:HG22	1:A:943:ARG:CZ	2.47	0.45
1:A:1041:VAL:CG1	1:A:1043:TYR:HE1	2.30	0.45
1:B:228:PHE:N	1:B:228:PHE:CD1	2.85	0.45
1:C:448:SER:O	1:C:452:THR:HG23	2.17	0.45
1:F:160:ILE:HG22	1:F:200:VAL:HG11	1.98	0.45
1:F:450:ILE:HG22	1:F:451:ASP:N	2.29	0.45
1:E:448:SER:O	1:E:452:THR:HG23	2.17	0.45
1:G:352:PRO:HA	1:G:356:PHE:CE1	2.52	0.45
1:G:1018:LEU:HD11	1:G:1024:LEU:HD11	1.98	0.45
1:D:653:LYS:O	1:D:943:ARG:HD3	2.15	0.45
1:D:930:GLN:O	1:D:934:LEU:HG	2.17	0.45
1:D:1018:LEU:HD11	1:D:1024:LEU:HD11	1.98	0.45
1:A:304:MET:HE1	1:A:399:CYS:HB2	1.99	0.45
1:A:960:LEU:CD2	1:A:964:MET:HB2	2.46	0.45
1:B:253:GLU:OE2	1:B:257:ARG:NH1	2.50	0.45
1:B:546:LEU:HD11	1:B:774:SER:HB2	1.98	0.45
1:B:618:VAL:O	1:B:979:TYR:OH	2.26	0.45
1:H:115:MET:C	1:H:116:PHE:HD1	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ARG:HD3	1:F:45:TYR:CE1	2.51	0.45
1:F:502:TYR:HD1	1:F:503:GLY:N	2.14	0.45
1:E:405:PHE:C	1:E:405:PHE:CD2	2.95	0.45
1:D:847:VAL:O	1:D:847:VAL:HG12	2.17	0.45
1:A:300:THR:O	1:A:303:GLU:HB2	2.16	0.45
1:A:1010:LEU:HD21	1:A:1031:ILE:CD1	2.44	0.45
1:B:437:HIS:CD2	1:B:439:ASP:N	2.73	0.45
1:B:543:HIS:ND1	1:B:551:VAL:HB	2.31	0.45
1:C:304:MET:HE1	1:C:399:CYS:HB2	1.99	0.45
1:C:368:SER:HA	1:C:419:PHE:CE1	2.52	0.45
1:C:794:LEU:HD12	1:C:795:ASP:O	2.17	0.45
1:F:657:VAL:HG22	1:F:943:ARG:CZ	2.47	0.45
1:F:960:LEU:CD2	1:F:964:MET:HB2	2.46	0.45
1:E:352:PRO:HA	1:E:356:PHE:CE1	2.51	0.45
1:E:618:VAL:O	1:E:979:TYR:OH	2.27	0.45
1:D:64:LEU:HD23	1:D:88:LEU:CD2	2.45	0.45
1:D:288:PHE:CD1	1:D:288:PHE:C	2.94	0.45
1:D:904:ILE:O	1:D:935:LYS:NZ	2.41	0.45
1:A:257:ARG:NH2	1:A:284:ASP:O	2.50	0.45
1:A:472:TYR:OH	1:A:1004:PHE:O	2.27	0.45
1:B:619:GLY:HA3	1:B:623:TYR:HE2	1.80	0.45
1:C:576:TRP:CD1	1:C:596:LEU:HD22	2.52	0.45
1:H:234:ILE:CD1	1:H:445:TYR:CZ	2.98	0.45
1:H:369:THR:HG1	1:H:415:ASN:ND2	2.10	0.45
1:H:693:LYS:HG2	1:H:731:THR:OG1	2.16	0.45
1:F:253:GLU:OE2	1:F:257:ARG:NH1	2.50	0.45
1:F:304:MET:HE1	1:F:399:CYS:HB2	1.99	0.45
1:F:778:MET:HG3	1:F:779:THR:N	2.32	0.45
1:E:54:GLY:HA3	1:E:62:ALA:CB	2.47	0.45
1:G:368:SER:HA	1:G:419:PHE:CE1	2.52	0.45
1:D:45:TYR:CE1	1:C:1047:ASN:CG	2.94	0.45
1:D:118:ASP:OD2	1:D:120:ILE:HG13	2.17	0.45
1:D:352:PRO:HA	1:D:356:PHE:CE1	2.51	0.45
1:D:1041:VAL:HG22	1:D:1054:ASN:OD1	2.17	0.45
1:A:44:ARG:HD3	1:A:45:TYR:CE1	2.52	0.45
1:A:450:ILE:HG22	1:A:451:ASP:N	2.30	0.45
1:B:367:ARG:NH1	1:B:1049:GLN:HB2	2.31	0.45
1:C:257:ARG:NH2	1:C:284:ASP:O	2.49	0.45
1:H:414:ARG:NH1	1:G:21:ARG:HD3	2.32	0.44
1:F:257:ARG:NH2	1:F:284:ASP:O	2.50	0.44
1:F:472:TYR:OH	1:F:1004:PHE:O	2.27	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:PHE:HA	1:E:45:TYR:CD2	2.52	0.44
1:G:70:ILE:HG21	1:G:101:GLU:HG3	1.98	0.44
1:G:607:MET:HE2	1:G:642:VAL:HG23	1.99	0.44
1:D:448:SER:O	1:D:452:THR:HG23	2.16	0.44
1:A:70:ILE:HG21	1:A:101:GLU:HG3	1.99	0.44
1:A:160:ILE:HG22	1:A:200:VAL:HG11	1.98	0.44
1:C:134:ILE:CG2	1:C:203:GLU:HB3	2.47	0.44
1:H:118:ASP:OD2	1:H:120:ILE:HG13	2.17	0.44
1:H:718:PRO:HG2	1:H:749:TYR:CD2	2.52	0.44
1:F:448:SER:O	1:F:452:THR:HG23	2.17	0.44
1:F:930:GLN:O	1:F:934:LEU:HG	2.17	0.44
1:E:331:PRO:HB2	1:E:335:ASP:HB2	1.97	0.44
1:E:367:ARG:NH1	1:E:1049:GLN:HB2	2.31	0.44
1:E:952:ASN:OD1	1:E:952:ASN:O	2.35	0.44
1:G:257:ARG:NH2	1:G:284:ASP:O	2.49	0.44
1:G:304:MET:HE1	1:G:399:CYS:HB2	1.99	0.44
1:A:17:ILE:HA	1:A:20:MET:HG3	1.99	0.44
1:A:253:GLU:OE2	1:A:257:ARG:NH1	2.50	0.44
1:B:54:GLY:HA3	1:B:62:ALA:CB	2.48	0.44
1:B:209:PRO:CG	1:B:280:LEU:HD23	2.48	0.44
1:C:17:ILE:O	1:C:21:ARG:HG3	2.17	0.44
1:C:70:ILE:HG21	1:C:101:GLU:HG3	1.98	0.44
1:C:352:PRO:HA	1:C:356:PHE:CE1	2.53	0.44
1:C:651:TRP:HE1	1:C:653:LYS:CB	2.31	0.44
1:H:448:SER:O	1:H:452:THR:HG23	2.16	0.44
1:F:319:ASP:OD2	1:F:321:TYR:HE2	2.00	0.44
1:F:368:SER:HA	1:F:419:PHE:CE1	2.51	0.44
1:E:266:MET:HE3	1:E:277:VAL:HG23	1.98	0.44
1:E:266:MET:HE1	1:E:291:VAL:CG1	2.48	0.44
1:G:741:HIS:CD2	1:G:775:GLN:HE21	2.36	0.44
1:G:794:LEU:HD12	1:G:795:ASP:O	2.17	0.44
1:D:253:GLU:OE2	1:D:257:ARG:NH1	2.50	0.44
1:C:365:THR:HG21	1:C:1051:ARG:CD	2.45	0.44
1:H:368:SER:HA	1:H:419:PHE:CE1	2.53	0.44
1:H:427:ASN:ND2	1:H:431:LEU:HD11	2.31	0.44
1:H:1041:VAL:HG22	1:H:1054:ASN:OD1	2.17	0.44
1:F:51:TYR:CE1	1:E:1021:GLY:HA2	2.50	0.44
1:E:234:ILE:CD1	1:E:445:TYR:CZ	2.98	0.44
1:E:626:ASN:OD1	1:E:950:PRO:HB3	2.17	0.44
1:D:712:MET:SD	1:D:712:MET:N	2.89	0.44
1:A:90:GLU:HA	1:A:113:LEU:HD22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ASN:OD1	1:B:950:PRO:HB3	2.17	0.44
1:C:68:ASN:O	1:C:72:ILE:HG13	2.17	0.44
1:C:607:MET:HE2	1:C:642:VAL:HG23	1.99	0.44
1:C:766:SER:O	1:C:767:SER:C	2.61	0.44
1:H:300:THR:O	1:H:303:GLU:HB2	2.17	0.44
1:E:134:ILE:CD1	1:E:287:TYR:CB	2.96	0.44
1:E:427:ASN:ND2	1:E:431:LEU:HD11	2.32	0.44
1:E:619:GLY:HA3	1:E:623:TYR:HE2	1.81	0.44
1:E:746:ASN:HD22	1:G:748:ILE:HG21	1.82	0.44
1:A:509:GLY:N	1:A:605:ASN:HB2	2.33	0.44
1:A:570:MET:HG3	1:A:573:PHE:CE1	2.52	0.44
1:A:1014:ILE:HD12	1:A:1016:VAL:HG12	2.00	0.44
1:B:44:ARG:HD3	1:B:45:TYR:CE1	2.52	0.44
1:B:821:ASN:OD1	1:B:821:ASN:N	2.49	0.44
1:B:952:ASN:OD1	1:B:952:ASN:O	2.35	0.44
1:C:718:PRO:HG2	1:C:749:TYR:CD2	2.52	0.44
1:F:709:ILE:HB	1:F:738:LEU:HD12	1.99	0.44
1:F:1014:ILE:HD12	1:F:1016:VAL:HG12	2.00	0.44
1:G:448:SER:O	1:G:452:THR:HG23	2.18	0.44
1:G:519:PRO:CB	1:G:705:HIS:NE2	2.78	0.44
1:G:718:PRO:HG2	1:G:749:TYR:CD2	2.52	0.44
1:D:17:ILE:O	1:D:21:ARG:HG3	2.18	0.44
1:D:115:MET:C	1:D:116:PHE:HD1	2.25	0.44
1:D:693:LYS:HG2	1:D:731:THR:OG1	2.17	0.44
1:A:778:MET:HG3	1:A:779:THR:N	2.31	0.44
1:B:266:MET:HE1	1:B:291:VAL:CG1	2.48	0.44
1:C:12:ARG:NH2	1:C:391:TYR:CD2	2.85	0.44
1:H:45:TYR:CE1	1:G:1047:ASN:CG	2.95	0.44
1:H:253:GLU:OE2	1:H:257:ARG:NH1	2.51	0.44
1:F:90:GLU:HA	1:F:113:LEU:HD22	2.00	0.44
1:F:607:MET:HE2	1:F:642:VAL:HG23	1.99	0.44
1:F:619:GLY:HA3	1:F:623:TYR:HE2	1.81	0.44
1:F:679:ILE:CD1	1:F:724:LEU:HD13	2.44	0.44
1:E:156:TYR:N	1:E:157:PRO:CD	2.80	0.44
1:A:54:GLY:HA3	1:A:62:ALA:CB	2.48	0.44
1:A:930:GLN:O	1:A:934:LEU:HG	2.17	0.44
1:B:42:PHE:HA	1:B:45:TYR:CD2	2.53	0.44
1:B:540:ARG:NH2	1:B:541:ASP:OD1	2.51	0.44
1:C:186:ARG:CZ	1:C:186:ARG:HB3	2.47	0.44
1:F:17:ILE:O	1:F:21:ARG:HG3	2.17	0.44
1:E:44:ARG:HD3	1:E:45:TYR:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ILE:O	1:D:106:VAL:HG23	2.18	0.44
1:D:234:ILE:CD1	1:D:445:TYR:CZ	2.99	0.44
1:A:234:ILE:CD1	1:A:445:TYR:CZ	2.99	0.44
1:A:319:ASP:OD2	1:A:321:TYR:HE2	2.01	0.44
1:C:519:PRO:CB	1:C:705:HIS:NE2	2.78	0.44
1:C:741:HIS:CD2	1:C:775:GLN:HE21	2.36	0.44
1:C:992:LYS:HE3	1:C:993:TYR:CE2	2.53	0.44
1:H:81:ILE:O	1:H:106:VAL:HG23	2.18	0.44
1:F:847:VAL:O	1:F:847:VAL:HG12	2.17	0.44
1:E:147:VAL:HG11	1:E:180:VAL:HG11	2.00	0.44
1:E:160:ILE:HD12	1:E:174:VAL:CG2	2.47	0.44
1:E:369:THR:OG1	1:E:370:GLY:N	2.50	0.44
1:E:505:GLN:C	1:E:506:ILE:HG12	2.43	0.44
1:E:607:MET:HE2	1:E:642:VAL:HG23	1.98	0.44
1:G:278:GLU:CB	1:G:289:ILE:CD1	2.96	0.44
1:D:45:TYR:CD1	1:C:1047:ASN:CB	2.97	0.44
1:B:228:PHE:N	1:B:228:PHE:HD1	2.16	0.44
1:B:266:MET:HE3	1:B:277:VAL:HG23	1.99	0.44
1:B:684:ARG:HH11	1:B:684:ARG:HA	1.83	0.44
1:H:13:GLY:C	1:H:17:ILE:HD12	2.43	0.43
1:F:157:PRO:C	1:F:205:CYS:HB2	2.43	0.43
1:F:570:MET:HG3	1:F:573:PHE:CE1	2.52	0.43
1:G:230:ARG:HD3	1:G:302:THR:OG1	2.18	0.43
1:G:278:GLU:HB2	1:G:289:ILE:CD1	2.48	0.43
1:D:969:THR:O	1:D:973:VAL:HG23	2.18	0.43
1:D:1033:GLU:HG3	1:D:1034:PRO:HD2	2.00	0.43
1:A:607:MET:HE2	1:A:642:VAL:HG23	1.99	0.43
1:B:746:ASN:HD22	1:C:748:ILE:HG21	1.83	0.43
1:F:54:GLY:HA3	1:F:62:ALA:CB	2.48	0.43
1:F:300:THR:O	1:F:303:GLU:HB2	2.17	0.43
1:E:228:PHE:N	1:E:228:PHE:CD1	2.87	0.43
1:D:898:TYR:HD1	1:D:928:LYS:HE3	1.81	0.43
1:A:131:ILE:O	1:A:131:ILE:HG12	2.14	0.43
1:A:754:ALA:HB1	1:A:759:VAL:CG1	2.49	0.43
1:B:331:PRO:HB2	1:B:335:ASP:HB2	1.98	0.43
1:C:278:GLU:HB2	1:C:289:ILE:CD1	2.48	0.43
1:C:472:TYR:OH	1:C:1004:PHE:O	2.28	0.43
1:H:712:MET:SD	1:H:712:MET:N	2.90	0.43
1:H:898:TYR:H	1:H:898:TYR:HD2	1.65	0.43
1:E:349:THR:HG23	1:E:393:SER:HB2	2.00	0.43
1:E:821:ASN:OD1	1:E:821:ASN:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:712:MET:SD	1:G:712:MET:N	2.88	0.43
1:D:607:MET:HE2	1:D:642:VAL:CG2	2.48	0.43
1:B:134:ILE:HG23	1:B:135:PRO:HD2	2.00	0.43
1:C:279:PHE:CA	1:C:289:ILE:HD11	2.48	0.43
1:C:600:ARG:HG3	1:C:639:GLY:HA3	1.99	0.43
1:H:304:MET:HE1	1:H:399:CYS:HB2	1.99	0.43
1:H:741:HIS:CE1	1:H:775:GLN:NE2	2.86	0.43
1:H:969:THR:O	1:H:973:VAL:HG23	2.18	0.43
1:F:234:ILE:CD1	1:F:445:TYR:CZ	2.99	0.43
1:G:81:ILE:O	1:G:106:VAL:HG23	2.18	0.43
1:D:12:ARG:HH21	1:D:38:ASP:CG	2.25	0.43
1:D:427:ASN:ND2	1:D:431:LEU:HD11	2.32	0.43
1:A:17:ILE:O	1:A:21:ARG:HG3	2.18	0.43
1:C:278:GLU:CB	1:C:289:ILE:CD1	2.96	0.43
1:C:737:HIS:CD2	1:C:737:HIS:C	2.97	0.43
1:H:709:ILE:HB	1:H:738:LEU:HD12	2.00	0.43
1:F:131:ILE:O	1:F:131:ILE:HG12	2.15	0.43
1:E:211:HIS:C	1:E:212:ILE:HD12	2.43	0.43
1:E:847:VAL:O	1:E:847:VAL:HG12	2.18	0.43
1:G:12:ARG:NH2	1:G:391:TYR:CD2	2.85	0.43
1:G:620:TYR:CE1	1:G:978:LEU:O	2.72	0.43
1:D:368:SER:HA	1:D:419:PHE:CE1	2.54	0.43
1:D:709:ILE:HB	1:D:738:LEU:HD12	2.00	0.43
1:B:174:VAL:HG12	1:B:176:SER:H	1.83	0.43
1:H:898:TYR:HD1	1:H:928:LYS:HE3	1.82	0.43
1:F:173:VAL:HG13	1:F:205:CYS:SG	2.58	0.43
1:E:847:VAL:CG1	1:E:889:GLN:OE1	2.67	0.43
1:G:288:PHE:CE2	1:G:291:VAL:HG23	2.54	0.43
1:G:600:ARG:HG3	1:G:639:GLY:HA3	1.99	0.43
1:A:619:GLY:HA3	1:A:623:TYR:HE2	1.82	0.43
1:A:1033:GLU:HG3	1:A:1034:PRO:HD2	2.00	0.43
1:B:352:PRO:HA	1:B:356:PHE:CE1	2.53	0.43
1:C:54:GLY:HA3	1:C:62:ALA:CB	2.48	0.43
1:C:230:ARG:HD3	1:C:302:THR:OG1	2.19	0.43
1:C:540:ARG:O	1:C:542:ALA:N	2.46	0.43
1:H:13:GLY:O	1:H:14:GLU:C	2.62	0.43
1:H:174:VAL:HG12	1:H:176:SER:H	1.84	0.43
1:H:519:PRO:HB2	1:H:705:HIS:CD2	2.53	0.43
1:E:17:ILE:O	1:E:21:ARG:HG3	2.18	0.43
1:E:288:PHE:CD1	1:E:289:ILE:N	2.86	0.43
1:E:288:PHE:CE2	1:E:291:VAL:HG23	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:GLY:HA3	1:G:62:ALA:CB	2.49	0.43
1:G:279:PHE:CA	1:G:289:ILE:HD11	2.48	0.43
1:A:81:ILE:HG13	1:A:103:ILE:HG21	2.00	0.43
1:A:347:ILE:C	1:A:395:LEU:HD12	2.42	0.43
1:A:368:SER:HA	1:A:419:PHE:CE1	2.53	0.43
1:A:806:TRP:O	1:A:807:GLU:C	2.61	0.43
1:A:847:VAL:O	1:A:847:VAL:HG12	2.17	0.43
1:B:234:ILE:CD1	1:B:445:TYR:CZ	2.99	0.43
1:B:427:ASN:ND2	1:B:431:LEU:HD11	2.33	0.43
1:B:603:ILE:CG1	1:B:608:PHE:CZ	3.00	0.43
1:B:607:MET:HE2	1:B:642:VAL:HG23	1.99	0.43
1:C:288:PHE:CE2	1:C:291:VAL:HG23	2.54	0.43
1:C:541:ASP:OD2	1:C:739:HIS:HE1	2.01	0.43
1:H:8:LEU:CA	1:H:31:VAL:CG2	2.89	0.43
1:H:600:ARG:HG3	1:H:639:GLY:HA3	2.00	0.43
1:F:51:TYR:CD1	1:E:1021:GLY:HA2	2.54	0.43
1:F:66:ILE:HG23	1:F:94:PHE:HD1	1.81	0.43
1:E:134:ILE:HG23	1:E:135:PRO:HD2	2.00	0.43
1:E:304:MET:HE1	1:E:399:CYS:HB2	1.99	0.43
1:E:603:ILE:CG1	1:E:608:PHE:CZ	3.00	0.43
1:G:540:ARG:O	1:G:542:ALA:N	2.46	0.43
1:G:737:HIS:CD2	1:G:737:HIS:C	2.97	0.43
1:G:959:GLU:O	1:G:963:LYS:HG2	2.18	0.43
1:A:126:ALA:CB	1:A:131:ILE:HD11	2.48	0.43
1:B:39:THR:HG22	1:B:44:ARG:HH21	1.82	0.43
1:B:266:MET:HE1	1:B:291:VAL:HG13	2.01	0.43
1:B:847:VAL:CG1	1:B:889:GLN:OE1	2.67	0.43
1:C:44:ARG:HD3	1:C:45:TYR:CE1	2.53	0.43
1:F:81:ILE:HG13	1:F:103:ILE:HG21	2.00	0.43
1:F:126:ALA:CB	1:F:131:ILE:HD11	2.48	0.43
1:F:347:ILE:C	1:F:395:LEU:HD12	2.42	0.43
1:F:867:PHE:N	1:F:867:PHE:CD1	2.85	0.43
1:E:39:THR:HG22	1:E:44:ARG:HH21	1.82	0.43
1:E:675:TYR:CE2	1:E:716:LEU:HD13	2.54	0.43
1:E:766:SER:O	1:E:767:SER:C	2.62	0.43
1:G:674:CYS:CB	1:G:712:MET:HE1	2.48	0.43
1:D:54:GLY:HA3	1:D:62:ALA:CB	2.48	0.43
1:D:718:PRO:HG2	1:D:749:TYR:CD2	2.53	0.43
1:D:778:MET:HG3	1:D:779:THR:N	2.34	0.43
1:D:841:GLN:HG2	1:D:853:TRP:CZ2	2.54	0.43
1:A:718:PRO:HG2	1:A:749:TYR:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:O	1:B:14:GLU:C	2.61	0.43
1:B:82:HIS:HB2	1:B:106:VAL:HG21	2.00	0.43
1:B:254:LEU:O	1:B:255:ARG:C	2.62	0.43
1:B:448:SER:O	1:B:452:THR:CG2	2.67	0.43
1:C:620:TYR:CE1	1:C:978:LEU:O	2.72	0.43
1:C:674:CYS:CB	1:C:712:MET:HE1	2.48	0.43
1:H:45:TYR:CD1	1:G:1047:ASN:CB	2.99	0.43
1:F:50:ALA:O	1:E:1021:GLY:O	2.37	0.43
1:F:209:PRO:HB2	1:F:280:LEU:HD22	2.01	0.43
1:E:607:MET:HE2	1:E:642:VAL:CG2	2.49	0.43
1:G:541:ASP:OD2	1:G:739:HIS:HE1	2.02	0.43
1:G:992:LYS:HE3	1:G:993:TYR:CE2	2.54	0.43
1:D:39:THR:HG22	1:D:44:ARG:HH21	1.84	0.43
1:D:674:CYS:CB	1:D:712:MET:HE1	2.49	0.43
1:D:898:TYR:H	1:D:898:TYR:HD2	1.65	0.43
1:A:563:MET:HB3	1:A:573:PHE:CE2	2.53	0.43
1:A:679:ILE:CD1	1:A:724:LEU:HD13	2.44	0.43
1:B:211:HIS:C	1:B:212:ILE:HD12	2.44	0.43
1:B:766:SER:O	1:B:767:SER:C	2.62	0.43
1:B:847:VAL:O	1:B:847:VAL:HG12	2.19	0.43
1:C:39:THR:HG22	1:C:44:ARG:HH21	1.83	0.43
1:H:39:THR:HG22	1:H:44:ARG:HH21	1.84	0.42
1:H:54:GLY:HA3	1:H:62:ALA:CB	2.49	0.42
1:H:631:PHE:O	1:H:635:SER:OG	2.37	0.42
1:H:867:PHE:N	1:H:867:PHE:CD1	2.85	0.42
1:H:1004:PHE:CD2	1:H:1004:PHE:C	2.97	0.42
1:H:1033:GLU:HG3	1:H:1034:PRO:HD2	2.01	0.42
1:F:519:PRO:HB2	1:F:705:HIS:CD2	2.54	0.42
1:F:754:ALA:HB1	1:F:759:VAL:CG1	2.49	0.42
1:E:82:HIS:HB2	1:E:106:VAL:HG21	2.00	0.42
1:E:448:SER:O	1:E:452:THR:CG2	2.67	0.42
1:A:519:PRO:HB2	1:A:705:HIS:CD2	2.54	0.42
1:A:867:PHE:N	1:A:867:PHE:CD1	2.86	0.42
1:B:304:MET:HE1	1:B:399:CYS:HB2	1.99	0.42
1:B:718:PRO:CG	1:B:749:TYR:CD2	3.02	0.42
1:C:194:ALA:C	1:C:195:PHE:CD2	2.95	0.42
1:C:348:THR:HG22	1:C:394:LEU:HA	2.01	0.42
1:C:427:ASN:ND2	1:C:431:LEU:HD11	2.34	0.42
1:C:712:MET:SD	1:C:712:MET:N	2.89	0.42
1:C:959:GLU:O	1:C:963:LYS:HG2	2.19	0.42
1:H:607:MET:HE2	1:H:642:VAL:CG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:674:CYS:CB	1:H:712:MET:HE1	2.49	0.42
1:F:39:THR:HG22	1:F:44:ARG:HH21	1.84	0.42
1:F:347:ILE:C	1:F:395:LEU:CD1	2.92	0.42
1:F:500:ILE:HG22	1:F:501:PRO:O	2.19	0.42
1:F:1033:GLU:HG3	1:F:1034:PRO:HD2	2.01	0.42
1:E:266:MET:HE1	1:E:291:VAL:HG13	2.01	0.42
1:E:712:MET:SD	1:E:712:MET:N	2.89	0.42
1:D:211:HIS:C	1:D:212:ILE:HD12	2.44	0.42
1:A:209:PRO:HB2	1:A:280:LEU:HD22	2.01	0.42
1:A:620:TYR:HD1	1:A:979:TYR:CE1	2.38	0.42
1:A:672:ALA:HA	1:A:708:GLY:O	2.20	0.42
1:A:709:ILE:HB	1:A:738:LEU:HD12	1.99	0.42
1:A:969:THR:O	1:A:973:VAL:HG23	2.19	0.42
1:B:288:PHE:CE2	1:B:291:VAL:HG23	2.54	0.42
1:B:349:THR:HG23	1:B:393:SER:HB2	2.01	0.42
1:C:134:ILE:HG23	1:C:135:PRO:HD2	1.99	0.42
1:C:211:HIS:C	1:C:212:ILE:HD12	2.45	0.42
1:C:1014:ILE:HD12	1:C:1016:VAL:HG12	2.01	0.42
1:H:12:ARG:HH21	1:H:38:ASP:CG	2.26	0.42
1:H:21:ARG:CZ	1:G:418:GLU:OE2	2.68	0.42
1:H:370:GLY:C	1:G:21:ARG:HH12	2.26	0.42
1:F:134:ILE:HG23	1:F:135:PRO:HD2	2.01	0.42
1:F:969:THR:O	1:F:973:VAL:HG23	2.19	0.42
1:E:600:ARG:HG3	1:E:639:GLY:HA3	2.01	0.42
1:G:1014:ILE:HD12	1:G:1016:VAL:HG12	2.01	0.42
1:D:600:ARG:HG3	1:D:639:GLY:HA3	2.01	0.42
1:A:39:THR:HG22	1:A:44:ARG:HH21	1.84	0.42
1:A:81:ILE:O	1:A:106:VAL:HG23	2.19	0.42
1:B:712:MET:SD	1:B:712:MET:N	2.89	0.42
1:H:134:ILE:HG21	1:H:203:GLU:HB2	2.01	0.42
1:F:428:ILE:HB	1:F:429:PRO:HD3	2.01	0.42
1:F:563:MET:HB3	1:F:573:PHE:CE2	2.54	0.42
1:E:228:PHE:N	1:E:228:PHE:HD1	2.18	0.42
1:E:490:PRO:HD2	1:E:492:TYR:CE2	2.54	0.42
1:G:44:ARG:HD3	1:G:45:TYR:CE1	2.54	0.42
1:G:304:MET:CE	1:G:399:CYS:CB	2.98	0.42
1:D:463:ARG:HG3	1:D:468:LYS:HE3	2.02	0.42
1:D:519:PRO:HB2	1:D:705:HIS:CD2	2.54	0.42
1:A:13:GLY:O	1:A:14:GLU:C	2.63	0.42
1:A:134:ILE:HG23	1:A:135:PRO:HD2	2.01	0.42
1:C:81:ILE:O	1:C:106:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:HA	1:C:184:PHE:CE2	2.54	0.42
1:F:81:ILE:O	1:F:106:VAL:HG23	2.19	0.42
1:F:620:TYR:HD1	1:F:979:TYR:CE1	2.38	0.42
1:F:713:ALA:HB3	1:F:715:LEU:HD12	1.99	0.42
1:E:373:GLY:O	1:E:400:THR:HA	2.19	0.42
1:G:17:ILE:O	1:G:21:ARG:HG3	2.20	0.42
1:G:1033:GLU:HG3	1:G:1034:PRO:HD2	2.00	0.42
1:D:8:LEU:CA	1:D:31:VAL:CG2	2.89	0.42
1:D:304:MET:HE1	1:D:399:CYS:HB2	2.00	0.42
1:D:680:ASP:HB3	1:A:787:ASN:ND2	2.35	0.42
1:D:741:HIS:CE1	1:D:775:GLN:NE2	2.87	0.42
1:B:600:ARG:HG3	1:B:639:GLY:HA3	2.01	0.42
1:B:675:TYR:CE2	1:B:716:LEU:HD13	2.54	0.42
1:B:754:ALA:HB1	1:B:759:VAL:CG1	2.49	0.42
1:C:509:GLY:N	1:C:605:ASN:HB2	2.34	0.42
1:H:115:MET:CG	1:H:125:GLN:HG3	2.48	0.42
1:H:680:ASP:HB3	1:F:787:ASN:ND2	2.35	0.42
1:F:718:PRO:HG2	1:F:749:TYR:CD2	2.54	0.42
1:E:348:THR:HG22	1:E:394:LEU:HA	2.01	0.42
1:E:718:PRO:CG	1:E:749:TYR:CD2	3.02	0.42
1:D:754:ALA:HB1	1:D:759:VAL:CG1	2.49	0.42
1:D:898:TYR:CD1	1:D:928:LYS:CE	2.99	0.42
1:A:288:PHE:CE2	1:A:291:VAL:HG23	2.55	0.42
1:A:519:PRO:CB	1:A:705:HIS:NE2	2.80	0.42
1:B:365:THR:CG2	1:B:1050:PRO:O	2.67	0.42
1:B:862:VAL:O	1:B:866:MET:N	2.52	0.42
1:H:41:SER:OG	1:H:43:HIS:HD2	2.02	0.42
1:H:224:ILE:HG22	1:H:263:VAL:HG13	2.02	0.42
1:F:1:MET:HE3	1:F:319:ASP:CG	2.45	0.42
1:F:288:PHE:CE2	1:F:291:VAL:HG23	2.55	0.42
1:E:144:ILE:HD12	1:E:145:LYS:H	1.83	0.42
1:E:304:MET:CE	1:E:399:CYS:HB2	2.49	0.42
1:E:828:TYR:CE2	1:G:783:TYR:HB3	2.54	0.42
1:E:862:VAL:O	1:E:866:MET:N	2.52	0.42
1:G:134:ILE:HG23	1:G:135:PRO:HD2	1.99	0.42
1:G:348:THR:HG22	1:G:394:LEU:HA	2.02	0.42
1:G:607:MET:HE2	1:G:642:VAL:CG2	2.50	0.42
1:D:631:PHE:O	1:D:635:SER:OG	2.38	0.42
1:D:867:PHE:N	1:D:867:PHE:CD1	2.86	0.42
1:A:347:ILE:C	1:A:395:LEU:CD1	2.93	0.42
1:A:766:SER:O	1:A:767:SER:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:MET:HE2	1:B:642:VAL:CG2	2.50	0.42
1:C:448:SER:O	1:C:452:THR:CG2	2.67	0.42
1:C:586:ARG:NH1	1:C:586:ARG:HB2	2.34	0.42
1:H:209:PRO:HB2	1:H:280:LEU:HD22	2.01	0.42
1:H:519:PRO:CB	1:H:705:HIS:NE2	2.80	0.42
1:H:754:ALA:HB1	1:H:759:VAL:CG1	2.49	0.42
1:H:1014:ILE:HD12	1:H:1016:VAL:HG12	2.01	0.42
1:G:39:THR:HG22	1:G:44:ARG:HH21	1.84	0.42
1:G:304:MET:CE	1:G:399:CYS:HB2	2.49	0.42
1:A:161:LYS:HB2	1:A:201:TYR:CE2	2.54	0.42
1:A:427:ASN:ND2	1:A:431:LEU:HD11	2.35	0.42
1:B:828:TYR:CE2	1:C:783:TYR:HB3	2.54	0.42
1:C:217:LEU:HD12	1:C:227:LEU:HD11	2.01	0.42
1:H:278:GLU:C	1:H:289:ILE:HD12	2.44	0.42
1:H:898:TYR:CD1	1:H:928:LYS:CE	2.99	0.42
1:E:754:ALA:HB1	1:E:759:VAL:CG1	2.49	0.42
1:G:427:ASN:ND2	1:G:431:LEU:HD11	2.35	0.42
1:D:134:ILE:HG21	1:D:203:GLU:HB2	2.02	0.42
1:D:209:PRO:HB2	1:D:280:LEU:HD22	2.01	0.42
1:A:1:MET:HE3	1:A:319:ASP:CG	2.45	0.42
1:A:428:ILE:HB	1:A:429:PRO:HD3	2.02	0.42
1:A:448:SER:O	1:A:452:THR:CG2	2.68	0.42
1:B:17:ILE:O	1:B:21:ARG:HG3	2.19	0.42
1:B:490:PRO:HD2	1:B:492:TYR:CE2	2.55	0.42
1:C:304:MET:CE	1:C:399:CYS:HB2	2.49	0.42
1:H:198:ASP:OD1	1:H:198:ASP:N	2.53	0.42
1:F:82:HIS:CD2	1:F:84:GLY:H	2.26	0.42
1:F:161:LYS:HB2	1:F:201:TYR:CE2	2.54	0.42
1:E:42:PHE:HA	1:E:45:TYR:HD2	1.83	0.42
1:D:224:ILE:HG22	1:D:263:VAL:HG13	2.02	0.42
1:A:66:ILE:HG23	1:A:94:PHE:HD1	1.83	0.42
1:B:348:THR:HG22	1:B:394:LEU:HA	2.02	0.42
1:C:607:MET:HE2	1:C:642:VAL:CG2	2.50	0.42
1:H:1:MET:HE3	1:H:319:ASP:CG	2.45	0.41
1:H:211:HIS:C	1:H:212:ILE:HD12	2.45	0.41
1:H:448:SER:O	1:H:452:THR:CG2	2.67	0.41
1:H:859:MET:HE2	1:H:859:MET:HA	2.01	0.41
1:F:509:GLY:N	1:F:605:ASN:HB2	2.35	0.41
1:E:13:GLY:O	1:E:14:GLU:C	2.62	0.41
1:E:1014:ILE:HD12	1:E:1016:VAL:HG12	2.01	0.41
1:G:586:ARG:NH1	1:G:586:ARG:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:754:ALA:HB1	1:G:759:VAL:CG1	2.50	0.41
1:D:174:VAL:CA	1:D:175:GLU:OE2	2.68	0.41
1:D:198:ASP:N	1:D:198:ASP:OD1	2.53	0.41
1:D:448:SER:O	1:D:452:THR:CG2	2.67	0.41
1:D:1014:ILE:HD12	1:D:1016:VAL:HG12	2.01	0.41
1:A:63:TYR:HB2	1:A:87:PHE:CE2	2.54	0.41
1:A:847:VAL:HB	1:A:849:LEU:CD1	2.50	0.41
1:B:133:VAL:HG12	1:B:134:ILE:N	2.35	0.41
1:B:304:MET:CE	1:B:399:CYS:HB2	2.50	0.41
1:B:675:TYR:HE2	1:B:716:LEU:HA	1.84	0.41
1:C:198:ASP:OD1	1:C:198:ASP:N	2.53	0.41
1:C:519:PRO:HB2	1:C:705:HIS:CD2	2.54	0.41
1:H:463:ARG:HG3	1:H:468:LYS:HE3	2.03	0.41
1:F:230:ARG:HD3	1:F:302:THR:OG1	2.20	0.41
1:E:672:ALA:HA	1:E:708:GLY:O	2.19	0.41
1:G:448:SER:O	1:G:452:THR:CG2	2.68	0.41
1:G:519:PRO:HB2	1:G:705:HIS:CD2	2.54	0.41
1:A:230:ARG:HD3	1:A:302:THR:OG1	2.20	0.41
1:A:600:ARG:HG3	1:A:639:GLY:HA3	2.02	0.41
1:H:134:ILE:HG23	1:H:135:PRO:HD2	2.02	0.41
1:H:280:LEU:HD23	1:H:280:LEU:HA	1.92	0.41
1:H:304:MET:CE	1:H:399:CYS:HB2	2.50	0.41
1:H:718:PRO:CG	1:H:749:TYR:CD2	3.04	0.41
1:H:841:GLN:HG2	1:H:853:TRP:CZ2	2.55	0.41
1:F:13:GLY:O	1:F:14:GLU:C	2.64	0.41
1:F:448:SER:O	1:F:452:THR:CG2	2.68	0.41
1:F:672:ALA:HA	1:F:708:GLY:O	2.21	0.41
1:E:212:ILE:HG23	1:E:229:GLU:HB2	2.02	0.41
1:G:144:ILE:HA	1:G:184:PHE:HE2	1.84	0.41
1:D:1:MET:HE3	1:D:319:ASP:CG	2.46	0.41
1:D:13:GLY:O	1:D:14:GLU:C	2.64	0.41
1:A:685:THR:O	1:A:688:THR:HG23	2.21	0.41
1:B:158:LEU:HA	1:B:205:CYS:H	1.85	0.41
1:B:1014:ILE:HD12	1:B:1016:VAL:HG12	2.02	0.41
1:B:1033:GLU:HG3	1:B:1034:PRO:HD2	2.01	0.41
1:C:41:SER:OG	1:C:43:HIS:HD2	2.03	0.41
1:C:85:TYR:CZ	1:C:297:VAL:HG22	2.55	0.41
1:C:754:ALA:HB1	1:C:759:VAL:CG1	2.50	0.41
1:C:1033:GLU:HG3	1:C:1034:PRO:HD2	2.01	0.41
1:F:519:PRO:CB	1:F:705:HIS:NE2	2.81	0.41
1:F:695:MET:HE3	1:F:695:MET:HB3	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:VAL:HG12	1:E:28:ILE:CG2	2.50	0.41
1:D:428:ILE:HB	1:D:429:PRO:HD3	2.02	0.41
1:D:628:ILE:O	1:D:632:VAL:HG23	2.21	0.41
1:D:679:ILE:CD1	1:D:724:LEU:HD13	2.45	0.41
1:D:859:MET:HE2	1:D:859:MET:HA	2.01	0.41
1:A:137:SER:CB	1:A:141:VAL:HG22	2.50	0.41
1:A:695:MET:HE3	1:A:695:MET:HB3	1.87	0.41
1:B:369:THR:OG1	1:B:370:GLY:N	2.53	0.41
1:H:17:ILE:HD11	1:H:43:HIS:CB	2.49	0.41
1:H:134:ILE:CG2	1:H:203:GLU:HB2	2.51	0.41
1:H:628:ILE:O	1:H:632:VAL:HG23	2.21	0.41
1:F:63:TYR:HB2	1:F:87:PHE:CE2	2.55	0.41
1:F:211:HIS:C	1:F:212:ILE:HD12	2.45	0.41
1:F:600:ARG:HG3	1:F:639:GLY:HA3	2.02	0.41
1:E:674:CYS:CB	1:E:712:MET:HE1	2.49	0.41
1:E:675:TYR:HE2	1:E:716:LEU:HA	1.84	0.41
1:G:41:SER:OG	1:G:43:HIS:HD2	2.03	0.41
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.92	0.41
1:A:82:HIS:CD2	1:A:84:GLY:H	2.26	0.41
1:B:265:LEU:C	1:B:265:LEU:HD12	2.46	0.41
1:B:948:MET:HA	1:B:948:MET:HE2	2.02	0.41
1:C:794:LEU:HD12	1:C:794:LEU:C	2.46	0.41
1:C:794:LEU:HD12	1:C:795:ASP:C	2.45	0.41
1:F:607:MET:HE2	1:F:642:VAL:CG2	2.50	0.41
1:G:13:GLY:O	1:G:14:GLU:C	2.63	0.41
1:G:95:ALA:O	1:G:99:GLU:HG3	2.21	0.41
1:G:194:ALA:C	1:G:195:PHE:CD2	2.97	0.41
1:G:313:SER:O	1:G:314:GLN:C	2.63	0.41
1:G:672:ALA:HA	1:G:708:GLY:O	2.20	0.41
1:D:115:MET:CG	1:D:125:GLN:HG3	2.49	0.41
1:B:7:VAL:HG12	1:B:28:ILE:CG2	2.50	0.41
1:B:672:ALA:HA	1:B:708:GLY:O	2.20	0.41
1:C:1:MET:HE3	1:C:319:ASP:CG	2.44	0.41
1:C:304:MET:CE	1:C:399:CYS:CB	2.99	0.41
1:H:428:ILE:HB	1:H:429:PRO:HD3	2.03	0.41
1:F:157:PRO:O	1:F:205:CYS:HB2	2.20	0.41
1:F:288:PHE:CD1	1:F:289:ILE:N	2.89	0.41
1:F:490:PRO:HD2	1:F:492:TYR:CE2	2.56	0.41
1:F:1044:PHE:HE2	1:F:1053:ILE:HD11	1.86	0.41
1:E:304:MET:CE	1:E:399:CYS:CB	2.98	0.41
1:E:1033:GLU:HG3	1:E:1034:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HE3	1:G:319:ASP:CG	2.45	0.41
1:G:134:ILE:CD1	1:G:287:TYR:CB	2.98	0.41
1:G:211:HIS:C	1:G:212:ILE:HD12	2.46	0.41
1:D:138:ASN:OD1	1:D:138:ASN:N	2.52	0.41
1:A:1:MET:HE3	1:A:319:ASP:OD2	2.20	0.41
1:A:198:ASP:OD1	1:A:198:ASP:N	2.54	0.41
1:A:470:LEU:HB3	1:A:1044:PHE:CE2	2.55	0.41
1:A:607:MET:HE2	1:A:642:VAL:CG2	2.50	0.41
1:B:450:ILE:CG2	1:B:451:ASP:N	2.84	0.41
1:B:631:PHE:O	1:B:635:SER:OG	2.38	0.41
1:F:67:GLU:O	1:F:71:GLU:HG2	2.21	0.41
1:F:427:ASN:ND2	1:F:431:LEU:HD11	2.36	0.41
1:F:847:VAL:HB	1:F:849:LEU:CD1	2.51	0.41
1:E:631:PHE:O	1:E:635:SER:OG	2.38	0.41
1:G:794:LEU:HD12	1:G:794:LEU:C	2.46	0.41
1:A:1:MET:CE	1:A:319:ASP:HB2	2.51	0.41
1:A:224:ILE:HG22	1:A:263:VAL:HG13	2.03	0.41
1:B:42:PHE:HA	1:B:45:TYR:HD2	1.84	0.41
1:B:373:GLY:O	1:B:400:THR:HA	2.20	0.41
1:C:672:ALA:HA	1:C:708:GLY:O	2.20	0.41
1:H:138:ASN:OD1	1:H:138:ASN:N	2.53	0.41
1:H:536:ASP:HB3	1:H:573:PHE:HD1	1.86	0.41
1:F:224:ILE:HG22	1:F:263:VAL:HG13	2.03	0.41
1:E:14:GLU:CD	1:E:397:LYS:HE2	2.44	0.41
1:E:133:VAL:HG12	1:E:134:ILE:N	2.36	0.41
1:E:254:LEU:O	1:E:255:ARG:C	2.64	0.41
1:G:509:GLY:N	1:G:605:ASN:HB2	2.35	0.41
1:G:1044:PHE:HE2	1:G:1053:ILE:HD11	1.85	0.41
1:D:41:SER:OG	1:D:43:HIS:HD2	2.03	0.41
1:D:134:ILE:HG23	1:D:135:PRO:HD2	2.03	0.41
1:D:1044:PHE:HE2	1:D:1053:ILE:HD11	1.85	0.41
1:A:67:GLU:O	1:A:71:GLU:HG2	2.21	0.41
1:A:211:HIS:C	1:A:212:ILE:HD12	2.46	0.41
1:A:304:MET:CE	1:A:399:CYS:HB2	2.50	0.41
1:A:490:PRO:HD2	1:A:492:TYR:CE2	2.56	0.41
1:B:212:ILE:HG23	1:B:229:GLU:HB2	2.03	0.41
1:B:304:MET:CE	1:B:399:CYS:CB	2.99	0.41
1:B:674:CYS:CB	1:B:712:MET:HE1	2.50	0.41
1:C:95:ALA:O	1:C:99:GLU:HG3	2.21	0.41
1:C:313:SER:O	1:C:314:GLN:C	2.64	0.41
1:C:502:TYR:CD1	1:C:502:TYR:C	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:PRO:CG	1:C:749:TYR:CD2	3.04	0.41
1:H:67:GLU:O	1:H:71:GLU:HG2	2.21	0.41
1:H:288:PHE:CD1	1:H:289:ILE:N	2.89	0.41
1:H:382:PHE:CD1	1:H:385:THR:HB	2.56	0.41
1:F:1:MET:HE3	1:F:319:ASP:OD2	2.21	0.41
1:F:1:MET:CE	1:F:319:ASP:HB2	2.51	0.41
1:F:88:LEU:HB3	1:F:94:PHE:CD2	2.56	0.41
1:F:685:THR:O	1:F:688:THR:HG23	2.21	0.41
1:E:265:LEU:C	1:E:265:LEU:HD12	2.46	0.41
1:E:612:LEU:CD1	1:E:612:LEU:C	2.94	0.41
1:G:1:MET:HE3	1:G:319:ASP:OD2	2.20	0.41
1:D:134:ILE:CG2	1:D:203:GLU:HB2	2.51	0.41
1:A:51:TYR:CE1	1:B:1021:GLY:HA2	2.54	0.41
1:B:12:ARG:NE	1:B:391:TYR:CD1	2.89	0.41
1:B:157:PRO:C	1:B:205:CYS:CB	2.94	0.41
1:C:1:MET:HE3	1:C:319:ASP:OD2	2.20	0.41
1:H:265:LEU:O	1:H:269:VAL:HG22	2.20	0.40
1:H:620:TYR:HD1	1:H:979:TYR:CE1	2.39	0.40
1:H:679:ILE:CD1	1:H:724:LEU:HD13	2.46	0.40
1:F:862:VAL:O	1:F:866:MET:N	2.53	0.40
1:F:911:ILE:O	1:F:915:MET:N	2.50	0.40
1:E:12:ARG:NE	1:E:391:TYR:CD1	2.90	0.40
1:E:365:THR:CG2	1:E:1050:PRO:O	2.68	0.40
1:G:198:ASP:O	1:G:200:VAL:CG2	2.68	0.40
1:G:373:GLY:O	1:G:400:THR:HA	2.20	0.40
1:G:651:TRP:HE1	1:G:653:LYS:CB	2.35	0.40
1:D:258:ILE:CG2	1:D:279:PHE:CD2	3.04	0.40
1:D:862:VAL:O	1:D:866:MET:N	2.54	0.40
1:C:134:ILE:CD1	1:C:287:TYR:CB	2.98	0.40
1:C:145:LYS:C	1:C:147:VAL:N	2.78	0.40
1:C:536:ASP:HB3	1:C:573:PHE:HD1	1.86	0.40
1:H:133:VAL:HG12	1:H:134:ILE:N	2.36	0.40
1:H:177:LYS:HG2	1:H:179:HIS:CE1	2.56	0.40
1:H:258:ILE:CG2	1:H:279:PHE:CD2	3.04	0.40
1:F:540:ARG:HH11	1:F:540:ARG:HD2	1.69	0.40
1:E:540:ARG:NH1	1:E:578:GLY:HA3	2.37	0.40
1:G:198:ASP:N	1:G:198:ASP:OD1	2.52	0.40
1:G:718:PRO:CG	1:G:749:TYR:CD2	3.05	0.40
1:D:278:GLU:C	1:D:289:ILE:HD12	2.46	0.40
1:D:620:TYR:HD1	1:D:979:TYR:CE1	2.39	0.40
1:A:212:ILE:HG23	1:A:229:GLU:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ALA:HB3	1:A:715:LEU:HD12	2.01	0.40
1:A:862:VAL:O	1:A:866:MET:N	2.53	0.40
1:A:1044:PHE:HE2	1:A:1053:ILE:HD11	1.86	0.40
1:B:14:GLU:CD	1:B:397:LYS:HE2	2.45	0.40
1:B:137:SER:CB	1:B:141:VAL:HG22	2.50	0.40
1:C:234:ILE:CD1	1:C:445:TYR:CZ	3.01	0.40
1:F:145:LYS:C	1:F:147:VAL:N	2.79	0.40
1:F:198:ASP:OD1	1:F:198:ASP:N	2.55	0.40
1:F:304:MET:CE	1:F:399:CYS:HB2	2.50	0.40
1:E:541:ASP:OD2	1:E:739:HIS:HE1	2.01	0.40
1:D:67:GLU:O	1:D:71:GLU:HG2	2.21	0.40
1:A:173:VAL:HG13	1:A:205:CYS:SG	2.61	0.40
1:B:540:ARG:NH2	1:B:541:ASP:CG	2.79	0.40
1:C:631:PHE:O	1:C:635:SER:OG	2.37	0.40
1:C:979:TYR:CB	1:C:982:VAL:HG22	2.51	0.40
1:C:1044:PHE:HE2	1:C:1053:ILE:HD11	1.86	0.40
1:H:862:VAL:O	1:H:866:MET:N	2.54	0.40
1:H:1044:PHE:HE2	1:H:1053:ILE:HD11	1.86	0.40
1:F:331:PRO:HG2	1:F:336:ILE:HG12	2.03	0.40
1:D:265:LEU:O	1:D:269:VAL:HG22	2.20	0.40
1:B:230:ARG:HD3	1:B:302:THR:OG1	2.21	0.40
1:B:541:ASP:OD2	1:B:739:HIS:HE1	2.02	0.40
1:B:612:LEU:CD1	1:B:612:LEU:C	2.94	0.40
1:H:230:ARG:HD3	1:H:302:THR:OG1	2.21	0.40
1:F:131:ILE:HD13	1:F:131:ILE:N	2.36	0.40
1:F:137:SER:CB	1:F:141:VAL:HG22	2.51	0.40
1:F:470:LEU:HB3	1:F:1044:PHE:CE2	2.56	0.40
1:E:540:ARG:NH2	1:E:541:ASP:CG	2.79	0.40
1:G:212:ILE:HG23	1:G:229:GLU:HB2	2.04	0.40
1:D:45:TYR:CZ	1:C:1047:ASN:O	2.74	0.40
1:D:304:MET:CE	1:D:399:CYS:HB2	2.51	0.40
1:D:536:ASP:HB3	1:D:573:PHE:HD1	1.87	0.40
1:A:373:GLY:O	1:A:400:THR:HA	2.22	0.40
1:B:628:ILE:O	1:B:632:VAL:HG23	2.21	0.40
1:C:288:PHE:CD1	1:C:289:ILE:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1048/1146 (91%)	988 (94%)	57 (5%)	3 (0%)	36	66
1	B	1021/1146 (89%)	966 (95%)	53 (5%)	2 (0%)	43	71
1	C	933/1146 (81%)	882 (94%)	47 (5%)	4 (0%)	30	60
1	D	1025/1146 (89%)	967 (94%)	55 (5%)	3 (0%)	36	66
1	E	1021/1146 (89%)	962 (94%)	56 (6%)	3 (0%)	36	66
1	F	1048/1146 (91%)	992 (95%)	54 (5%)	2 (0%)	43	71
1	G	934/1146 (82%)	881 (94%)	49 (5%)	4 (0%)	30	60
1	H	1025/1146 (89%)	966 (94%)	56 (6%)	3 (0%)	36	66
All	All	8055/9168 (88%)	7604 (94%)	427 (5%)	24 (0%)	36	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	273	ASN
1	F	273	ASN
1	E	273	ASN
1	G	176	SER
1	G	273	ASN
1	D	273	ASN
1	A	273	ASN
1	B	273	ASN
1	C	176	SER
1	C	273	ASN
1	A	176	SER
1	F	176	SER
1	D	176	SER
1	H	997	THR
1	E	506	ILE
1	G	506	ILE
1	C	506	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1035	ILE
1	E	1035	ILE
1	G	1035	ILE
1	D	1035	ILE
1	B	1035	ILE
1	C	1035	ILE
1	A	1035	ILE

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	814/981 (83%)	699 (86%)	115 (14%)	3	16
1	B	719/981 (73%)	617 (86%)	102 (14%)	3	15
1	C	676/981 (69%)	579 (86%)	97 (14%)	3	15
1	D	819/981 (84%)	705 (86%)	114 (14%)	3	16
1	E	719/981 (73%)	618 (86%)	101 (14%)	3	16
1	F	814/981 (83%)	700 (86%)	114 (14%)	3	16
1	G	677/981 (69%)	581 (86%)	96 (14%)	3	15
1	H	819/981 (84%)	706 (86%)	113 (14%)	3	16
All	All	6057/7848 (77%)	5205 (86%)	852 (14%)	3	16

All (852) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	ARG
1	H	7	VAL
1	H	12	ARG
1	H	20	MET
1	H	31	VAL
1	H	39	THR
1	H	44	ARG
1	H	57	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	60	ILE
1	H	70	ILE
1	H	71	GLU
1	H	76	SER
1	H	88	LEU
1	H	92	ILE
1	H	106	VAL
1	H	110	SER
1	H	116	PHE
1	H	121	LYS
1	H	127	LEU
1	H	134	ILE
1	H	177	LYS
1	H	183	SER
1	H	198	ASP
1	H	203	GLU
1	H	207	MET
1	H	223	ASN
1	H	239	GLN
1	H	248	ASN
1	H	251	THR
1	H	252	SER
1	H	254	LEU
1	H	265	LEU
1	H	269	VAL
1	H	289	ILE
1	H	290	GLU
1	H	294	ARG
1	H	295	VAL
1	H	304	MET
1	H	323	LEU
1	H	334	GLU
1	H	350	GLU
1	H	356	PHE
1	H	360	THR
1	H	364	ASP
1	H	367	ARG
1	H	369	THR
1	H	377	ASP
1	H	382	PHE
1	H	392	ASP
1	H	393	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	405	PHE
1	H	407	GLN
1	H	419	PHE
1	H	434	VAL
1	H	436	ARG
1	H	453	THR
1	H	461	HIS
1	H	462	ILE
1	H	478	VAL
1	H	499	LYS
1	H	504	SER
1	H	507	SER
1	H	517	LYS
1	H	531	GLU
1	H	533	LEU
1	H	540	ARG
1	H	545	SER
1	H	547	LEU
1	H	549	THR
1	H	558	GLN
1	H	572	SER
1	H	576	TRP
1	H	600	ARG
1	H	613	ARG
1	H	635	SER
1	H	645	VAL
1	H	657	VAL
1	H	658	SER
1	H	668	ILE
1	H	682	ASP
1	H	688	THR
1	H	695	MET
1	H	698	GLU
1	H	717	LYS
1	H	719	GLN
1	H	723	ARG
1	H	727	GLU
1	H	734	VAL
1	H	748	ILE
1	H	781	LEU
1	H	792	THR
1	H	825	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	845	ILE
1	H	858	GLU
1	H	867	PHE
1	H	870	ILE
1	H	890	ASN
1	H	891	GLU
1	H	895	GLU
1	H	896	ASP
1	H	898	TYR
1	H	918	ILE
1	H	928	LYS
1	H	942	ASP
1	H	960	LEU
1	H	974	ILE
1	H	1016	VAL
1	H	1018	LEU
1	H	1020	LYS
1	H	1040	ARG
1	H	1051	ARG
1	H	1053	ILE
1	H	1059	ASN
1	F	7	VAL
1	F	20	MET
1	F	39	THR
1	F	44	ARG
1	F	57	LYS
1	F	60	ILE
1	F	71	GLU
1	F	76	SER
1	F	92	ILE
1	F	106	VAL
1	F	110	SER
1	F	115	MET
1	F	121	LYS
1	F	127	LEU
1	F	131	ILE
1	F	134	ILE
1	F	159	MET
1	F	163	SER
1	F	183	SER
1	F	195	PHE
1	F	198	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	205	CYS
1	F	207	MET
1	F	239	GLN
1	F	251	THR
1	F	252	SER
1	F	254	LEU
1	F	265	LEU
1	F	269	VAL
1	F	289	ILE
1	F	294	ARG
1	F	295	VAL
1	F	304	MET
1	F	323	LEU
1	F	326	GLN
1	F	334	GLU
1	F	360	THR
1	F	367	ARG
1	F	369	THR
1	F	382	PHE
1	F	392	ASP
1	F	393	SER
1	F	395	LEU
1	F	403	MET
1	F	405	PHE
1	F	407	GLN
1	F	419	PHE
1	F	434	VAL
1	F	436	ARG
1	F	453	THR
1	F	462	ILE
1	F	463	ARG
1	F	476	VAL
1	F	504	SER
1	F	505	GLN
1	F	507	SER
1	F	510	THR
1	F	513	ILE
1	F	520	GLU
1	F	531	GLU
1	F	540	ARG
1	F	545	SER
1	F	547	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	549	THR
1	F	558	GLN
1	F	572	SER
1	F	576	TRP
1	F	600	ARG
1	F	635	SER
1	F	645	VAL
1	F	652	ILE
1	F	657	VAL
1	F	658	SER
1	F	668	ILE
1	F	682	ASP
1	F	688	THR
1	F	695	MET
1	F	698	GLU
1	F	717	LYS
1	F	719	GLN
1	F	723	ARG
1	F	727	GLU
1	F	734	VAL
1	F	748	ILE
1	F	781	LEU
1	F	792	THR
1	F	794	LEU
1	F	820	LEU
1	F	825	THR
1	F	845	ILE
1	F	867	PHE
1	F	870	ILE
1	F	890	ASN
1	F	891	GLU
1	F	895	GLU
1	F	896	ASP
1	F	897	VAL
1	F	918	ILE
1	F	940	LEU
1	F	942	ASP
1	F	943	ARG
1	F	957	LYS
1	F	960	LEU
1	F	974	ILE
1	F	1016	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1018	LEU
1	F	1030	SER
1	F	1031	ILE
1	F	1040	ARG
1	F	1049	GLN
1	F	1053	ILE
1	F	1054	ASN
1	F	1056	GLN
1	F	1059	ASN
1	E	1	MET
1	E	7	VAL
1	E	20	MET
1	E	27	LYS
1	E	39	THR
1	E	44	ARG
1	E	58	LYS
1	E	76	SER
1	E	88	LEU
1	E	92	ILE
1	E	103	ILE
1	E	106	VAL
1	E	110	SER
1	E	115	MET
1	E	127	LEU
1	E	134	ILE
1	E	144	ILE
1	E	163	SER
1	E	183	SER
1	E	184	PHE
1	E	198	ASP
1	E	207	MET
1	E	228	PHE
1	E	237	ARG
1	E	248	ASN
1	E	251	THR
1	E	252	SER
1	E	254	LEU
1	E	265	LEU
1	E	269	VAL
1	E	280	LEU
1	E	289	ILE
1	E	294	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	304	MET
1	E	323	LEU
1	E	326	GLN
1	E	334	GLU
1	E	349	THR
1	E	350	GLU
1	E	356	PHE
1	E	357	MET
1	E	360	THR
1	E	364	ASP
1	E	367	ARG
1	E	369	THR
1	E	377	ASP
1	E	382	PHE
1	E	392	ASP
1	E	393	SER
1	E	403	MET
1	E	405	PHE
1	E	407	GLN
1	E	419	PHE
1	E	434	VAL
1	E	436	ARG
1	E	453	THR
1	E	463	ARG
1	E	476	VAL
1	E	504	SER
1	E	505	GLN
1	E	507	SER
1	E	510	THR
1	E	531	GLU
1	E	540	ARG
1	E	545	SER
1	E	547	LEU
1	E	549	THR
1	E	558	GLN
1	E	567	LEU
1	E	572	SER
1	E	576	TRP
1	E	600	ARG
1	E	612	LEU
1	E	613	ARG
1	E	635	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	645	VAL
1	E	657	VAL
1	E	658	SER
1	E	668	ILE
1	E	682	ASP
1	E	684	ARG
1	E	688	THR
1	E	724	LEU
1	E	748	ILE
1	E	781	LEU
1	E	825	THR
1	E	858	GLU
1	E	890	ASN
1	E	891	GLU
1	E	895	GLU
1	E	896	ASP
1	E	898	TYR
1	E	920	GLN
1	E	927	GLU
1	E	949	GLU
1	E	952	ASN
1	E	960	LEU
1	E	974	ILE
1	E	1016	VAL
1	E	1040	ARG
1	E	1053	ILE
1	G	3	ARG
1	G	7	VAL
1	G	12	ARG
1	G	20	MET
1	G	39	THR
1	G	44	ARG
1	G	57	LYS
1	G	60	ILE
1	G	64	LEU
1	G	71	GLU
1	G	76	SER
1	G	88	LEU
1	G	92	ILE
1	G	106	VAL
1	G	110	SER
1	G	115	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	134	ILE
1	G	163	SER
1	G	172	ARG
1	G	174	VAL
1	G	179	HIS
1	G	183	SER
1	G	186	ARG
1	G	195	PHE
1	G	198	ASP
1	G	205	CYS
1	G	207	MET
1	G	248	ASN
1	G	251	THR
1	G	252	SER
1	G	254	LEU
1	G	265	LEU
1	G	269	VAL
1	G	289	ILE
1	G	294	ARG
1	G	295	VAL
1	G	304	MET
1	G	323	LEU
1	G	326	GLN
1	G	334	GLU
1	G	339	HIS
1	G	350	GLU
1	G	356	PHE
1	G	360	THR
1	G	364	ASP
1	G	367	ARG
1	G	369	THR
1	G	377	ASP
1	G	392	ASP
1	G	393	SER
1	G	405	PHE
1	G	407	GLN
1	G	419	PHE
1	G	434	VAL
1	G	436	ARG
1	G	453	THR
1	G	458	LYS
1	G	462	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	476	VAL
1	G	494	GLU
1	G	502	TYR
1	G	504	SER
1	G	506	ILE
1	G	507	SER
1	G	510	THR
1	G	531	GLU
1	G	540	ARG
1	G	545	SER
1	G	547	LEU
1	G	549	THR
1	G	558	GLN
1	G	572	SER
1	G	576	TRP
1	G	588	LEU
1	G	600	ARG
1	G	635	SER
1	G	657	VAL
1	G	658	SER
1	G	668	ILE
1	G	682	ASP
1	G	688	THR
1	G	698	GLU
1	G	717	LYS
1	G	737	HIS
1	G	748	ILE
1	G	781	LEU
1	G	792	THR
1	G	794	LEU
1	G	960	LEU
1	G	962	GLU
1	G	989	MET
1	G	1016	VAL
1	G	1018	LEU
1	G	1040	ARG
1	G	1053	ILE
1	G	1059	ASN
1	D	3	ARG
1	D	7	VAL
1	D	12	ARG
1	D	20	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	31	VAL
1	D	39	THR
1	D	44	ARG
1	D	57	LYS
1	D	60	ILE
1	D	70	ILE
1	D	71	GLU
1	D	76	SER
1	D	88	LEU
1	D	92	ILE
1	D	106	VAL
1	D	110	SER
1	D	116	PHE
1	D	121	LYS
1	D	127	LEU
1	D	134	ILE
1	D	177	LYS
1	D	183	SER
1	D	198	ASP
1	D	203	GLU
1	D	207	MET
1	D	223	ASN
1	D	239	GLN
1	D	248	ASN
1	D	251	THR
1	D	252	SER
1	D	254	LEU
1	D	265	LEU
1	D	269	VAL
1	D	289	ILE
1	D	290	GLU
1	D	294	ARG
1	D	295	VAL
1	D	304	MET
1	D	323	LEU
1	D	334	GLU
1	D	339	HIS
1	D	350	GLU
1	D	356	PHE
1	D	360	THR
1	D	364	ASP
1	D	367	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	369	THR
1	D	377	ASP
1	D	382	PHE
1	D	392	ASP
1	D	393	SER
1	D	405	PHE
1	D	407	GLN
1	D	419	PHE
1	D	434	VAL
1	D	436	ARG
1	D	453	THR
1	D	461	HIS
1	D	462	ILE
1	D	478	VAL
1	D	499	LYS
1	D	504	SER
1	D	507	SER
1	D	517	LYS
1	D	520	GLU
1	D	531	GLU
1	D	533	LEU
1	D	540	ARG
1	D	545	SER
1	D	547	LEU
1	D	549	THR
1	D	558	GLN
1	D	572	SER
1	D	576	TRP
1	D	600	ARG
1	D	613	ARG
1	D	635	SER
1	D	645	VAL
1	D	657	VAL
1	D	658	SER
1	D	668	ILE
1	D	682	ASP
1	D	688	THR
1	D	695	MET
1	D	698	GLU
1	D	717	LYS
1	D	719	GLN
1	D	723	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	727	GLU
1	D	734	VAL
1	D	748	ILE
1	D	781	LEU
1	D	792	THR
1	D	825	THR
1	D	845	ILE
1	D	858	GLU
1	D	867	PHE
1	D	870	ILE
1	D	890	ASN
1	D	891	GLU
1	D	895	GLU
1	D	896	ASP
1	D	898	TYR
1	D	918	ILE
1	D	928	LYS
1	D	942	ASP
1	D	960	LEU
1	D	974	ILE
1	D	1016	VAL
1	D	1018	LEU
1	D	1020	LYS
1	D	1040	ARG
1	D	1053	ILE
1	D	1059	ASN
1	A	7	VAL
1	A	20	MET
1	A	39	THR
1	A	44	ARG
1	A	57	LYS
1	A	60	ILE
1	A	71	GLU
1	A	76	SER
1	A	92	ILE
1	A	106	VAL
1	A	110	SER
1	A	115	MET
1	A	121	LYS
1	A	127	LEU
1	A	131	ILE
1	A	134	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	MET
1	A	163	SER
1	A	176	SER
1	A	183	SER
1	A	195	PHE
1	A	198	ASP
1	A	205	CYS
1	A	207	MET
1	A	239	GLN
1	A	251	THR
1	A	252	SER
1	A	253	GLU
1	A	254	LEU
1	A	265	LEU
1	A	269	VAL
1	A	289	ILE
1	A	294	ARG
1	A	295	VAL
1	A	304	MET
1	A	323	LEU
1	A	326	GLN
1	A	334	GLU
1	A	360	THR
1	A	367	ARG
1	A	369	THR
1	A	382	PHE
1	A	392	ASP
1	A	393	SER
1	A	395	LEU
1	A	403	MET
1	A	405	PHE
1	A	407	GLN
1	A	419	PHE
1	A	434	VAL
1	A	436	ARG
1	A	453	THR
1	A	462	ILE
1	A	463	ARG
1	A	476	VAL
1	A	504	SER
1	A	507	SER
1	A	510	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	513	ILE
1	A	520	GLU
1	A	531	GLU
1	A	540	ARG
1	A	545	SER
1	A	547	LEU
1	A	549	THR
1	A	558	GLN
1	A	572	SER
1	A	576	TRP
1	A	600	ARG
1	A	635	SER
1	A	645	VAL
1	A	652	ILE
1	A	657	VAL
1	A	658	SER
1	A	668	ILE
1	A	682	ASP
1	A	688	THR
1	A	695	MET
1	A	698	GLU
1	A	717	LYS
1	A	719	GLN
1	A	723	ARG
1	A	727	GLU
1	A	734	VAL
1	A	748	ILE
1	A	781	LEU
1	A	792	THR
1	A	794	LEU
1	A	820	LEU
1	A	825	THR
1	A	845	ILE
1	A	867	PHE
1	A	870	ILE
1	A	890	ASN
1	A	891	GLU
1	A	895	GLU
1	A	896	ASP
1	A	897	VAL
1	A	918	ILE
1	A	940	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	942	ASP
1	A	943	ARG
1	A	957	LYS
1	A	960	LEU
1	A	974	ILE
1	A	1016	VAL
1	A	1018	LEU
1	A	1030	SER
1	A	1031	ILE
1	A	1040	ARG
1	A	1049	GLN
1	A	1053	ILE
1	A	1054	ASN
1	A	1056	GLN
1	A	1059	ASN
1	B	1	MET
1	B	7	VAL
1	B	20	MET
1	B	27	LYS
1	B	39	THR
1	B	44	ARG
1	B	58	LYS
1	B	76	SER
1	B	88	LEU
1	B	92	ILE
1	B	103	ILE
1	B	106	VAL
1	B	110	SER
1	B	115	MET
1	B	127	LEU
1	B	134	ILE
1	B	144	ILE
1	B	158	LEU
1	B	163	SER
1	B	183	SER
1	B	184	PHE
1	B	198	ASP
1	B	207	MET
1	B	228	PHE
1	B	237	ARG
1	B	248	ASN
1	B	251	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	SER
1	B	254	LEU
1	B	265	LEU
1	B	269	VAL
1	B	280	LEU
1	B	289	ILE
1	B	294	ARG
1	B	304	MET
1	B	323	LEU
1	B	326	GLN
1	B	334	GLU
1	B	349	THR
1	B	350	GLU
1	B	356	PHE
1	B	357	MET
1	B	360	THR
1	B	364	ASP
1	B	367	ARG
1	B	369	THR
1	B	377	ASP
1	B	382	PHE
1	B	392	ASP
1	B	393	SER
1	B	405	PHE
1	B	407	GLN
1	B	434	VAL
1	B	436	ARG
1	B	453	THR
1	B	463	ARG
1	B	476	VAL
1	B	502	TYR
1	B	504	SER
1	B	505	GLN
1	B	506	ILE
1	B	510	THR
1	B	531	GLU
1	B	540	ARG
1	B	545	SER
1	B	547	LEU
1	B	549	THR
1	B	558	GLN
1	B	567	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	572	SER
1	B	576	TRP
1	B	600	ARG
1	B	612	LEU
1	B	613	ARG
1	B	635	SER
1	B	645	VAL
1	B	657	VAL
1	B	658	SER
1	B	668	ILE
1	B	682	ASP
1	B	684	ARG
1	B	688	THR
1	B	724	LEU
1	B	748	ILE
1	B	781	LEU
1	B	825	THR
1	B	858	GLU
1	B	890	ASN
1	B	891	GLU
1	B	895	GLU
1	B	896	ASP
1	B	898	TYR
1	B	920	GLN
1	B	927	GLU
1	B	949	GLU
1	B	952	ASN
1	B	960	LEU
1	B	974	ILE
1	B	1016	VAL
1	B	1040	ARG
1	B	1053	ILE
1	B	1059	ASN
1	C	3	ARG
1	C	7	VAL
1	C	12	ARG
1	C	20	MET
1	C	39	THR
1	C	44	ARG
1	C	57	LYS
1	C	60	ILE
1	C	64	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	71	GLU
1	C	76	SER
1	C	88	LEU
1	C	92	ILE
1	C	106	VAL
1	C	110	SER
1	C	115	MET
1	C	134	ILE
1	C	172	ARG
1	C	174	VAL
1	C	175	GLU
1	C	179	HIS
1	C	183	SER
1	C	186	ARG
1	C	195	PHE
1	C	198	ASP
1	C	203	GLU
1	C	205	CYS
1	C	207	MET
1	C	227	LEU
1	C	248	ASN
1	C	251	THR
1	C	252	SER
1	C	254	LEU
1	C	265	LEU
1	C	269	VAL
1	C	289	ILE
1	C	294	ARG
1	C	295	VAL
1	C	304	MET
1	C	323	LEU
1	C	326	GLN
1	C	334	GLU
1	C	339	HIS
1	C	350	GLU
1	C	356	PHE
1	C	360	THR
1	C	364	ASP
1	C	367	ARG
1	C	369	THR
1	C	377	ASP
1	C	392	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	393	SER
1	C	405	PHE
1	C	407	GLN
1	C	434	VAL
1	C	436	ARG
1	C	453	THR
1	C	458	LYS
1	C	462	ILE
1	C	476	VAL
1	C	494	GLU
1	C	502	TYR
1	C	504	SER
1	C	506	ILE
1	C	507	SER
1	C	510	THR
1	C	531	GLU
1	C	540	ARG
1	C	545	SER
1	C	547	LEU
1	C	549	THR
1	C	558	GLN
1	C	572	SER
1	C	576	TRP
1	C	588	LEU
1	C	600	ARG
1	C	635	SER
1	C	651	TRP
1	C	657	VAL
1	C	658	SER
1	C	668	ILE
1	C	682	ASP
1	C	688	THR
1	C	698	GLU
1	C	717	LYS
1	C	737	HIS
1	C	748	ILE
1	C	781	LEU
1	C	792	THR
1	C	794	LEU
1	C	960	LEU
1	C	962	GLU
1	C	989	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1016	VAL
1	C	1040	ARG
1	C	1053	ILE
1	C	1059	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	2	ASN
1	H	43	HIS
1	H	82	HIS
1	H	112	HIS
1	H	221	HIS
1	H	223	ASN
1	H	226	HIS
1	H	292	ASN
1	H	333	GLN
1	H	337	HIS
1	H	354	ASN
1	H	383	GLN
1	H	415	ASN
1	H	479	ASN
1	H	558	GLN
1	H	602	GLN
1	H	719	GLN
1	H	741	HIS
1	H	787	ASN
1	H	842	GLN
1	H	1047	ASN
1	F	2	ASN
1	F	43	HIS
1	F	82	HIS
1	F	112	HIS
1	F	179	HIS
1	F	223	ASN
1	F	226	HIS
1	F	292	ASN
1	F	333	GLN
1	F	337	HIS
1	F	383	GLN
1	F	415	ASN
1	F	461	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	479	ASN
1	F	505	GLN
1	F	558	GLN
1	F	565	HIS
1	F	602	GLN
1	F	719	GLN
1	F	741	HIS
1	F	787	ASN
1	F	865	GLN
1	F	1047	ASN
1	E	43	HIS
1	E	82	HIS
1	E	112	HIS
1	E	221	HIS
1	E	223	ASN
1	E	226	HIS
1	E	292	ASN
1	E	333	GLN
1	E	337	HIS
1	E	354	ASN
1	E	383	GLN
1	E	415	ASN
1	E	437	HIS
1	E	479	ASN
1	E	558	GLN
1	E	746	ASN
1	E	787	ASN
1	E	842	GLN
1	E	865	GLN
1	E	1047	ASN
1	E	1049	GLN
1	G	2	ASN
1	G	43	HIS
1	G	82	HIS
1	G	112	HIS
1	G	221	HIS
1	G	223	ASN
1	G	226	HIS
1	G	292	ASN
1	G	333	GLN
1	G	337	HIS
1	G	415	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	479	ASN
1	G	558	GLN
1	G	602	GLN
1	G	737	HIS
1	G	746	ASN
1	G	787	ASN
1	G	830	HIS
1	D	2	ASN
1	D	43	HIS
1	D	82	HIS
1	D	112	HIS
1	D	221	HIS
1	D	223	ASN
1	D	226	HIS
1	D	292	ASN
1	D	333	GLN
1	D	337	HIS
1	D	354	ASN
1	D	383	GLN
1	D	415	ASN
1	D	479	ASN
1	D	558	GLN
1	D	602	GLN
1	D	719	GLN
1	D	741	HIS
1	D	787	ASN
1	D	842	GLN
1	D	1047	ASN
1	A	2	ASN
1	A	43	HIS
1	A	82	HIS
1	A	112	HIS
1	A	179	HIS
1	A	223	ASN
1	A	226	HIS
1	A	292	ASN
1	A	333	GLN
1	A	337	HIS
1	A	383	GLN
1	A	415	ASN
1	A	461	HIS
1	A	479	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	558	GLN
1	A	602	GLN
1	A	719	GLN
1	A	741	HIS
1	A	787	ASN
1	A	865	GLN
1	A	1047	ASN
1	B	43	HIS
1	B	82	HIS
1	B	112	HIS
1	B	221	HIS
1	B	223	ASN
1	B	226	HIS
1	B	292	ASN
1	B	333	GLN
1	B	337	HIS
1	B	354	ASN
1	B	383	GLN
1	B	415	ASN
1	B	437	HIS
1	B	479	ASN
1	B	558	GLN
1	B	622	ASN
1	B	746	ASN
1	B	787	ASN
1	B	842	GLN
1	B	865	GLN
1	B	1047	ASN
1	B	1049	GLN
1	C	2	ASN
1	C	43	HIS
1	C	82	HIS
1	C	112	HIS
1	C	221	HIS
1	C	223	ASN
1	C	226	HIS
1	C	292	ASN
1	C	333	GLN
1	C	337	HIS
1	C	415	ASN
1	C	479	ASN
1	C	558	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	565	HIS
1	C	602	GLN
1	C	622	ASN
1	C	737	HIS
1	C	746	ASN
1	C	787	ASN
1	C	830	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1052/1146 (91%)	-1.14	4 (0%) 88 78	74, 124, 168, 201	0
1	B	1031/1146 (89%)	-0.97	2 (0%) 91 85	72, 153, 205, 246	0
1	C	941/1146 (82%)	-0.93	4 (0%) 88 78	72, 147, 212, 265	0
1	D	1029/1146 (89%)	-1.13	1 (0%) 92 90	58, 118, 188, 231	0
1	E	1031/1146 (89%)	-0.98	6 (0%) 85 72	68, 149, 205, 248	0
1	F	1052/1146 (91%)	-1.16	4 (0%) 88 78	72, 123, 168, 204	0
1	G	942/1146 (82%)	-1.00	4 (0%) 88 78	70, 141, 208, 267	0
1	H	1029/1146 (89%)	-1.13	0 100 100	59, 114, 185, 232	0
All	All	8107/9168 (88%)	-1.06	25 (0%) 90 82	58, 132, 199, 267	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	569	ASN	3.3
1	A	1017	GLU	2.8
1	E	575	MET	2.7
1	C	757	ALA	2.7
1	A	1018	LEU	2.5
1	A	1052	GLU	2.5
1	E	576	TRP	2.4
1	D	116	PHE	2.3
1	E	108	PRO	2.3
1	F	1052	GLU	2.3
1	G	551	VAL	2.2
1	E	572	SER	2.2
1	G	141	VAL	2.2
1	G	292	ASN	2.2
1	F	1017	GLU	2.2
1	E	998	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	147	VAL	2.1
1	C	538	THR	2.1
1	A	1023	ILE	2.1
1	C	595	ARG	2.1
1	B	568	PRO	2.1
1	F	1018	LEU	2.0
1	G	674	CYS	2.0
1	E	293	PRO	2.0
1	F	1050	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.