Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:29 pm BST

PDB ID	:	3ZVJ
Title	:	Crystal structure of high molecular weight (HMW) form of Peroxiredoxin I from Schistosoma mansoni
Authors	:	Saccoccia, F.; Angelucci, F.; Bellelli, A.; Boumis, G.; Brunori, M.; Miele, A.E.
Deposited on	:	2011-07-25
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

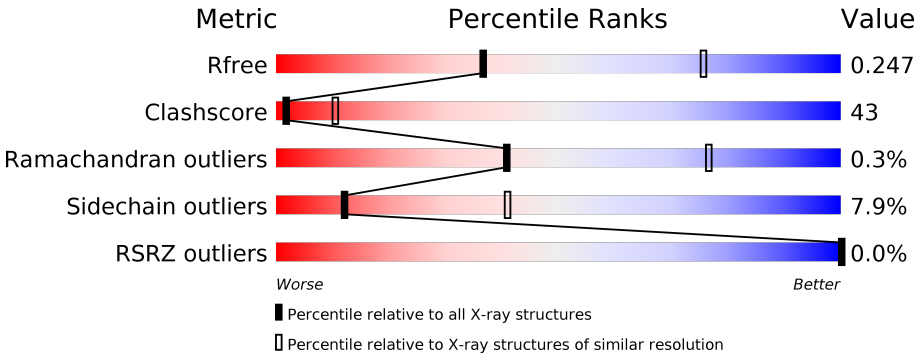
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	30% 41% 5% 25%
1	B	219	24% 49% • 24%
1	C	219	25% 51% • 21%
1	E	219	26% 47% 5% 23%
1	F	219	30% 45% • 21%
1	G	219	31% 42% 5% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	219	32% 43% 22%
1	I	219	26% 45% 6% 24%
1	J	219	25% 47% 6% 22%
1	K	219	28% 46% 22%
1	L	219	30% 43% 5% 22%
1	M	219	25% 51% 22%
1	N	219	33% 40% 25%
1	O	219	28% 44% 24%
1	P	219	29% 43% 24%
1	Q	219	21% 49% 26%
1	R	219	30% 42% 23%
1	S	219	30% 43% 6% 21%
1	T	219	28% 47% 22%
2	D	219	28% 44% 5% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26988 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 THIOREDOXIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1324	848	224	246	6			
1	B	166	Total	C	N	O	S	0	0	0
			1331	852	225	248	6			
1	C	174	Total	C	N	O	S	0	0	0
			1385	884	234	260	7			
1	E	169	Total	C	N	O	S	0	0	0
			1351	864	229	253	5			
1	F	172	Total	C	N	O	S	0	0	0
			1367	872	231	257	7			
1	G	172	Total	C	N	O	S	0	0	0
			1372	877	232	256	7			
1	H	171	Total	C	N	O	S	0	0	0
			1364	873	230	254	7			
1	I	167	Total	C	N	O	S	0	0	0
			1337	855	226	250	6			
1	J	171	Total	C	N	O	S	0	0	0
			1364	873	230	254	7			
1	K	170	Total	C	N	O	S	0	0	0
			1357	867	229	254	7			
1	L	171	Total	C	N	O	S	0	0	0
			1364	872	230	255	7			
1	M	171	Total	C	N	O	S	0	0	0
			1361	869	230	256	6			
1	N	165	Total	C	N	O	S	0	0	0
			1322	845	224	248	5			
1	O	167	Total	C	N	O	S	0	0	0
			1337	854	226	251	6			
1	P	167	Total	C	N	O	S	0	0	0
			1335	854	226	249	6			
1	Q	163	Total	C	N	O	S	0	0	0
			1311	840	222	244	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	168	Total	C	N	O	S	0	0	0
			1338	854	227	251	6			
1	S	172	Total	C	N	O	S	0	0	0
			1367	872	231	257	7			
1	T	170	Total	C	N	O	S	0	0	0
			1357	867	229	254	7			

There are 646 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP O97161
A	-32	ARG	-	expression tag	UNP O97161
A	-31	GLY	-	expression tag	UNP O97161
A	-30	SER	-	expression tag	UNP O97161
A	-29	HIS	-	expression tag	UNP O97161
A	-28	HIS	-	expression tag	UNP O97161
A	-27	HIS	-	expression tag	UNP O97161
A	-26	HIS	-	expression tag	UNP O97161
A	-25	HIS	-	expression tag	UNP O97161
A	-24	HIS	-	expression tag	UNP O97161
A	-23	GLY	-	expression tag	UNP O97161
A	-22	MET	-	expression tag	UNP O97161
A	-21	ALA	-	expression tag	UNP O97161
A	-20	SER	-	expression tag	UNP O97161
A	-19	MET	-	expression tag	UNP O97161
A	-18	THR	-	expression tag	UNP O97161
A	-17	GLY	-	expression tag	UNP O97161
A	-16	GLY	-	expression tag	UNP O97161
A	-15	GLN	-	expression tag	UNP O97161
A	-14	GLN	-	expression tag	UNP O97161
A	-13	MET	-	expression tag	UNP O97161
A	-12	GLY	-	expression tag	UNP O97161
A	-11	ARG	-	expression tag	UNP O97161
A	-10	ASP	-	expression tag	UNP O97161
A	-9	LEU	-	expression tag	UNP O97161
A	-8	TYR	-	expression tag	UNP O97161
A	-7	ASP	-	expression tag	UNP O97161
A	-6	ASP	-	expression tag	UNP O97161
A	-5	ASP	-	expression tag	UNP O97161
A	-4	ASP	-	expression tag	UNP O97161
A	-3	LYS	-	expression tag	UNP O97161
A	-2	GLY	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP O97161
A	0	THR	-	expression tag	UNP O97161
B	-33	MET	-	expression tag	UNP O97161
B	-32	ARG	-	expression tag	UNP O97161
B	-31	GLY	-	expression tag	UNP O97161
B	-30	SER	-	expression tag	UNP O97161
B	-29	HIS	-	expression tag	UNP O97161
B	-28	HIS	-	expression tag	UNP O97161
B	-27	HIS	-	expression tag	UNP O97161
B	-26	HIS	-	expression tag	UNP O97161
B	-25	HIS	-	expression tag	UNP O97161
B	-24	HIS	-	expression tag	UNP O97161
B	-23	GLY	-	expression tag	UNP O97161
B	-22	MET	-	expression tag	UNP O97161
B	-21	ALA	-	expression tag	UNP O97161
B	-20	SER	-	expression tag	UNP O97161
B	-19	MET	-	expression tag	UNP O97161
B	-18	THR	-	expression tag	UNP O97161
B	-17	GLY	-	expression tag	UNP O97161
B	-16	GLY	-	expression tag	UNP O97161
B	-15	GLN	-	expression tag	UNP O97161
B	-14	GLN	-	expression tag	UNP O97161
B	-13	MET	-	expression tag	UNP O97161
B	-12	GLY	-	expression tag	UNP O97161
B	-11	ARG	-	expression tag	UNP O97161
B	-10	ASP	-	expression tag	UNP O97161
B	-9	LEU	-	expression tag	UNP O97161
B	-8	TYR	-	expression tag	UNP O97161
B	-7	ASP	-	expression tag	UNP O97161
B	-6	ASP	-	expression tag	UNP O97161
B	-5	ASP	-	expression tag	UNP O97161
B	-4	ASP	-	expression tag	UNP O97161
B	-3	LYS	-	expression tag	UNP O97161
B	-2	GLY	-	expression tag	UNP O97161
B	-1	SER	-	expression tag	UNP O97161
B	0	THR	-	expression tag	UNP O97161
C	-33	MET	-	expression tag	UNP O97161
C	-32	ARG	-	expression tag	UNP O97161
C	-31	GLY	-	expression tag	UNP O97161
C	-30	SER	-	expression tag	UNP O97161
C	-29	HIS	-	expression tag	UNP O97161
C	-28	HIS	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-27	HIS	-	expression tag	UNP O97161
C	-26	HIS	-	expression tag	UNP O97161
C	-25	HIS	-	expression tag	UNP O97161
C	-24	HIS	-	expression tag	UNP O97161
C	-23	GLY	-	expression tag	UNP O97161
C	-22	MET	-	expression tag	UNP O97161
C	-21	ALA	-	expression tag	UNP O97161
C	-20	SER	-	expression tag	UNP O97161
C	-19	MET	-	expression tag	UNP O97161
C	-18	THR	-	expression tag	UNP O97161
C	-17	GLY	-	expression tag	UNP O97161
C	-16	GLY	-	expression tag	UNP O97161
C	-15	GLN	-	expression tag	UNP O97161
C	-14	GLN	-	expression tag	UNP O97161
C	-13	MET	-	expression tag	UNP O97161
C	-12	GLY	-	expression tag	UNP O97161
C	-11	ARG	-	expression tag	UNP O97161
C	-10	ASP	-	expression tag	UNP O97161
C	-9	LEU	-	expression tag	UNP O97161
C	-8	TYR	-	expression tag	UNP O97161
C	-7	ASP	-	expression tag	UNP O97161
C	-6	ASP	-	expression tag	UNP O97161
C	-5	ASP	-	expression tag	UNP O97161
C	-4	ASP	-	expression tag	UNP O97161
C	-3	LYS	-	expression tag	UNP O97161
C	-2	GLY	-	expression tag	UNP O97161
C	-1	SER	-	expression tag	UNP O97161
C	0	THR	-	expression tag	UNP O97161
E	-33	MET	-	expression tag	UNP O97161
E	-32	ARG	-	expression tag	UNP O97161
E	-31	GLY	-	expression tag	UNP O97161
E	-30	SER	-	expression tag	UNP O97161
E	-29	HIS	-	expression tag	UNP O97161
E	-28	HIS	-	expression tag	UNP O97161
E	-27	HIS	-	expression tag	UNP O97161
E	-26	HIS	-	expression tag	UNP O97161
E	-25	HIS	-	expression tag	UNP O97161
E	-24	HIS	-	expression tag	UNP O97161
E	-23	GLY	-	expression tag	UNP O97161
E	-22	MET	-	expression tag	UNP O97161
E	-21	ALA	-	expression tag	UNP O97161
E	-20	SER	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	expression tag	UNP O97161
E	-18	THR	-	expression tag	UNP O97161
E	-17	GLY	-	expression tag	UNP O97161
E	-16	GLY	-	expression tag	UNP O97161
E	-15	GLN	-	expression tag	UNP O97161
E	-14	GLN	-	expression tag	UNP O97161
E	-13	MET	-	expression tag	UNP O97161
E	-12	GLY	-	expression tag	UNP O97161
E	-11	ARG	-	expression tag	UNP O97161
E	-10	ASP	-	expression tag	UNP O97161
E	-9	LEU	-	expression tag	UNP O97161
E	-8	TYR	-	expression tag	UNP O97161
E	-7	ASP	-	expression tag	UNP O97161
E	-6	ASP	-	expression tag	UNP O97161
E	-5	ASP	-	expression tag	UNP O97161
E	-4	ASP	-	expression tag	UNP O97161
E	-3	LYS	-	expression tag	UNP O97161
E	-2	GLY	-	expression tag	UNP O97161
E	-1	SER	-	expression tag	UNP O97161
E	0	THR	-	expression tag	UNP O97161
F	-33	MET	-	expression tag	UNP O97161
F	-32	ARG	-	expression tag	UNP O97161
F	-31	GLY	-	expression tag	UNP O97161
F	-30	SER	-	expression tag	UNP O97161
F	-29	HIS	-	expression tag	UNP O97161
F	-28	HIS	-	expression tag	UNP O97161
F	-27	HIS	-	expression tag	UNP O97161
F	-26	HIS	-	expression tag	UNP O97161
F	-25	HIS	-	expression tag	UNP O97161
F	-24	HIS	-	expression tag	UNP O97161
F	-23	GLY	-	expression tag	UNP O97161
F	-22	MET	-	expression tag	UNP O97161
F	-21	ALA	-	expression tag	UNP O97161
F	-20	SER	-	expression tag	UNP O97161
F	-19	MET	-	expression tag	UNP O97161
F	-18	THR	-	expression tag	UNP O97161
F	-17	GLY	-	expression tag	UNP O97161
F	-16	GLY	-	expression tag	UNP O97161
F	-15	GLN	-	expression tag	UNP O97161
F	-14	GLN	-	expression tag	UNP O97161
F	-13	MET	-	expression tag	UNP O97161
F	-12	GLY	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	ARG	-	expression tag	UNP O97161
F	-10	ASP	-	expression tag	UNP O97161
F	-9	LEU	-	expression tag	UNP O97161
F	-8	TYR	-	expression tag	UNP O97161
F	-7	ASP	-	expression tag	UNP O97161
F	-6	ASP	-	expression tag	UNP O97161
F	-5	ASP	-	expression tag	UNP O97161
F	-4	ASP	-	expression tag	UNP O97161
F	-3	LYS	-	expression tag	UNP O97161
F	-2	GLY	-	expression tag	UNP O97161
F	-1	SER	-	expression tag	UNP O97161
F	0	THR	-	expression tag	UNP O97161
G	-33	MET	-	expression tag	UNP O97161
G	-32	ARG	-	expression tag	UNP O97161
G	-31	GLY	-	expression tag	UNP O97161
G	-30	SER	-	expression tag	UNP O97161
G	-29	HIS	-	expression tag	UNP O97161
G	-28	HIS	-	expression tag	UNP O97161
G	-27	HIS	-	expression tag	UNP O97161
G	-26	HIS	-	expression tag	UNP O97161
G	-25	HIS	-	expression tag	UNP O97161
G	-24	HIS	-	expression tag	UNP O97161
G	-23	GLY	-	expression tag	UNP O97161
G	-22	MET	-	expression tag	UNP O97161
G	-21	ALA	-	expression tag	UNP O97161
G	-20	SER	-	expression tag	UNP O97161
G	-19	MET	-	expression tag	UNP O97161
G	-18	THR	-	expression tag	UNP O97161
G	-17	GLY	-	expression tag	UNP O97161
G	-16	GLY	-	expression tag	UNP O97161
G	-15	GLN	-	expression tag	UNP O97161
G	-14	GLN	-	expression tag	UNP O97161
G	-13	MET	-	expression tag	UNP O97161
G	-12	GLY	-	expression tag	UNP O97161
G	-11	ARG	-	expression tag	UNP O97161
G	-10	ASP	-	expression tag	UNP O97161
G	-9	LEU	-	expression tag	UNP O97161
G	-8	TYR	-	expression tag	UNP O97161
G	-7	ASP	-	expression tag	UNP O97161
G	-6	ASP	-	expression tag	UNP O97161
G	-5	ASP	-	expression tag	UNP O97161
G	-4	ASP	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	LYS	-	expression tag	UNP O97161
G	-2	GLY	-	expression tag	UNP O97161
G	-1	SER	-	expression tag	UNP O97161
G	0	THR	-	expression tag	UNP O97161
H	-33	MET	-	expression tag	UNP O97161
H	-32	ARG	-	expression tag	UNP O97161
H	-31	GLY	-	expression tag	UNP O97161
H	-30	SER	-	expression tag	UNP O97161
H	-29	HIS	-	expression tag	UNP O97161
H	-28	HIS	-	expression tag	UNP O97161
H	-27	HIS	-	expression tag	UNP O97161
H	-26	HIS	-	expression tag	UNP O97161
H	-25	HIS	-	expression tag	UNP O97161
H	-24	HIS	-	expression tag	UNP O97161
H	-23	GLY	-	expression tag	UNP O97161
H	-22	MET	-	expression tag	UNP O97161
H	-21	ALA	-	expression tag	UNP O97161
H	-20	SER	-	expression tag	UNP O97161
H	-19	MET	-	expression tag	UNP O97161
H	-18	THR	-	expression tag	UNP O97161
H	-17	GLY	-	expression tag	UNP O97161
H	-16	GLY	-	expression tag	UNP O97161
H	-15	GLN	-	expression tag	UNP O97161
H	-14	GLN	-	expression tag	UNP O97161
H	-13	MET	-	expression tag	UNP O97161
H	-12	GLY	-	expression tag	UNP O97161
H	-11	ARG	-	expression tag	UNP O97161
H	-10	ASP	-	expression tag	UNP O97161
H	-9	LEU	-	expression tag	UNP O97161
H	-8	TYR	-	expression tag	UNP O97161
H	-7	ASP	-	expression tag	UNP O97161
H	-6	ASP	-	expression tag	UNP O97161
H	-5	ASP	-	expression tag	UNP O97161
H	-4	ASP	-	expression tag	UNP O97161
H	-3	LYS	-	expression tag	UNP O97161
H	-2	GLY	-	expression tag	UNP O97161
H	-1	SER	-	expression tag	UNP O97161
H	0	THR	-	expression tag	UNP O97161
I	-33	MET	-	expression tag	UNP O97161
I	-32	ARG	-	expression tag	UNP O97161
I	-31	GLY	-	expression tag	UNP O97161
I	-30	SER	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-29	HIS	-	expression tag	UNP O97161
I	-28	HIS	-	expression tag	UNP O97161
I	-27	HIS	-	expression tag	UNP O97161
I	-26	HIS	-	expression tag	UNP O97161
I	-25	HIS	-	expression tag	UNP O97161
I	-24	HIS	-	expression tag	UNP O97161
I	-23	GLY	-	expression tag	UNP O97161
I	-22	MET	-	expression tag	UNP O97161
I	-21	ALA	-	expression tag	UNP O97161
I	-20	SER	-	expression tag	UNP O97161
I	-19	MET	-	expression tag	UNP O97161
I	-18	THR	-	expression tag	UNP O97161
I	-17	GLY	-	expression tag	UNP O97161
I	-16	GLY	-	expression tag	UNP O97161
I	-15	GLN	-	expression tag	UNP O97161
I	-14	GLN	-	expression tag	UNP O97161
I	-13	MET	-	expression tag	UNP O97161
I	-12	GLY	-	expression tag	UNP O97161
I	-11	ARG	-	expression tag	UNP O97161
I	-10	ASP	-	expression tag	UNP O97161
I	-9	LEU	-	expression tag	UNP O97161
I	-8	TYR	-	expression tag	UNP O97161
I	-7	ASP	-	expression tag	UNP O97161
I	-6	ASP	-	expression tag	UNP O97161
I	-5	ASP	-	expression tag	UNP O97161
I	-4	ASP	-	expression tag	UNP O97161
I	-3	LYS	-	expression tag	UNP O97161
I	-2	GLY	-	expression tag	UNP O97161
I	-1	SER	-	expression tag	UNP O97161
I	0	THR	-	expression tag	UNP O97161
J	-33	MET	-	expression tag	UNP O97161
J	-32	ARG	-	expression tag	UNP O97161
J	-31	GLY	-	expression tag	UNP O97161
J	-30	SER	-	expression tag	UNP O97161
J	-29	HIS	-	expression tag	UNP O97161
J	-28	HIS	-	expression tag	UNP O97161
J	-27	HIS	-	expression tag	UNP O97161
J	-26	HIS	-	expression tag	UNP O97161
J	-25	HIS	-	expression tag	UNP O97161
J	-24	HIS	-	expression tag	UNP O97161
J	-23	GLY	-	expression tag	UNP O97161
J	-22	MET	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	-21	ALA	-	expression tag	UNP O97161
J	-20	SER	-	expression tag	UNP O97161
J	-19	MET	-	expression tag	UNP O97161
J	-18	THR	-	expression tag	UNP O97161
J	-17	GLY	-	expression tag	UNP O97161
J	-16	GLY	-	expression tag	UNP O97161
J	-15	GLN	-	expression tag	UNP O97161
J	-14	GLN	-	expression tag	UNP O97161
J	-13	MET	-	expression tag	UNP O97161
J	-12	GLY	-	expression tag	UNP O97161
J	-11	ARG	-	expression tag	UNP O97161
J	-10	ASP	-	expression tag	UNP O97161
J	-9	LEU	-	expression tag	UNP O97161
J	-8	TYR	-	expression tag	UNP O97161
J	-7	ASP	-	expression tag	UNP O97161
J	-6	ASP	-	expression tag	UNP O97161
J	-5	ASP	-	expression tag	UNP O97161
J	-4	ASP	-	expression tag	UNP O97161
J	-3	LYS	-	expression tag	UNP O97161
J	-2	GLY	-	expression tag	UNP O97161
J	-1	SER	-	expression tag	UNP O97161
J	0	THR	-	expression tag	UNP O97161
K	-33	MET	-	expression tag	UNP O97161
K	-32	ARG	-	expression tag	UNP O97161
K	-31	GLY	-	expression tag	UNP O97161
K	-30	SER	-	expression tag	UNP O97161
K	-29	HIS	-	expression tag	UNP O97161
K	-28	HIS	-	expression tag	UNP O97161
K	-27	HIS	-	expression tag	UNP O97161
K	-26	HIS	-	expression tag	UNP O97161
K	-25	HIS	-	expression tag	UNP O97161
K	-24	HIS	-	expression tag	UNP O97161
K	-23	GLY	-	expression tag	UNP O97161
K	-22	MET	-	expression tag	UNP O97161
K	-21	ALA	-	expression tag	UNP O97161
K	-20	SER	-	expression tag	UNP O97161
K	-19	MET	-	expression tag	UNP O97161
K	-18	THR	-	expression tag	UNP O97161
K	-17	GLY	-	expression tag	UNP O97161
K	-16	GLY	-	expression tag	UNP O97161
K	-15	GLN	-	expression tag	UNP O97161
K	-14	GLN	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-13	MET	-	expression tag	UNP O97161
K	-12	GLY	-	expression tag	UNP O97161
K	-11	ARG	-	expression tag	UNP O97161
K	-10	ASP	-	expression tag	UNP O97161
K	-9	LEU	-	expression tag	UNP O97161
K	-8	TYR	-	expression tag	UNP O97161
K	-7	ASP	-	expression tag	UNP O97161
K	-6	ASP	-	expression tag	UNP O97161
K	-5	ASP	-	expression tag	UNP O97161
K	-4	ASP	-	expression tag	UNP O97161
K	-3	LYS	-	expression tag	UNP O97161
K	-2	GLY	-	expression tag	UNP O97161
K	-1	SER	-	expression tag	UNP O97161
K	0	THR	-	expression tag	UNP O97161
L	-33	MET	-	expression tag	UNP O97161
L	-32	ARG	-	expression tag	UNP O97161
L	-31	GLY	-	expression tag	UNP O97161
L	-30	SER	-	expression tag	UNP O97161
L	-29	HIS	-	expression tag	UNP O97161
L	-28	HIS	-	expression tag	UNP O97161
L	-27	HIS	-	expression tag	UNP O97161
L	-26	HIS	-	expression tag	UNP O97161
L	-25	HIS	-	expression tag	UNP O97161
L	-24	HIS	-	expression tag	UNP O97161
L	-23	GLY	-	expression tag	UNP O97161
L	-22	MET	-	expression tag	UNP O97161
L	-21	ALA	-	expression tag	UNP O97161
L	-20	SER	-	expression tag	UNP O97161
L	-19	MET	-	expression tag	UNP O97161
L	-18	THR	-	expression tag	UNP O97161
L	-17	GLY	-	expression tag	UNP O97161
L	-16	GLY	-	expression tag	UNP O97161
L	-15	GLN	-	expression tag	UNP O97161
L	-14	GLN	-	expression tag	UNP O97161
L	-13	MET	-	expression tag	UNP O97161
L	-12	GLY	-	expression tag	UNP O97161
L	-11	ARG	-	expression tag	UNP O97161
L	-10	ASP	-	expression tag	UNP O97161
L	-9	LEU	-	expression tag	UNP O97161
L	-8	TYR	-	expression tag	UNP O97161
L	-7	ASP	-	expression tag	UNP O97161
L	-6	ASP	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	ASP	-	expression tag	UNP O97161
L	-4	ASP	-	expression tag	UNP O97161
L	-3	LYS	-	expression tag	UNP O97161
L	-2	GLY	-	expression tag	UNP O97161
L	-1	SER	-	expression tag	UNP O97161
L	0	THR	-	expression tag	UNP O97161
M	-33	MET	-	expression tag	UNP O97161
M	-32	ARG	-	expression tag	UNP O97161
M	-31	GLY	-	expression tag	UNP O97161
M	-30	SER	-	expression tag	UNP O97161
M	-29	HIS	-	expression tag	UNP O97161
M	-28	HIS	-	expression tag	UNP O97161
M	-27	HIS	-	expression tag	UNP O97161
M	-26	HIS	-	expression tag	UNP O97161
M	-25	HIS	-	expression tag	UNP O97161
M	-24	HIS	-	expression tag	UNP O97161
M	-23	GLY	-	expression tag	UNP O97161
M	-22	MET	-	expression tag	UNP O97161
M	-21	ALA	-	expression tag	UNP O97161
M	-20	SER	-	expression tag	UNP O97161
M	-19	MET	-	expression tag	UNP O97161
M	-18	THR	-	expression tag	UNP O97161
M	-17	GLY	-	expression tag	UNP O97161
M	-16	GLY	-	expression tag	UNP O97161
M	-15	GLN	-	expression tag	UNP O97161
M	-14	GLN	-	expression tag	UNP O97161
M	-13	MET	-	expression tag	UNP O97161
M	-12	GLY	-	expression tag	UNP O97161
M	-11	ARG	-	expression tag	UNP O97161
M	-10	ASP	-	expression tag	UNP O97161
M	-9	LEU	-	expression tag	UNP O97161
M	-8	TYR	-	expression tag	UNP O97161
M	-7	ASP	-	expression tag	UNP O97161
M	-6	ASP	-	expression tag	UNP O97161
M	-5	ASP	-	expression tag	UNP O97161
M	-4	ASP	-	expression tag	UNP O97161
M	-3	LYS	-	expression tag	UNP O97161
M	-2	GLY	-	expression tag	UNP O97161
M	-1	SER	-	expression tag	UNP O97161
M	0	THR	-	expression tag	UNP O97161
N	-33	MET	-	expression tag	UNP O97161
N	-32	ARG	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	-31	GLY	-	expression tag	UNP O97161
N	-30	SER	-	expression tag	UNP O97161
N	-29	HIS	-	expression tag	UNP O97161
N	-28	HIS	-	expression tag	UNP O97161
N	-27	HIS	-	expression tag	UNP O97161
N	-26	HIS	-	expression tag	UNP O97161
N	-25	HIS	-	expression tag	UNP O97161
N	-24	HIS	-	expression tag	UNP O97161
N	-23	GLY	-	expression tag	UNP O97161
N	-22	MET	-	expression tag	UNP O97161
N	-21	ALA	-	expression tag	UNP O97161
N	-20	SER	-	expression tag	UNP O97161
N	-19	MET	-	expression tag	UNP O97161
N	-18	THR	-	expression tag	UNP O97161
N	-17	GLY	-	expression tag	UNP O97161
N	-16	GLY	-	expression tag	UNP O97161
N	-15	GLN	-	expression tag	UNP O97161
N	-14	GLN	-	expression tag	UNP O97161
N	-13	MET	-	expression tag	UNP O97161
N	-12	GLY	-	expression tag	UNP O97161
N	-11	ARG	-	expression tag	UNP O97161
N	-10	ASP	-	expression tag	UNP O97161
N	-9	LEU	-	expression tag	UNP O97161
N	-8	TYR	-	expression tag	UNP O97161
N	-7	ASP	-	expression tag	UNP O97161
N	-6	ASP	-	expression tag	UNP O97161
N	-5	ASP	-	expression tag	UNP O97161
N	-4	ASP	-	expression tag	UNP O97161
N	-3	LYS	-	expression tag	UNP O97161
N	-2	GLY	-	expression tag	UNP O97161
N	-1	SER	-	expression tag	UNP O97161
N	0	THR	-	expression tag	UNP O97161
O	-33	MET	-	expression tag	UNP O97161
O	-32	ARG	-	expression tag	UNP O97161
O	-31	GLY	-	expression tag	UNP O97161
O	-30	SER	-	expression tag	UNP O97161
O	-29	HIS	-	expression tag	UNP O97161
O	-28	HIS	-	expression tag	UNP O97161
O	-27	HIS	-	expression tag	UNP O97161
O	-26	HIS	-	expression tag	UNP O97161
O	-25	HIS	-	expression tag	UNP O97161
O	-24	HIS	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	-23	GLY	-	expression tag	UNP O97161
O	-22	MET	-	expression tag	UNP O97161
O	-21	ALA	-	expression tag	UNP O97161
O	-20	SER	-	expression tag	UNP O97161
O	-19	MET	-	expression tag	UNP O97161
O	-18	THR	-	expression tag	UNP O97161
O	-17	GLY	-	expression tag	UNP O97161
O	-16	GLY	-	expression tag	UNP O97161
O	-15	GLN	-	expression tag	UNP O97161
O	-14	GLN	-	expression tag	UNP O97161
O	-13	MET	-	expression tag	UNP O97161
O	-12	GLY	-	expression tag	UNP O97161
O	-11	ARG	-	expression tag	UNP O97161
O	-10	ASP	-	expression tag	UNP O97161
O	-9	LEU	-	expression tag	UNP O97161
O	-8	TYR	-	expression tag	UNP O97161
O	-7	ASP	-	expression tag	UNP O97161
O	-6	ASP	-	expression tag	UNP O97161
O	-5	ASP	-	expression tag	UNP O97161
O	-4	ASP	-	expression tag	UNP O97161
O	-3	LYS	-	expression tag	UNP O97161
O	-2	GLY	-	expression tag	UNP O97161
O	-1	SER	-	expression tag	UNP O97161
O	0	THR	-	expression tag	UNP O97161
P	-33	MET	-	expression tag	UNP O97161
P	-32	ARG	-	expression tag	UNP O97161
P	-31	GLY	-	expression tag	UNP O97161
P	-30	SER	-	expression tag	UNP O97161
P	-29	HIS	-	expression tag	UNP O97161
P	-28	HIS	-	expression tag	UNP O97161
P	-27	HIS	-	expression tag	UNP O97161
P	-26	HIS	-	expression tag	UNP O97161
P	-25	HIS	-	expression tag	UNP O97161
P	-24	HIS	-	expression tag	UNP O97161
P	-23	GLY	-	expression tag	UNP O97161
P	-22	MET	-	expression tag	UNP O97161
P	-21	ALA	-	expression tag	UNP O97161
P	-20	SER	-	expression tag	UNP O97161
P	-19	MET	-	expression tag	UNP O97161
P	-18	THR	-	expression tag	UNP O97161
P	-17	GLY	-	expression tag	UNP O97161
P	-16	GLY	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	-15	GLN	-	expression tag	UNP O97161
P	-14	GLN	-	expression tag	UNP O97161
P	-13	MET	-	expression tag	UNP O97161
P	-12	GLY	-	expression tag	UNP O97161
P	-11	ARG	-	expression tag	UNP O97161
P	-10	ASP	-	expression tag	UNP O97161
P	-9	LEU	-	expression tag	UNP O97161
P	-8	TYR	-	expression tag	UNP O97161
P	-7	ASP	-	expression tag	UNP O97161
P	-6	ASP	-	expression tag	UNP O97161
P	-5	ASP	-	expression tag	UNP O97161
P	-4	ASP	-	expression tag	UNP O97161
P	-3	LYS	-	expression tag	UNP O97161
P	-2	GLY	-	expression tag	UNP O97161
P	-1	SER	-	expression tag	UNP O97161
P	0	THR	-	expression tag	UNP O97161
Q	-33	MET	-	expression tag	UNP O97161
Q	-32	ARG	-	expression tag	UNP O97161
Q	-31	GLY	-	expression tag	UNP O97161
Q	-30	SER	-	expression tag	UNP O97161
Q	-29	HIS	-	expression tag	UNP O97161
Q	-28	HIS	-	expression tag	UNP O97161
Q	-27	HIS	-	expression tag	UNP O97161
Q	-26	HIS	-	expression tag	UNP O97161
Q	-25	HIS	-	expression tag	UNP O97161
Q	-24	HIS	-	expression tag	UNP O97161
Q	-23	GLY	-	expression tag	UNP O97161
Q	-22	MET	-	expression tag	UNP O97161
Q	-21	ALA	-	expression tag	UNP O97161
Q	-20	SER	-	expression tag	UNP O97161
Q	-19	MET	-	expression tag	UNP O97161
Q	-18	THR	-	expression tag	UNP O97161
Q	-17	GLY	-	expression tag	UNP O97161
Q	-16	GLY	-	expression tag	UNP O97161
Q	-15	GLN	-	expression tag	UNP O97161
Q	-14	GLN	-	expression tag	UNP O97161
Q	-13	MET	-	expression tag	UNP O97161
Q	-12	GLY	-	expression tag	UNP O97161
Q	-11	ARG	-	expression tag	UNP O97161
Q	-10	ASP	-	expression tag	UNP O97161
Q	-9	LEU	-	expression tag	UNP O97161
Q	-8	TYR	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-7	ASP	-	expression tag	UNP O97161
Q	-6	ASP	-	expression tag	UNP O97161
Q	-5	ASP	-	expression tag	UNP O97161
Q	-4	ASP	-	expression tag	UNP O97161
Q	-3	LYS	-	expression tag	UNP O97161
Q	-2	GLY	-	expression tag	UNP O97161
Q	-1	SER	-	expression tag	UNP O97161
Q	0	THR	-	expression tag	UNP O97161
R	-33	MET	-	expression tag	UNP O97161
R	-32	ARG	-	expression tag	UNP O97161
R	-31	GLY	-	expression tag	UNP O97161
R	-30	SER	-	expression tag	UNP O97161
R	-29	HIS	-	expression tag	UNP O97161
R	-28	HIS	-	expression tag	UNP O97161
R	-27	HIS	-	expression tag	UNP O97161
R	-26	HIS	-	expression tag	UNP O97161
R	-25	HIS	-	expression tag	UNP O97161
R	-24	HIS	-	expression tag	UNP O97161
R	-23	GLY	-	expression tag	UNP O97161
R	-22	MET	-	expression tag	UNP O97161
R	-21	ALA	-	expression tag	UNP O97161
R	-20	SER	-	expression tag	UNP O97161
R	-19	MET	-	expression tag	UNP O97161
R	-18	THR	-	expression tag	UNP O97161
R	-17	GLY	-	expression tag	UNP O97161
R	-16	GLY	-	expression tag	UNP O97161
R	-15	GLN	-	expression tag	UNP O97161
R	-14	GLN	-	expression tag	UNP O97161
R	-13	MET	-	expression tag	UNP O97161
R	-12	GLY	-	expression tag	UNP O97161
R	-11	ARG	-	expression tag	UNP O97161
R	-10	ASP	-	expression tag	UNP O97161
R	-9	LEU	-	expression tag	UNP O97161
R	-8	TYR	-	expression tag	UNP O97161
R	-7	ASP	-	expression tag	UNP O97161
R	-6	ASP	-	expression tag	UNP O97161
R	-5	ASP	-	expression tag	UNP O97161
R	-4	ASP	-	expression tag	UNP O97161
R	-3	LYS	-	expression tag	UNP O97161
R	-2	GLY	-	expression tag	UNP O97161
R	-1	SER	-	expression tag	UNP O97161
R	0	THR	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	-33	MET	-	expression tag	UNP O97161
S	-32	ARG	-	expression tag	UNP O97161
S	-31	GLY	-	expression tag	UNP O97161
S	-30	SER	-	expression tag	UNP O97161
S	-29	HIS	-	expression tag	UNP O97161
S	-28	HIS	-	expression tag	UNP O97161
S	-27	HIS	-	expression tag	UNP O97161
S	-26	HIS	-	expression tag	UNP O97161
S	-25	HIS	-	expression tag	UNP O97161
S	-24	HIS	-	expression tag	UNP O97161
S	-23	GLY	-	expression tag	UNP O97161
S	-22	MET	-	expression tag	UNP O97161
S	-21	ALA	-	expression tag	UNP O97161
S	-20	SER	-	expression tag	UNP O97161
S	-19	MET	-	expression tag	UNP O97161
S	-18	THR	-	expression tag	UNP O97161
S	-17	GLY	-	expression tag	UNP O97161
S	-16	GLY	-	expression tag	UNP O97161
S	-15	GLN	-	expression tag	UNP O97161
S	-14	GLN	-	expression tag	UNP O97161
S	-13	MET	-	expression tag	UNP O97161
S	-12	GLY	-	expression tag	UNP O97161
S	-11	ARG	-	expression tag	UNP O97161
S	-10	ASP	-	expression tag	UNP O97161
S	-9	LEU	-	expression tag	UNP O97161
S	-8	TYR	-	expression tag	UNP O97161
S	-7	ASP	-	expression tag	UNP O97161
S	-6	ASP	-	expression tag	UNP O97161
S	-5	ASP	-	expression tag	UNP O97161
S	-4	ASP	-	expression tag	UNP O97161
S	-3	LYS	-	expression tag	UNP O97161
S	-2	GLY	-	expression tag	UNP O97161
S	-1	SER	-	expression tag	UNP O97161
S	0	THR	-	expression tag	UNP O97161
T	-33	MET	-	expression tag	UNP O97161
T	-32	ARG	-	expression tag	UNP O97161
T	-31	GLY	-	expression tag	UNP O97161
T	-30	SER	-	expression tag	UNP O97161
T	-29	HIS	-	expression tag	UNP O97161
T	-28	HIS	-	expression tag	UNP O97161
T	-27	HIS	-	expression tag	UNP O97161
T	-26	HIS	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	-25	HIS	-	expression tag	UNP O97161
T	-24	HIS	-	expression tag	UNP O97161
T	-23	GLY	-	expression tag	UNP O97161
T	-22	MET	-	expression tag	UNP O97161
T	-21	ALA	-	expression tag	UNP O97161
T	-20	SER	-	expression tag	UNP O97161
T	-19	MET	-	expression tag	UNP O97161
T	-18	THR	-	expression tag	UNP O97161
T	-17	GLY	-	expression tag	UNP O97161
T	-16	GLY	-	expression tag	UNP O97161
T	-15	GLN	-	expression tag	UNP O97161
T	-14	GLN	-	expression tag	UNP O97161
T	-13	MET	-	expression tag	UNP O97161
T	-12	GLY	-	expression tag	UNP O97161
T	-11	ARG	-	expression tag	UNP O97161
T	-10	ASP	-	expression tag	UNP O97161
T	-9	LEU	-	expression tag	UNP O97161
T	-8	TYR	-	expression tag	UNP O97161
T	-7	ASP	-	expression tag	UNP O97161
T	-6	ASP	-	expression tag	UNP O97161
T	-5	ASP	-	expression tag	UNP O97161
T	-4	ASP	-	expression tag	UNP O97161
T	-3	LYS	-	expression tag	UNP O97161
T	-2	GLY	-	expression tag	UNP O97161
T	-1	SER	-	expression tag	UNP O97161
T	0	THR	-	expression tag	UNP O97161

- Molecule 2 is a protein called THIOREDOXIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	168	Total	C	N	O	S	0	0	0
			1344	860	227	251	6			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-33	MET	-	expression tag	UNP O97161
D	-32	ARG	-	expression tag	UNP O97161
D	-31	GLY	-	expression tag	UNP O97161
D	-30	SER	-	expression tag	UNP O97161
D	-29	HIS	-	expression tag	UNP O97161
D	-28	HIS	-	expression tag	UNP O97161

Continued on next page...

Continued from previous page...

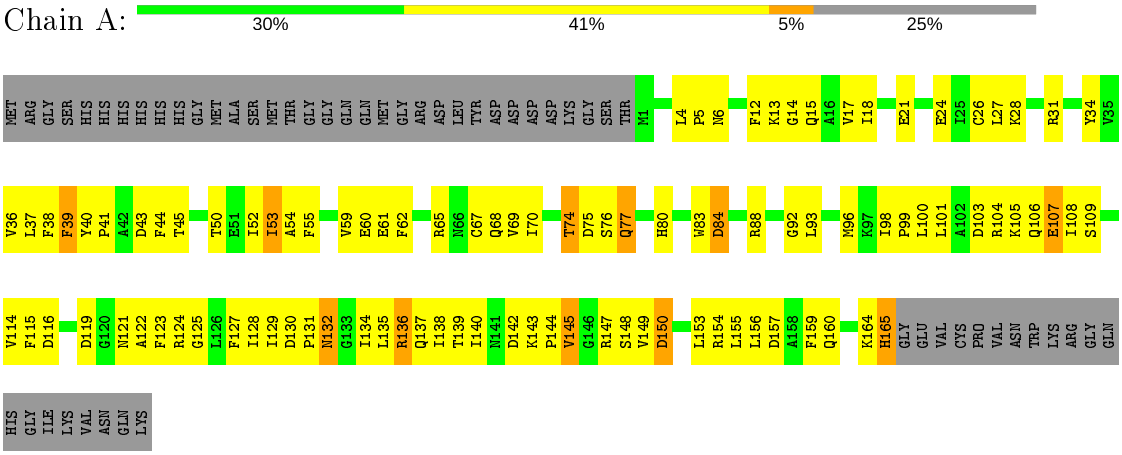
Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	HIS	-	expression tag	UNP O97161
D	-26	HIS	-	expression tag	UNP O97161
D	-25	HIS	-	expression tag	UNP O97161
D	-24	HIS	-	expression tag	UNP O97161
D	-23	GLY	-	expression tag	UNP O97161
D	-22	MET	-	expression tag	UNP O97161
D	-21	ALA	-	expression tag	UNP O97161
D	-20	SER	-	expression tag	UNP O97161
D	-19	MET	-	expression tag	UNP O97161
D	-18	THR	-	expression tag	UNP O97161
D	-17	GLY	-	expression tag	UNP O97161
D	-16	GLY	-	expression tag	UNP O97161
D	-15	GLN	-	expression tag	UNP O97161
D	-14	GLN	-	expression tag	UNP O97161
D	-13	MET	-	expression tag	UNP O97161
D	-12	GLY	-	expression tag	UNP O97161
D	-11	ARG	-	expression tag	UNP O97161
D	-10	ASP	-	expression tag	UNP O97161
D	-9	LEU	-	expression tag	UNP O97161
D	-8	TYR	-	expression tag	UNP O97161
D	-7	ASP	-	expression tag	UNP O97161
D	-6	ASP	-	expression tag	UNP O97161
D	-5	ASP	-	expression tag	UNP O97161
D	-4	ASP	-	expression tag	UNP O97161
D	-3	LYS	-	expression tag	UNP O97161
D	-2	GLY	-	expression tag	UNP O97161
D	-1	SER	-	expression tag	UNP O97161
D	0	THR	-	expression tag	UNP O97161
D	140	LEU	ILE	conflict	UNP O97161

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

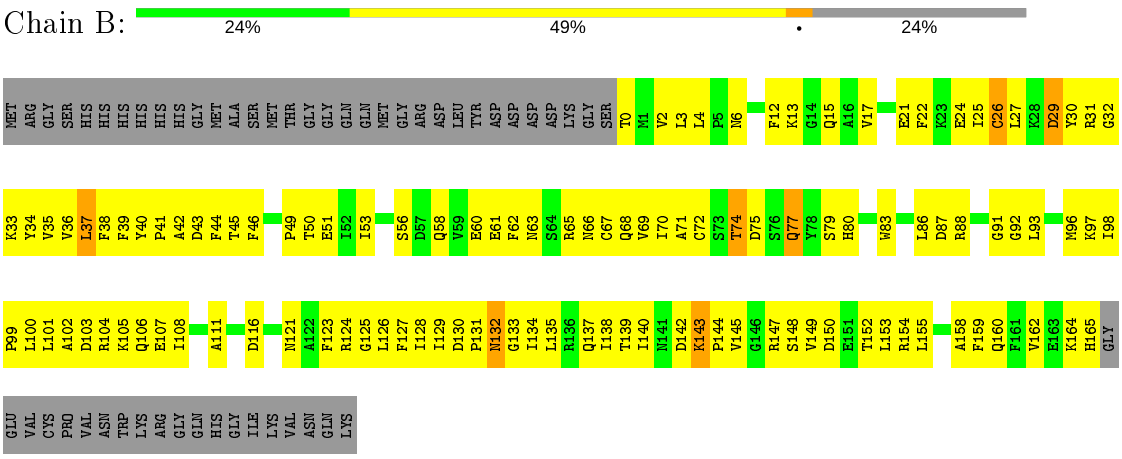
- Molecule 1: THIOREDOXIN PEROXIDASE

Chain A:



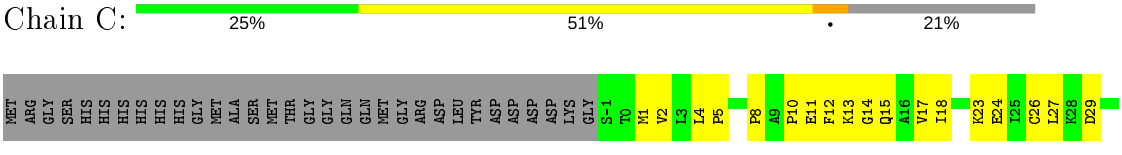
- Molecule 1: THIOREDOXIN PEROXIDASE

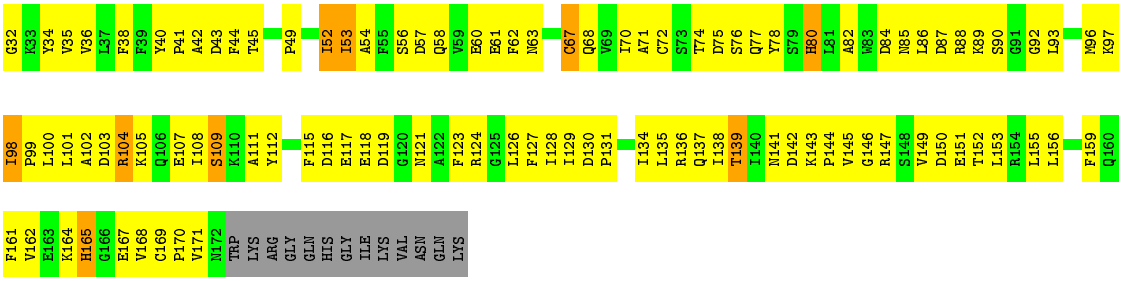
Chain B:



- Molecule 1: THIOREDOXIN PEROXIDASE

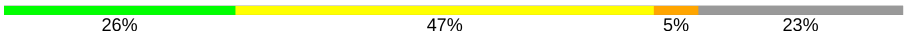
Chain C:

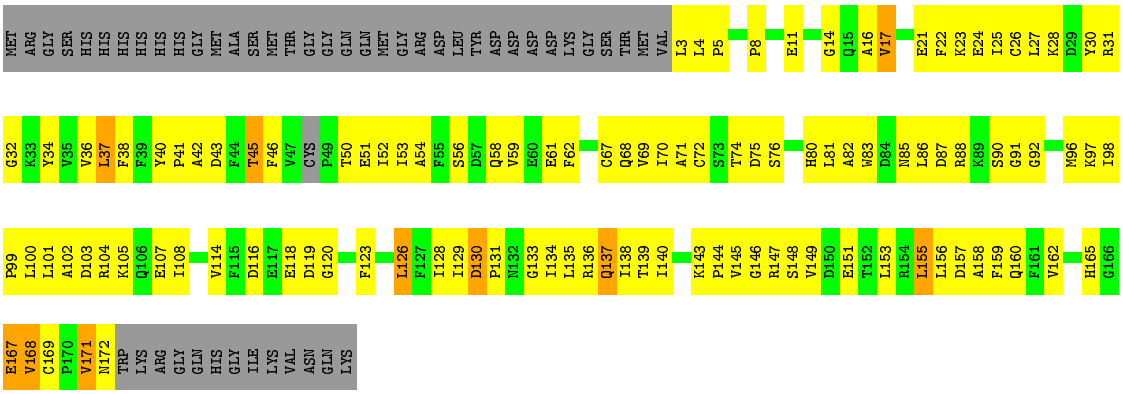




• Molecule 1: THIOREDOXIN PEROXIDASE

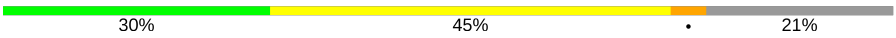
Chain E:

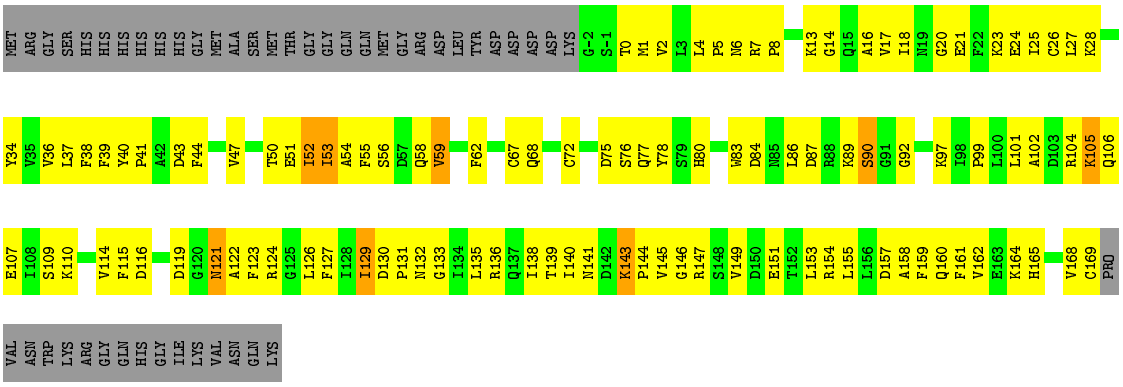




• Molecule 1: THIOREDOXIN PEROXIDASE

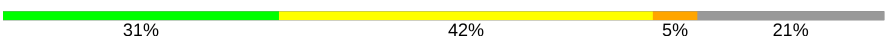
Chain F:

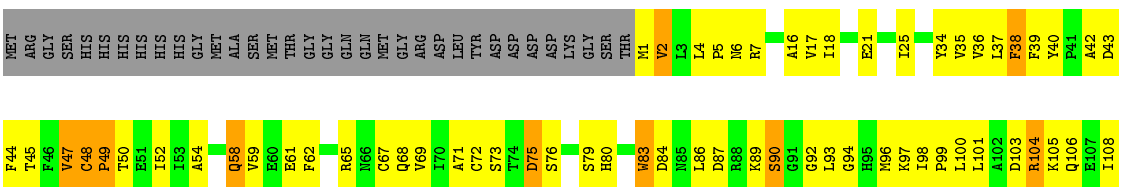


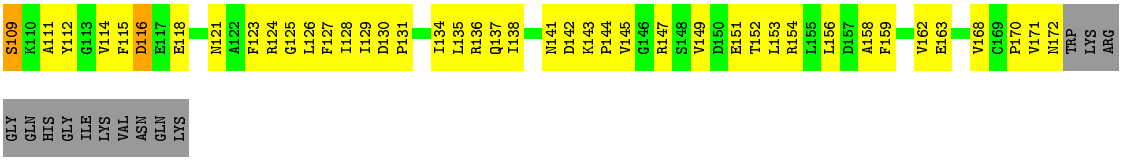


• Molecule 1: THIOREDOXIN PEROXIDASE

Chain G:

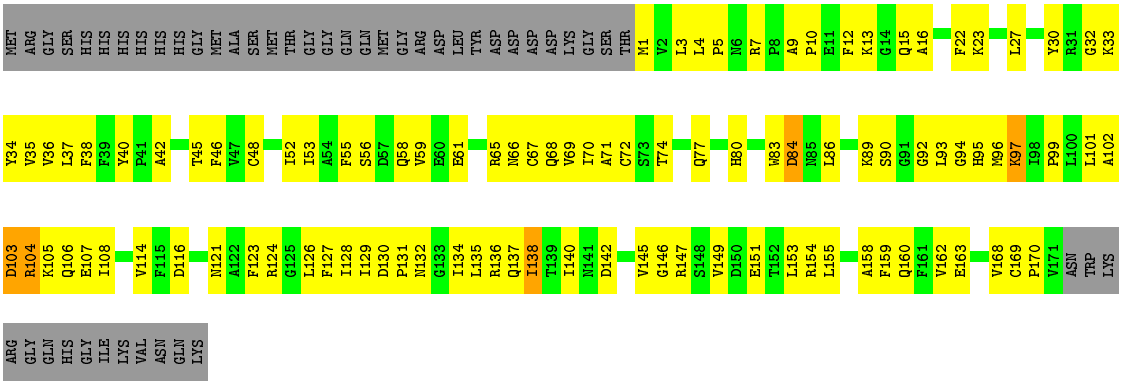






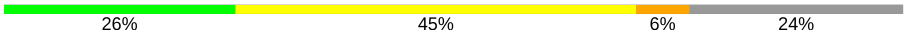
• Molecule 1: THIOREDOXIN PEROXIDASE

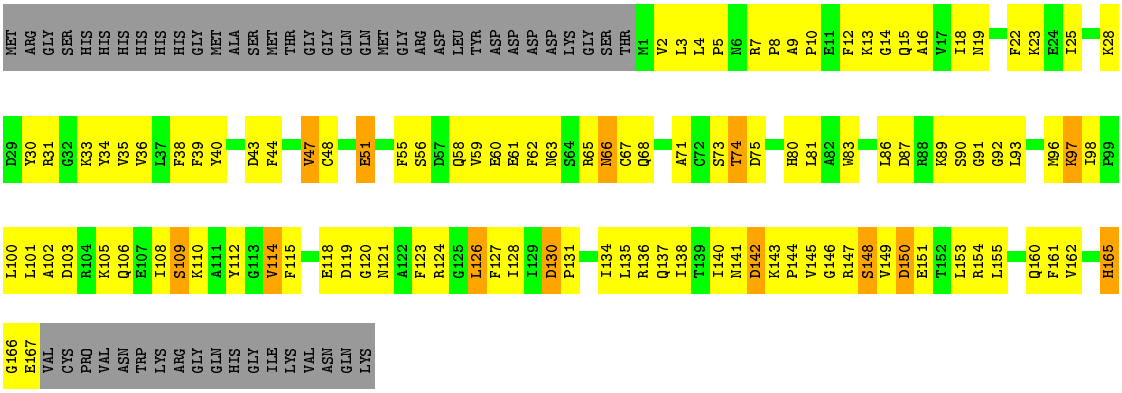
Chain H:



• Molecule 1: THIOREDOXIN PEROXIDASE

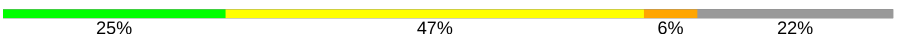
Chain I:

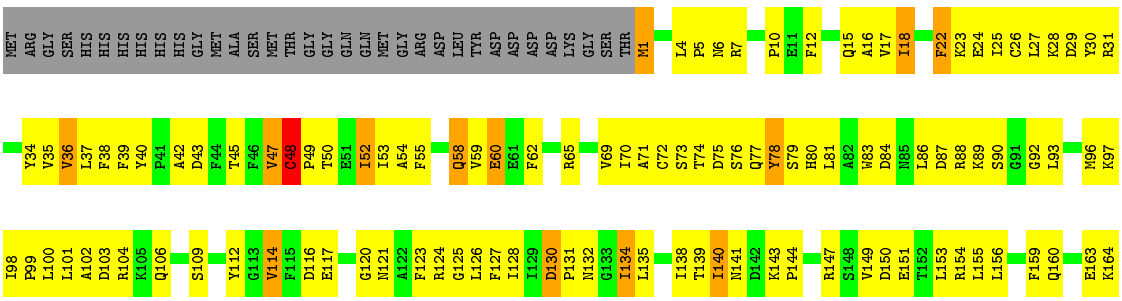




• Molecule 1: THIOREDOXIN PEROXIDASE

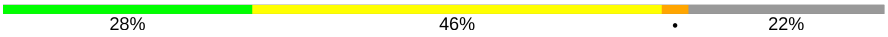
Chain J:

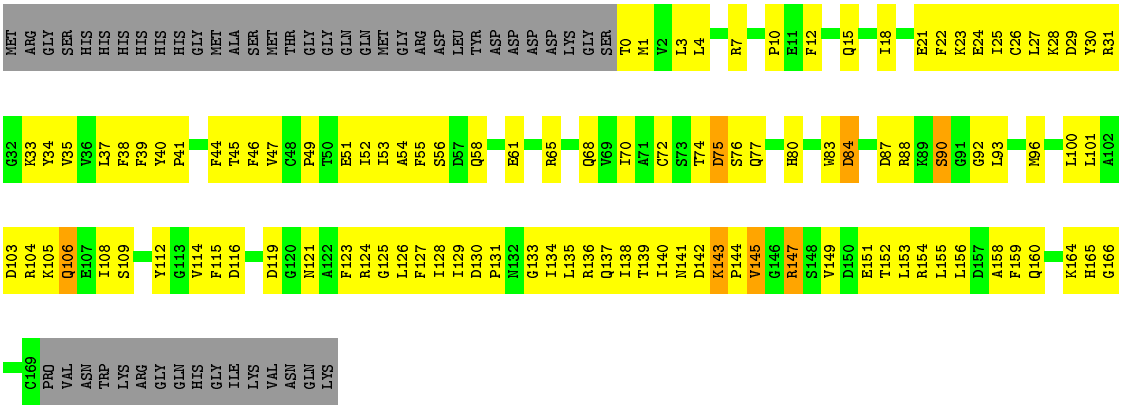




- Molecule 1: THIOREDOXIN PEROXIDASE

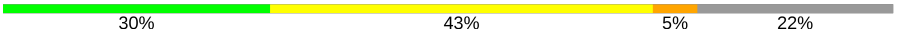
Chain K:

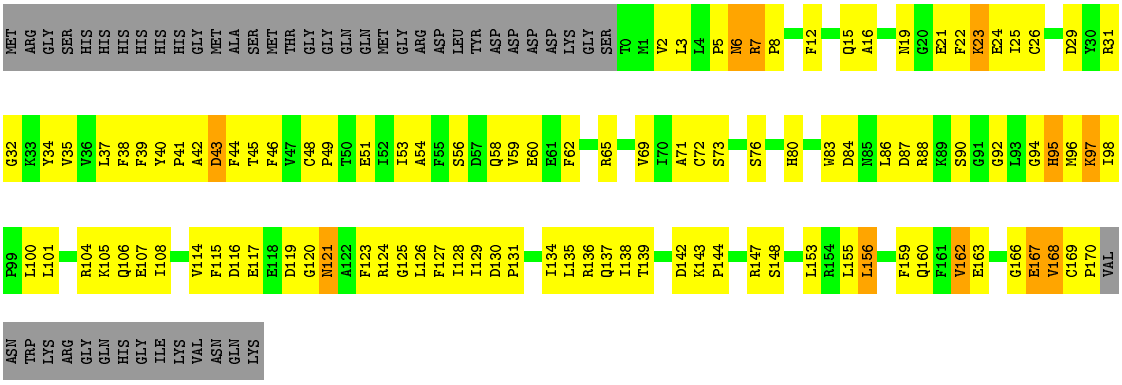




- Molecule 1: THIOREDOXIN PEROXIDASE

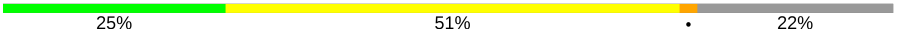
Chain L:

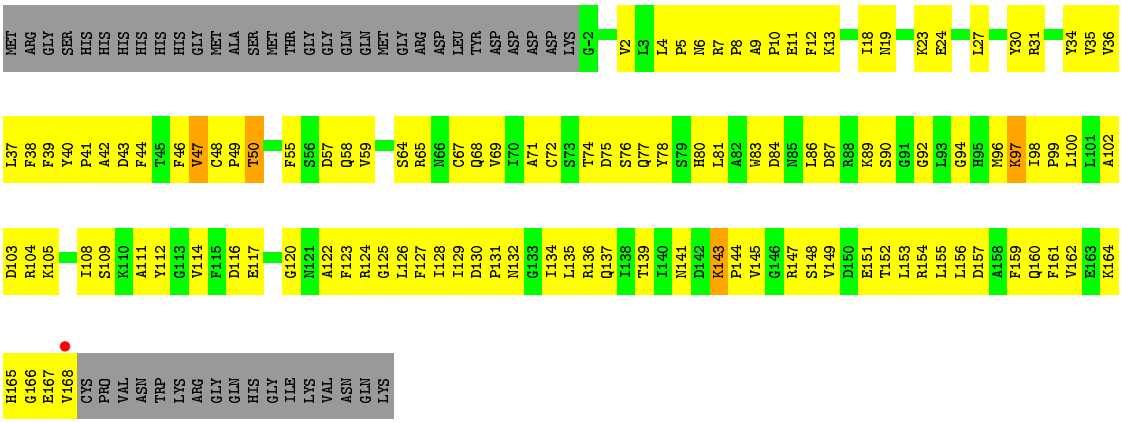




- Molecule 1: THIOREDOXIN PEROXIDASE

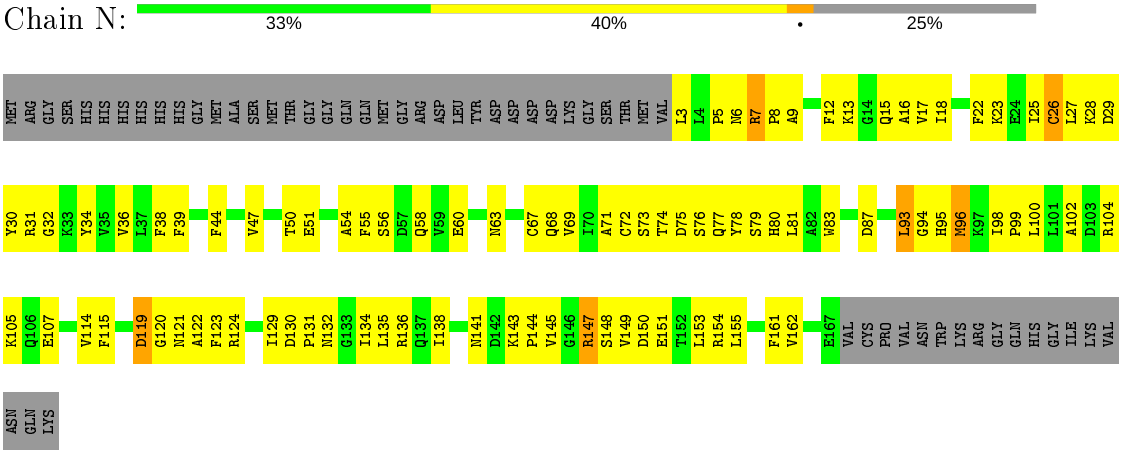
Chain M:





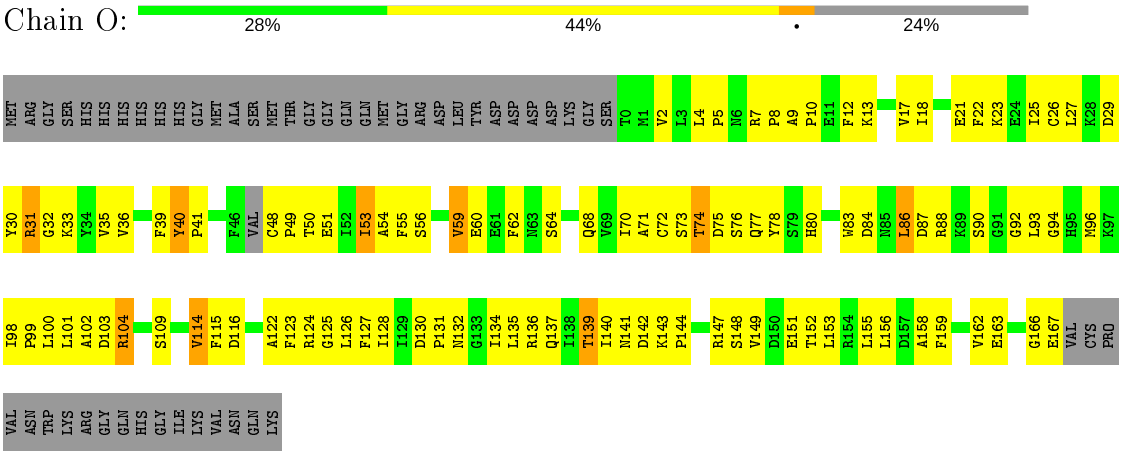
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain N:



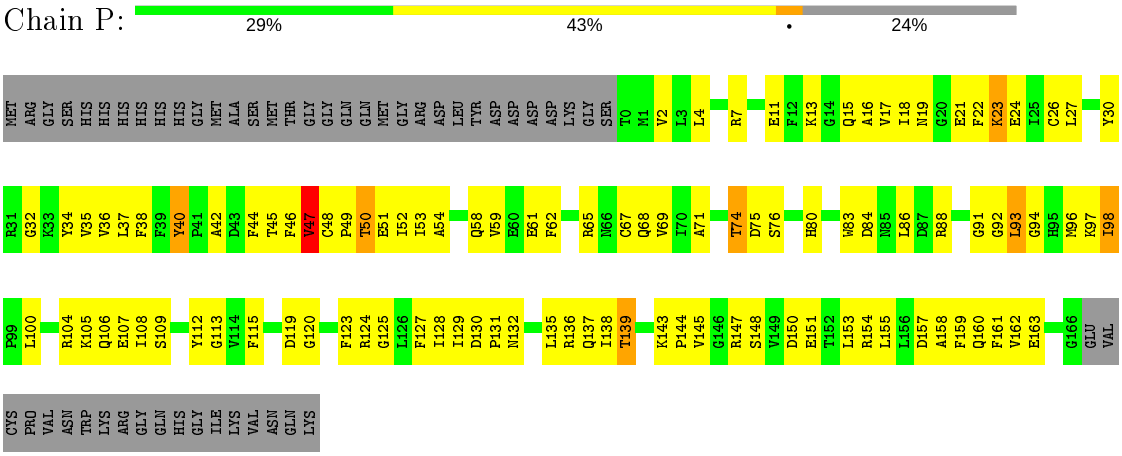
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain O:



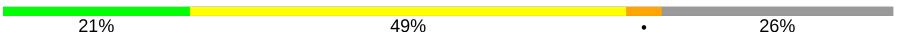
• Molecule 1: THIOREDOXIN PEROXIDASE

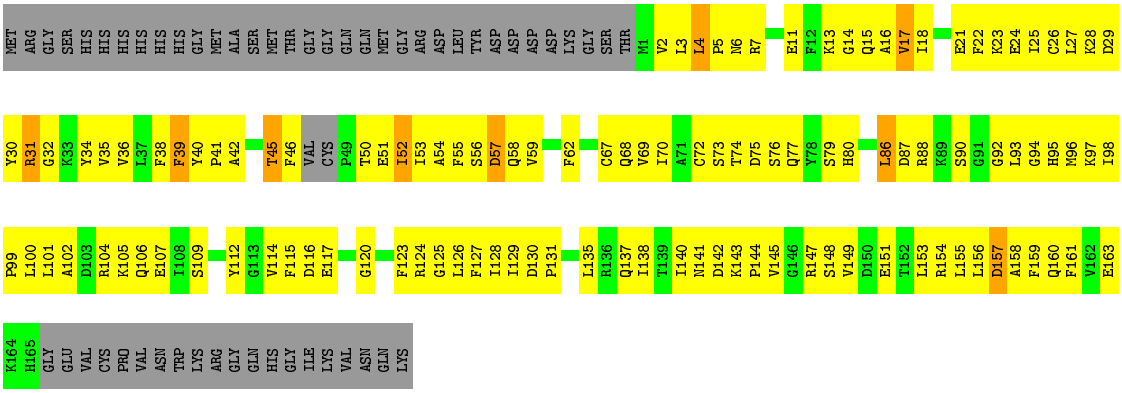
Chain P:



• Molecule 1: THIOREDOXIN PEROXIDASE

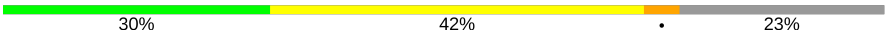
Chain Q:

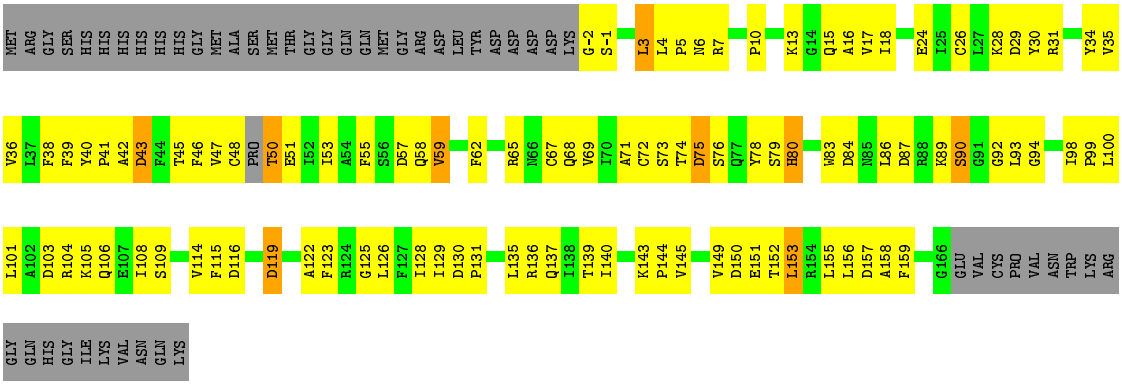




• Molecule 1: THIOREDOXIN PEROXIDASE

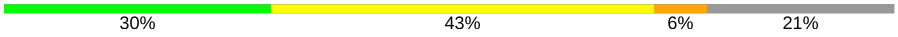
Chain R:

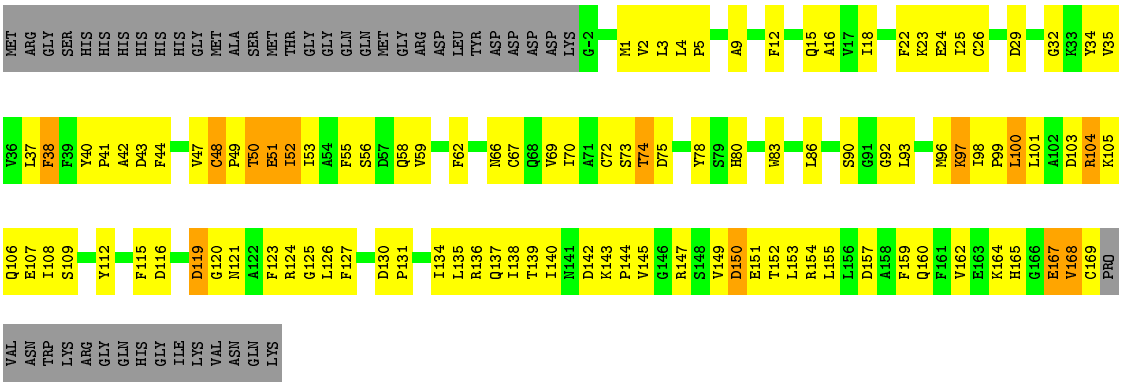




• Molecule 1: THIOREDOXIN PEROXIDASE

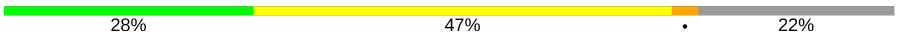
Chain S:

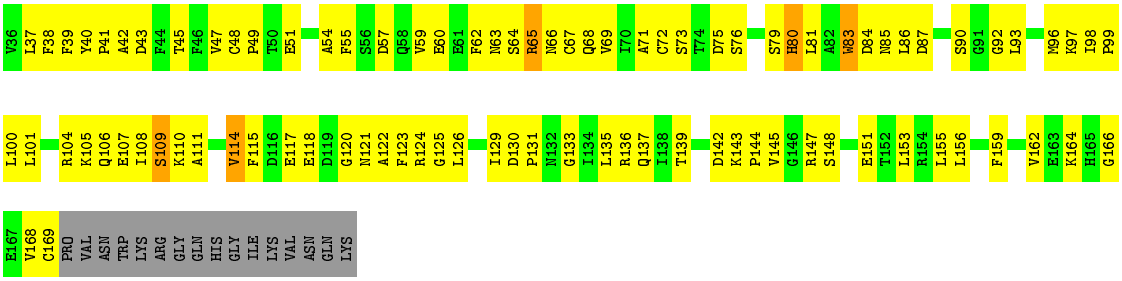




• Molecule 1: THIOREDOXIN PEROXIDASE

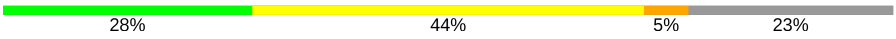
Chain T:

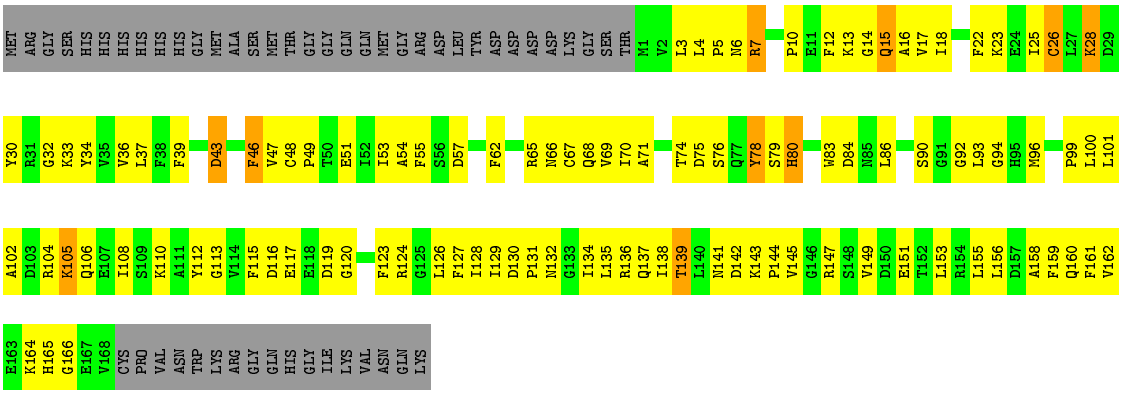




- Molecule 2: THIOREDOXIN PEROXIDASE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.91Å 204.94Å 126.84Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	29.86 – 3.00 29.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.86-3.00) 95.5 (29.86-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.270 0.212 , 0.247	Depositor DCC
R_{free} test set	5627 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , -5.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.400 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for L,-K,H	Depositor
Outliers	0 of 112406 reflections	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	26988	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.39	0/1354	0.51	0/1829
1	B	0.38	0/1361	0.52	0/1839
1	C	0.37	0/1416	0.51	0/1915
1	E	0.39	0/1381	0.53	0/1865
1	F	0.39	0/1397	0.54	0/1887
1	G	0.38	0/1403	0.55	0/1897
1	H	0.36	0/1395	0.50	0/1886
1	I	0.37	0/1367	0.53	0/1846
1	J	0.39	0/1395	0.53	0/1886
1	K	0.37	0/1387	0.52	0/1874
1	L	0.38	0/1395	0.51	0/1886
1	M	0.40	0/1391	0.55	0/1879
1	N	0.37	0/1352	0.54	0/1826
1	O	0.38	0/1366	0.52	0/1843
1	P	0.39	0/1365	0.53	0/1844
1	Q	0.37	0/1340	0.53	0/1807
1	R	0.39	0/1366	0.53	0/1842
1	S	0.37	0/1397	0.55	0/1887
1	T	0.37	0/1387	0.53	0/1874
2	D	0.38	0/1374	0.52	0/1856
All	All	0.38	0/27589	0.53	0/37268

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	P	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	49	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1324	0	1301	121	0
1	B	1331	0	1308	128	0
1	C	1385	0	1358	135	0
1	E	1351	0	1320	124	0
1	F	1367	0	1339	119	0
1	G	1372	0	1346	127	0
1	H	1364	0	1340	115	0
1	I	1337	0	1310	124	0
1	J	1364	0	1340	142	0
1	K	1357	0	1331	113	0
1	L	1364	0	1338	126	0
1	M	1361	0	1334	124	0
1	N	1322	0	1289	100	0
1	O	1337	0	1307	124	0
1	P	1335	0	1311	126	0
1	Q	1311	0	1287	126	0
1	R	1338	0	1311	111	0
1	S	1367	0	1339	132	0
1	T	1357	0	1331	128	0
2	D	1344	0	1319	138	0
All	All	26988	0	26459	2301	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 43.

All (2301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:15:GLN:HG2	1:S:24:GLU:HG2	1.18	1.14
1:O:40:TYR:HE1	1:O:73:SER:HB3	1.05	1.12
1:S:51:GLU:HA	1:S:51:GLU:OE1	1.43	1.10
2:D:84:ASP:HA	2:D:93:LEU:HB2	1.28	1.10
1:T:60:GLU:HA	1:T:63:ASN:HB2	1.25	1.09
2:D:15:GLN:HA	2:D:15:GLN:HE21	1.17	1.08
1:A:61:GLU:HB3	1:A:65:ARG:HE	1.21	1.04
1:I:28:LYS:HA	1:I:31:ARG:HE	1.20	1.03
1:I:2:VAL:HA	1:J:1:MET:HA	1.41	1.01
1:O:40:TYR:CE1	1:O:73:SER:HB3	1.97	1.00
1:I:162:VAL:HA	1:I:166:GLY:HA3	1.41	1.00
1:O:41:PRO:HG3	1:O:143:LYS:HG2	1.43	0.99
1:S:47:VAL:CG2	1:S:51:GLU:HG2	1.92	0.98
1:H:93:LEU:HB3	1:H:96:MET:HG2	1.45	0.98
1:S:52:ILE:N	1:S:52:ILE:HD13	1.78	0.98
1:L:128:ILE:HG13	1:L:137:GLN:HB3	1.46	0.96
1:J:58:GLN:HA	1:J:58:GLN:HE21	1.31	0.95
1:L:40:TYR:HB2	1:L:41:PRO:HD2	1.48	0.95
1:O:86:LEU:HD11	1:O:90:SER:HB3	1.46	0.95
1:E:40:TYR:HB2	1:E:41:PRO:HD2	1.47	0.95
1:E:140:ILE:HB	1:F:138:ILE:HB	1.45	0.94
1:Q:128:ILE:HD12	1:Q:137:GLN:HB3	1.49	0.94
1:N:147:ARG:H	1:N:147:ARG:HE	1.16	0.94
1:J:47:VAL:HG22	1:J:48:CYS:H	1.32	0.93
1:K:109:SER:HB3	1:K:115:PHE:HB2	1.48	0.93
1:R:75:ASP:HB2	1:R:80:HIS:HE1	1.33	0.93
1:L:65:ARG:HG2	1:L:160:GLN:HE22	1.31	0.93
1:G:65:ARG:HH21	1:G:153:LEU:HD23	1.35	0.92
1:C:119:ASP:HB3	1:C:121:ASN:ND2	1.83	0.92
1:T:62:PHE:HB3	1:T:67:CYS:HB3	1.50	0.92
1:R:75:ASP:HB2	1:R:80:HIS:CE1	2.05	0.91
1:S:47:VAL:HG21	1:S:51:GLU:HG2	1.52	0.91
2:D:126:LEU:HD12	2:D:147:ARG:HD2	1.50	0.91
1:Q:11:GLU:HG2	1:Q:27:LEU:HB3	1.53	0.91
1:J:125:GLY:HA2	1:J:140:ILE:HA	1.49	0.90
1:S:4:LEU:HB3	1:T:123:PHE:HE2	1.32	0.90
1:K:58:GLN:OE1	1:K:61:GLU:HG3	1.72	0.90
1:R:48:CYS:HB2	1:R:51:GLU:H	1.36	0.90
1:C:119:ASP:HB3	1:C:121:ASN:HD21	1.36	0.89
2:D:47:VAL:HG12	2:D:48:CYS:H	1.36	0.89
1:N:56:SER:HB2	1:N:96:MET:HG3	1.53	0.89
1:O:84:ASP:HA	1:O:93:LEU:HB2	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:124:ARG:HB3	1:T:147:ARG:HH12	1.37	0.89
1:K:53:ILE:HA	1:K:56:SER:HB3	1.51	0.89
1:N:18:ILE:HD12	1:N:23:LYS:HB2	1.55	0.89
1:K:4:LEU:HB2	1:K:7:ARG:HD2	1.53	0.88
1:C:62:PHE:HB3	1:C:67:CYS:HB3	1.55	0.88
2:D:136:ARG:HB3	2:D:159:PHE:CE2	2.07	0.88
1:G:87:ASP:OD2	1:G:89:LYS:HB2	1.74	0.88
1:S:4:LEU:HB3	1:T:123:PHE:CE2	2.08	0.88
2:D:14:GLY:HA3	2:D:101:LEU:HD11	1.55	0.88
1:Q:22:PHE:HE1	1:Q:77:GLN:HB2	1.40	0.87
1:M:55:PHE:CE1	1:M:149:VAL:HG22	2.10	0.87
1:O:142:ASP:OD2	1:O:144:PRO:HD2	1.75	0.87
1:K:10:PRO:HB2	1:K:112:TYR:CE1	2.10	0.87
1:B:164:LYS:HD2	1:B:165:HIS:CE1	2.09	0.86
1:R:4:LEU:HD12	1:R:7:ARG:HE	1.39	0.86
1:T:32:GLY:HA2	1:T:131:PRO:HB3	1.55	0.86
1:A:132:ASN:HD22	1:A:132:ASN:H	1.24	0.86
1:R:130:ASP:HB2	1:R:131:PRO:HD2	1.58	0.86
1:K:143:LYS:HG3	1:K:144:PRO:HD3	1.56	0.86
1:L:124:ARG:HB3	1:L:147:ARG:NH2	1.91	0.85
1:E:76:SER:HA	1:E:102:ALA:HB1	1.56	0.85
1:J:24:GLU:HB3	1:K:24:GLU:HB3	1.56	0.85
1:A:34:TYR:HB2	1:A:67:CYS:HB2	1.58	0.85
1:P:53:ILE:HD13	1:P:88:ARG:HD3	1.58	0.85
1:O:86:LEU:HD12	1:O:87:ASP:N	1.90	0.85
2:D:124:ARG:HG2	2:D:147:ARG:HH12	1.42	0.84
1:A:28:LYS:HE3	1:A:31:ARG:HE	1.41	0.84
1:J:83:TRP:CD1	1:J:92:GLY:HA2	2.12	0.84
1:C:17:VAL:HB	1:C:100:LEU:HB2	1.60	0.84
1:F:41:PRO:O	1:F:121:ASN:HB3	1.78	0.84
1:T:12:PHE:HB2	1:T:108:ILE:HG13	1.58	0.84
1:A:104:ARG:HG3	1:J:120:GLY:O	1.78	0.83
1:I:75:ASP:HB2	1:I:80:HIS:HE1	1.42	0.83
1:J:86:LEU:HD21	1:J:90:SER:HB3	1.60	0.83
1:I:86:LEU:HB3	1:I:92:GLY:HA3	1.61	0.83
1:E:123:PHE:HE2	1:F:4:LEU:HD23	1.43	0.83
1:P:109:SER:HB2	1:P:115:PHE:HB2	1.61	0.83
1:S:126:LEU:HB3	1:S:139:THR:HB	1.59	0.83
1:B:104:ARG:O	1:B:106:GLN:HG3	1.79	0.83
1:E:74:THR:HG21	1:E:120:GLY:O	1.79	0.82
1:S:41:PRO:HD3	1:S:124:ARG:HG2	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:VAL:HB	1:C:129:ILE:HB	1.61	0.82
1:P:4:LEU:HB2	1:P:7:ARG:HD3	1.58	0.82
1:A:75:ASP:HB2	1:A:80:HIS:HE1	1.45	0.82
1:J:150:ASP:HA	1:J:153:LEU:HD23	1.61	0.82
1:B:96:MET:HG3	1:B:100:LEU:HD11	1.60	0.82
1:Q:69:VAL:O	1:Q:99:PRO:HD2	1.80	0.82
1:I:28:LYS:O	1:I:31:ARG:HG2	1.80	0.81
1:E:17:VAL:HG21	1:E:80:HIS:HB3	1.61	0.81
2:D:34:TYR:CE1	2:D:131:PRO:HD3	2.16	0.81
1:N:149:VAL:O	1:N:153:LEU:HD13	1.81	0.81
1:G:76:SER:HB3	1:G:104:ARG:NH2	1.95	0.81
1:Q:22:PHE:CE1	1:Q:77:GLN:HB2	2.16	0.81
1:N:8:PRO:HA	1:N:134:ILE:HA	1.63	0.81
1:E:30:TYR:HE2	1:E:68:GLN:HG2	1.45	0.80
1:H:4:LEU:HB2	1:H:7:ARG:HD3	1.60	0.80
1:Q:143:LYS:HB2	1:Q:144:PRO:HD3	1.63	0.80
1:B:0:THR:HB	1:B:2:VAL:HG13	1.62	0.80
1:I:8:PRO:HA	1:I:134:ILE:HA	1.63	0.80
1:T:126:LEU:HB3	1:T:139:THR:HB	1.62	0.80
1:I:25:ILE:HD11	1:I:101:LEU:HD13	1.64	0.80
1:L:69:VAL:HB	1:L:98:ILE:HG21	1.63	0.80
2:D:6:ASN:O	2:D:7:ARG:HD2	1.82	0.79
1:H:124:ARG:HH11	1:H:147:ARG:HH21	1.26	0.79
1:B:155:LEU:HB3	1:B:159:PHE:HE2	1.46	0.79
1:L:76:SER:HB3	1:L:104:ARG:HH11	1.47	0.79
1:H:36:VAL:HG22	1:H:128:ILE:HG12	1.63	0.79
1:A:61:GLU:HB3	1:A:65:ARG:NE	1.98	0.79
1:S:169:CYS:HB3	1:T:48:CYS:SG	2.23	0.79
1:M:152:THR:HA	1:M:155:LEU:HG	1.63	0.78
1:O:162:VAL:HG21	1:P:145:VAL:HG22	1.63	0.78
1:P:120:GLY:HA3	1:Q:104:ARG:HG3	1.65	0.78
1:R:152:THR:HA	1:R:155:LEU:HD12	1.62	0.78
2:D:86:LEU:HG	2:D:92:GLY:HA3	1.62	0.78
1:I:83:TRP:HB3	1:I:93:LEU:HD12	1.66	0.78
1:C:18:ILE:HD13	1:C:23:LYS:HB2	1.65	0.78
1:H:168:VAL:HG12	1:H:169:CYS:H	1.47	0.78
1:S:26:CYS:HB3	1:S:29:ASP:OD1	1.83	0.78
1:T:28:LYS:HA	1:T:31:ARG:NE	1.98	0.78
2:D:135:LEU:HD12	2:D:136:ARG:H	1.47	0.78
1:G:84:ASP:HA	1:G:93:LEU:HB2	1.65	0.78
1:N:15:GLN:HE21	1:N:22:PHE:HB3	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:HA	1:B:153:LEU:HD22	1.65	0.78
1:L:65:ARG:HG2	1:L:160:GLN:NE2	1.99	0.78
1:L:167:GLU:HG2	1:L:169:CYS:SG	2.23	0.78
1:A:150:ASP:HA	1:A:153:LEU:HD13	1.65	0.77
1:S:53:ILE:HD11	1:S:93:LEU:HA	1.66	0.77
1:S:127:PHE:CE1	1:S:138:ILE:HG23	2.18	0.77
1:S:47:VAL:HG23	1:S:51:GLU:HG2	1.64	0.77
1:I:10:PRO:HG2	1:I:112:TYR:CZ	2.18	0.77
2:D:86:LEU:HD11	2:D:90:SER:HB2	1.66	0.77
1:G:76:SER:HB3	1:G:104:ARG:HH22	1.48	0.77
1:M:41:PRO:HA	1:M:122:ALA:H	1.49	0.77
1:N:119:ASP:HB2	1:N:121:ASN:OD1	1.85	0.77
1:P:148:SER:HB3	1:P:151:GLU:HB3	1.67	0.77
1:S:15:GLN:CG	1:S:24:GLU:HG2	2.07	0.77
1:E:138:ILE:HB	1:F:140:ILE:HB	1.65	0.77
1:R:59:VAL:HA	1:R:62:PHE:HD2	1.48	0.77
2:D:46:PHE:H	2:D:46:PHE:HD1	1.30	0.77
1:I:38:PHE:HB3	1:I:126:LEU:HG	1.67	0.77
1:I:22:PHE:O	1:I:23:LYS:HD2	1.85	0.77
1:N:15:GLN:NE2	1:N:22:PHE:HB3	1.98	0.77
1:T:28:LYS:O	1:T:31:ARG:HD3	1.83	0.77
1:G:86:LEU:HG	1:G:92:GLY:HA3	1.66	0.76
2:D:5:PRO:O	2:D:135:LEU:HG	1.85	0.76
1:L:39:PHE:CE1	1:L:114:VAL:HG21	2.20	0.76
1:K:58:GLN:OE1	1:K:61:GLU:CG	2.34	0.76
1:E:5:PRO:HB3	1:E:136:ARG:O	1.85	0.76
1:I:28:LYS:HA	1:I:31:ARG:NE	1.97	0.76
1:S:55:PHE:CE2	1:S:149:VAL:HA	2.21	0.76
1:K:51:GLU:HG3	1:K:52:ILE:H	1.49	0.76
1:S:127:PHE:HE1	1:S:138:ILE:HG23	1.51	0.76
1:S:47:VAL:HG21	1:S:51:GLU:CG	2.15	0.76
1:T:162:VAL:HG13	1:T:166:GLY:HA2	1.67	0.76
1:C:56:SER:OG	1:C:96:MET:HB2	1.86	0.76
1:H:130:ASP:HB2	1:H:131:PRO:HD2	1.68	0.76
1:K:128:ILE:HG22	1:K:136:ARG:HB3	1.68	0.76
1:B:70:ILE:HG12	1:B:99:PRO:HG2	1.69	0.75
1:E:51:GLU:OE1	1:E:146:GLY:HA2	1.85	0.75
1:H:103:ASP:HB2	1:H:108:ILE:HD12	1.68	0.75
1:P:51:GLU:OE2	1:P:124:ARG:HD3	1.86	0.75
1:I:141:ASN:HD22	1:I:145:VAL:HG12	1.51	0.75
1:Q:6:ASN:O	1:Q:7:ARG:HG3	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LYS:HE3	1:C:24:GLU:OE2	1.87	0.75
1:E:123:PHE:CE2	1:F:4:LEU:HD23	2.20	0.75
1:G:149:VAL:HG12	1:G:153:LEU:HD13	1.69	0.74
1:P:30:TYR:CE2	1:P:68:GLN:HG2	2.23	0.74
1:Q:57:ASP:HA	1:Q:97:LYS:HD3	1.69	0.74
1:E:30:TYR:CE2	1:E:68:GLN:HG2	2.21	0.74
1:Q:34:TYR:CD1	1:Q:130:ASP:HA	2.22	0.74
1:J:124:ARG:HB2	1:J:141:ASN:HB2	1.69	0.74
1:R:5:PRO:HA	1:R:135:LEU:HD23	1.69	0.74
1:H:22:PHE:CE1	1:H:77:GLN:HB2	2.22	0.74
1:J:80:HIS:CD2	1:J:102:ALA:HB2	2.22	0.74
2:D:17:VAL:HB	2:D:100:LEU:HB2	1.68	0.74
1:O:88:ARG:HH12	1:O:94:GLY:HA3	1.53	0.74
1:A:14:GLY:O	1:A:24:GLU:HG3	1.88	0.74
2:D:15:GLN:HA	2:D:15:GLN:NE2	1.99	0.74
1:K:7:ARG:HH11	1:K:7:ARG:HG3	1.51	0.74
1:T:124:ARG:CB	1:T:147:ARG:HH12	2.01	0.73
1:I:35:VAL:HG22	1:I:68:GLN:HB3	1.69	0.73
1:H:131:PRO:HG3	1:Q:163:GLU:HG3	1.70	0.73
1:A:109:SER:HB3	1:A:115:PHE:HB2	1.70	0.73
1:N:26:CYS:O	1:N:29:ASP:HB2	1.89	0.73
1:T:28:LYS:HA	1:T:31:ARG:HE	1.53	0.73
1:E:103:ASP:HB2	1:E:108:ILE:HD12	1.70	0.73
1:H:84:ASP:OD2	1:H:95:HIS:HA	1.88	0.73
1:O:130:ASP:OD2	1:O:134:ILE:HB	1.89	0.73
1:S:74:THR:HA	1:S:103:ASP:O	1.87	0.73
2:D:93:LEU:HD22	2:D:96:MET:HE3	1.71	0.73
1:N:115:PHE:HA	1:N:122:ALA:HA	1.71	0.73
1:B:124:ARG:HE	1:B:143:LYS:HA	1.54	0.73
1:C:124:ARG:HH11	1:C:147:ARG:NH2	1.86	0.73
1:E:56:SER:O	1:E:59:VAL:HG23	1.88	0.73
1:H:36:VAL:HG13	1:H:126:LEU:HD21	1.71	0.73
1:K:0:THR:HG22	1:K:1:MET:H	1.54	0.73
1:B:83:TRP:CD1	1:B:92:GLY:HA2	2.24	0.73
1:O:13:LYS:HG2	1:O:25:ILE:O	1.89	0.73
1:K:105:LYS:HD3	1:T:118:GLU:O	1.89	0.73
1:B:32:GLY:CA	1:B:131:PRO:HB3	2.19	0.73
1:I:154:ARG:HH22	1:J:147:ARG:HA	1.53	0.73
1:I:126:LEU:HD12	1:I:147:ARG:HD2	1.71	0.72
1:T:30:TYR:O	1:T:31:ARG:HD2	1.89	0.72
1:F:50:THR:HA	1:F:54:ALA:HB2	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:7:ARG:HD2	1:N:7:ARG:H	1.54	0.72
1:O:88:ARG:NH1	1:O:94:GLY:HA3	2.04	0.72
1:Q:112:TYR:HB3	1:Q:127:PHE:CZ	2.23	0.72
1:F:129:ILE:HG22	1:F:133:GLY:HA2	1.69	0.72
1:O:22:PHE:CE2	1:O:77:GLN:HB3	2.23	0.72
1:G:130:ASP:OD2	1:G:134:ILE:HB	1.90	0.72
1:L:128:ILE:HB	1:L:136:ARG:HB2	1.71	0.72
1:S:116:ASP:HB2	1:S:123:PHE:CE1	2.25	0.72
1:F:62:PHE:HB3	1:F:67:CYS:O	1.89	0.72
1:N:7:ARG:CD	1:N:7:ARG:H	2.03	0.72
1:Q:116:ASP:HB2	1:Q:123:PHE:CE2	2.25	0.72
1:M:59:VAL:HG21	1:M:97:LYS:HB3	1.71	0.72
1:O:151:GLU:HG3	1:O:155:LEU:HD11	1.71	0.72
1:Q:55:PHE:CZ	1:Q:149:VAL:HA	2.24	0.72
1:Q:13:LYS:HG3	1:Q:26:CYS:SG	2.29	0.72
1:A:15:GLN:HG2	1:A:77:GLN:OE1	1.89	0.72
1:L:126:LEU:HB3	1:L:139:THR:HB	1.70	0.72
1:A:148:SER:HB2	1:B:154:ARG:CZ	2.20	0.72
1:G:39:PHE:CD2	1:G:114:VAL:HG21	2.25	0.72
1:C:98:ILE:HG13	1:C:99:PRO:HD2	1.72	0.72
1:O:158:ALA:O	1:O:162:VAL:HG23	1.90	0.72
1:O:162:VAL:O	1:O:166:GLY:HA2	1.90	0.72
1:O:5:PRO:HB3	1:O:136:ARG:O	1.90	0.72
1:S:51:GLU:OE1	1:S:51:GLU:CA	2.30	0.72
1:C:82:ALA:HA	1:C:85:ASN:HD22	1.53	0.71
2:D:23:LYS:HE3	1:O:23:LYS:HB2	1.72	0.71
1:I:161:PHE:CE2	1:I:166:GLY:HA2	2.25	0.71
1:R:126:LEU:HB3	1:R:139:THR:HB	1.70	0.71
1:T:162:VAL:HA	1:T:166:GLY:H	1.54	0.71
1:T:69:VAL:O	1:T:99:PRO:HD2	1.90	0.71
1:H:16:ALA:HB2	1:H:101:LEU:HD12	1.71	0.71
1:F:4:LEU:O	1:F:135:LEU:HD23	1.91	0.71
1:R:4:LEU:HB2	1:R:7:ARG:HD3	1.72	0.71
1:T:124:ARG:HB3	1:T:147:ARG:NH1	2.06	0.71
1:F:106:GLN:HB3	1:F:110:LYS:HE3	1.72	0.71
1:I:75:ASP:HB2	1:I:80:HIS:CE1	2.25	0.71
1:Q:75:ASP:HB3	1:Q:79:SER:CB	2.21	0.71
1:T:32:GLY:CA	1:T:131:PRO:HB3	2.20	0.71
1:F:87:ASP:OD1	1:F:90:SER:HB3	1.91	0.71
1:R:36:VAL:HG22	1:R:128:ILE:HG12	1.70	0.71
1:T:41:PRO:HD3	1:T:124:ARG:HG2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HG3	1:A:155:LEU:HD13	1.72	0.71
1:K:15:GLN:HG2	1:K:77:GLN:NE2	2.05	0.71
1:P:75:ASP:CG	1:Q:104:ARG:HH22	1.93	0.71
1:R:73:SER:HB3	1:R:80:HIS:NE2	2.05	0.71
1:S:136:ARG:HB3	1:S:159:PHE:CE1	2.26	0.71
1:C:123:PHE:CD2	2:D:4:LEU:HD12	2.26	0.71
2:D:126:LEU:HD23	2:D:127:PHE:N	2.06	0.70
1:G:109:SER:HB3	1:G:115:PHE:HB2	1.72	0.70
1:L:59:VAL:HG21	1:L:97:LYS:HG2	1.71	0.70
1:E:67:CYS:HB2	1:E:156:LEU:HD21	1.73	0.70
1:E:162:VAL:HG12	1:E:167:GLU:HA	1.72	0.70
1:H:3:LEU:O	1:H:4:LEU:HD23	1.91	0.70
1:L:38:PHE:HB2	1:L:147:ARG:HH22	1.56	0.70
1:C:34:TYR:CE1	1:C:131:PRO:HD3	2.26	0.70
1:E:96:MET:HG3	1:E:100:LEU:HD21	1.73	0.70
1:Q:124:ARG:HB3	1:Q:147:ARG:HD3	1.73	0.70
1:B:75:ASP:HA	1:B:104:ARG:NH1	2.07	0.70
2:D:117:GLU:O	1:E:105:LYS:HE3	1.90	0.70
1:E:123:PHE:CE2	1:F:5:PRO:HD2	2.27	0.70
1:M:144:PRO:HB2	1:N:162:VAL:HG21	1.73	0.70
1:T:130:ASP:OD1	1:T:131:PRO:HD2	1.91	0.70
1:J:40:TYR:CE2	1:J:73:SER:HB2	2.26	0.70
1:Q:148:SER:OG	1:Q:151:GLU:HB3	1.91	0.70
1:F:36:VAL:HG13	1:F:126:LEU:HD21	1.74	0.70
1:N:147:ARG:N	1:N:147:ARG:HE	1.88	0.70
1:T:39:PHE:HB2	1:T:125:GLY:H	1.56	0.70
1:C:127:PHE:CE2	1:C:138:ILE:HG23	2.27	0.69
1:E:80:HIS:CD2	1:E:102:ALA:HB2	2.27	0.69
1:F:51:GLU:HG2	1:F:147:ARG:HB2	1.73	0.69
1:L:48:CYS:HB2	1:L:49:PRO:HD3	1.74	0.69
1:N:75:ASP:HB2	1:N:80:HIS:NE2	2.07	0.69
1:O:86:LEU:HD12	1:O:87:ASP:H	1.57	0.69
1:I:10:PRO:HG2	1:I:112:TYR:CE2	2.27	0.69
1:R:50:THR:OG1	1:R:53:ILE:HB	1.93	0.69
1:P:135:LEU:HD12	1:P:136:ARG:H	1.55	0.69
1:C:12:PHE:CE1	1:C:27:LEU:HB2	2.27	0.69
1:S:103:ASP:HB2	1:S:108:ILE:HD12	1.75	0.69
1:F:80:HIS:HE1	1:F:102:ALA:HB2	1.55	0.69
1:P:50:THR:HA	1:P:53:ILE:HD12	1.75	0.69
1:C:149:VAL:HB	1:C:153:LEU:HD13	1.74	0.69
1:E:53:ILE:HD13	1:E:88:ARG:HD2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:LYS:HG2	1:O:23:LYS:HD3	1.74	0.69
1:P:109:SER:CB	1:P:115:PHE:HB2	2.23	0.69
1:G:128:ILE:HD12	1:G:137:GLN:HB3	1.75	0.68
1:J:15:GLN:HE22	1:J:24:GLU:HB2	1.58	0.68
1:L:126:LEU:HB2	1:L:147:ARG:HH11	1.58	0.68
1:L:71:ALA:HB3	1:L:100:LEU:HD23	1.75	0.68
1:C:126:LEU:HB3	1:C:139:THR:HB	1.75	0.68
1:G:138:ILE:HB	1:H:140:ILE:HG22	1.74	0.68
1:S:52:ILE:N	1:S:52:ILE:CD1	2.49	0.68
1:C:15:GLN:NE2	1:C:24:GLU:HB2	2.08	0.68
1:M:148:SER:HB2	1:N:154:ARG:NE	2.08	0.68
1:T:72:CYS:HB2	1:T:101:LEU:HB3	1.75	0.68
1:G:149:VAL:HG12	1:G:153:LEU:CD1	2.24	0.68
1:H:105:LYS:O	1:H:106:GLN:HB2	1.93	0.68
1:I:34:TYR:CE1	1:I:131:PRO:HD3	2.29	0.68
1:H:169:CYS:HB3	1:H:170:PRO:HD2	1.74	0.68
1:J:12:PHE:CE2	1:J:27:LEU:HD13	2.28	0.68
1:R:40:TYR:CZ	1:R:73:SER:HB2	2.29	0.68
1:M:143:LYS:N	1:M:144:PRO:HD2	2.08	0.68
1:R:48:CYS:CB	1:R:51:GLU:H	2.05	0.68
1:G:159:PHE:HE1	1:H:142:ASP:HB2	1.60	0.67
1:J:60:GLU:HA	1:J:60:GLU:OE1	1.94	0.67
1:T:75:ASP:HB2	1:T:80:HIS:HE1	1.59	0.67
1:A:17:VAL:O	1:A:99:PRO:HA	1.93	0.67
1:E:3:LEU:HD12	1:E:4:LEU:H	1.59	0.67
1:E:123:PHE:CD2	1:F:5:PRO:HD2	2.29	0.67
1:O:22:PHE:HE2	1:O:77:GLN:HB3	1.57	0.67
1:I:55:PHE:CE1	1:I:149:VAL:HG22	2.28	0.67
1:I:145:VAL:HG21	1:J:159:PHE:CE1	2.29	0.67
1:H:93:LEU:HD13	1:H:96:MET:HG3	1.75	0.67
1:I:135:LEU:HD11	1:I:137:GLN:O	1.93	0.67
1:S:5:PRO:HD3	1:S:138:ILE:CD1	2.24	0.67
2:D:155:LEU:O	2:D:159:PHE:HD1	1.78	0.67
1:L:12:PHE:HB2	1:L:108:ILE:HG12	1.77	0.67
1:L:124:ARG:HB3	1:L:147:ARG:CZ	2.24	0.67
1:F:38:PHE:CE2	1:F:51:GLU:O	2.48	0.67
1:J:125:GLY:HA2	1:J:139:THR:O	1.95	0.67
1:M:155:LEU:O	1:M:159:PHE:HD2	1.78	0.67
1:O:80:HIS:ND1	1:O:100:LEU:HB3	2.08	0.67
1:Q:142:ASP:CG	1:Q:144:PRO:HD2	2.15	0.67
1:A:39:PHE:O	1:A:124:ARG:HA	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASP:HB3	1:C:123:PHE:CE2	2.30	0.67
1:C:146:GLY:O	1:C:147:ARG:HG3	1.95	0.67
1:P:65:ARG:NH1	1:P:157:ASP:HB3	2.10	0.67
1:B:38:PHE:CZ	1:B:71:ALA:HB2	2.30	0.67
2:D:4:LEU:HB2	2:D:7:ARG:HD3	1.76	0.67
1:F:78:TYR:HB3	1:G:45:THR:HB	1.75	0.67
1:N:3:LEU:HB2	1:N:138:ILE:HD13	1.75	0.67
1:T:105:LYS:HB2	1:T:107:GLU:HG3	1.75	0.67
1:C:11:GLU:OE1	1:C:27:LEU:HB3	1.95	0.67
1:C:155:LEU:O	1:C:159:PHE:HD1	1.77	0.67
1:J:116:ASP:HB2	1:J:123:PHE:CE2	2.30	0.67
1:N:16:ALA:HA	1:N:100:LEU:O	1.95	0.67
2:D:33:LYS:O	2:D:131:PRO:HA	1.94	0.66
2:D:93:LEU:HD22	2:D:96:MET:CE	2.25	0.66
1:H:35:VAL:O	1:H:128:ILE:HA	1.96	0.66
1:T:129:ILE:HG12	1:T:135:LEU:HD13	1.77	0.66
1:L:32:GLY:HA2	1:L:131:PRO:HB3	1.77	0.66
1:M:162:VAL:HB	1:M:167:GLU:HB3	1.76	0.66
1:R:47:VAL:O	1:R:50:THR:HA	1.94	0.66
1:A:5:PRO:O	1:A:6:ASN:HB3	1.96	0.66
1:C:32:GLY:HA2	1:C:131:PRO:HB3	1.77	0.66
1:F:24:GLU:OE1	1:F:24:GLU:HA	1.93	0.66
1:K:15:GLN:HG2	1:K:77:GLN:HE21	1.59	0.66
1:P:11:GLU:OE1	1:P:27:LEU:HD23	1.95	0.66
1:F:52:ILE:HG22	1:F:53:ILE:N	2.09	0.66
1:H:86:LEU:HB3	1:H:92:GLY:HA3	1.76	0.66
1:I:9:ALA:HB2	1:I:135:LEU:HB2	1.76	0.66
1:B:13:LYS:HG3	1:B:25:ILE:O	1.96	0.66
1:B:70:ILE:HG23	1:B:99:PRO:HB2	1.78	0.66
1:B:42:ALA:O	1:B:45:THR:HG22	1.95	0.66
2:D:26:CYS:SG	2:D:28:LYS:HE3	2.35	0.66
1:G:48:CYS:O	1:G:50:THR:N	2.27	0.66
1:M:128:ILE:HB	1:M:137:GLN:HB3	1.78	0.66
1:B:88:ARG:HA	1:B:92:GLY:O	1.96	0.66
1:J:69:VAL:O	1:J:99:PRO:HD2	1.96	0.66
1:L:42:ALA:HB3	1:L:45:THR:HG23	1.78	0.66
1:N:76:SER:HB3	1:N:104:ARG:NE	2.10	0.66
1:S:145:VAL:HG21	1:T:159:PHE:CE1	2.31	0.66
2:D:127:PHE:HA	2:D:137:GLN:O	1.96	0.66
1:M:164:LYS:HG2	1:M:165:HIS:ND1	2.10	0.66
1:M:75:ASP:O	1:M:102:ALA:HB1	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LEU:HD12	1:E:70:ILE:O	1.96	0.65
1:L:43:ASP:HA	1:L:83:TRP:CE3	2.31	0.65
1:S:75:ASP:HB2	1:S:80:HIS:CE1	2.32	0.65
1:B:33:LYS:HA	1:B:66:ASN:HD21	1.61	0.65
1:M:4:LEU:HD21	1:N:114:VAL:HA	1.77	0.65
1:R:86:LEU:HG	1:R:87:ASP:H	1.60	0.65
1:B:17:VAL:HA	1:B:21:GLU:O	1.96	0.65
1:B:33:LYS:HA	1:B:66:ASN:ND2	2.11	0.65
1:H:93:LEU:HB3	1:H:96:MET:CG	2.22	0.65
1:K:103:ASP:OD2	1:K:108:ILE:HB	1.95	0.65
1:C:109:SER:HB3	1:C:115:PHE:HB2	1.78	0.65
2:D:76:SER:HB3	2:D:79:SER:OG	1.97	0.65
1:I:60:GLU:HA	1:I:63:ASN:HB2	1.77	0.65
1:A:105:LYS:HB3	1:A:107:GLU:OE2	1.96	0.65
1:B:12:PHE:HE1	1:B:27:LEU:HD13	1.61	0.65
1:B:61:GLU:O	1:B:65:ARG:HG3	1.97	0.65
1:C:11:GLU:OE2	1:C:27:LEU:HD23	1.96	0.65
1:L:37:LEU:HD12	1:L:38:PHE:N	2.12	0.65
1:O:148:SER:HB2	1:P:154:ARG:NE	2.12	0.65
1:M:59:VAL:HG21	1:M:97:LYS:CB	2.27	0.65
1:B:71:ALA:HB3	1:B:100:LEU:HD23	1.78	0.65
1:G:65:ARG:HD2	1:G:156:LEU:HD23	1.77	0.65
1:I:71:ALA:HB3	1:I:100:LEU:HD23	1.78	0.65
1:I:154:ARG:NH2	1:J:147:ARG:HA	2.11	0.65
1:T:86:LEU:HB3	1:T:92:GLY:HA3	1.78	0.65
1:B:74:THR:O	1:B:104:ARG:HD3	1.97	0.64
1:G:5:PRO:HG2	1:H:123:PHE:CD1	2.32	0.64
2:D:54:ALA:HA	2:D:57:ASP:OD2	1.97	0.64
1:E:43:ASP:HA	1:E:83:TRP:CZ3	2.31	0.64
1:I:144:PRO:HB3	1:J:167:GLU:HG3	1.79	0.64
1:N:31:ARG:HD3	1:N:131:PRO:O	1.96	0.64
1:E:129:ILE:HG23	1:E:134:ILE:O	1.97	0.64
1:F:136:ARG:HB3	1:F:159:PHE:CE2	2.32	0.64
1:O:72:CYS:SG	1:O:101:LEU:HG	2.37	0.64
1:O:41:PRO:CG	1:O:143:LYS:HG2	2.25	0.64
1:R:87:ASP:OD2	1:R:89:LYS:HB2	1.97	0.64
1:T:45:THR:O	1:T:49:PRO:HG3	1.97	0.64
1:O:86:LEU:HG	1:O:92:GLY:N	2.12	0.64
1:P:65:ARG:HD2	1:P:160:GLN:HE22	1.62	0.64
1:S:164:LYS:HB3	1:S:165:HIS:CD2	2.32	0.64
1:S:52:ILE:H	1:S:52:ILE:HD13	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:159:PHE:CD2	1:P:145:VAL:HG21	2.33	0.64
1:Q:55:PHE:CE2	1:Q:149:VAL:HA	2.32	0.64
1:Q:34:TYR:HD1	1:Q:130:ASP:HA	1.61	0.64
1:S:12:PHE:HB2	1:S:108:ILE:HG12	1.79	0.64
1:H:126:LEU:HD23	1:H:127:PHE:N	2.12	0.64
1:L:163:GLU:O	1:L:163:GLU:HG2	1.97	0.64
1:P:65:ARG:HH21	1:P:153:LEU:HD23	1.62	0.64
1:S:55:PHE:HE2	1:S:149:VAL:HA	1.58	0.64
1:A:96:MET:HG2	1:A:100:LEU:HD21	1.80	0.64
1:H:168:VAL:HG12	1:H:169:CYS:N	2.12	0.64
1:S:5:PRO:HD3	1:S:138:ILE:HD12	1.80	0.64
1:S:75:ASP:HB2	1:S:80:HIS:HE1	1.63	0.64
1:H:137:GLN:NE2	1:H:155:LEU:HD13	2.12	0.64
1:I:34:TYR:CE1	1:I:160:GLN:HG2	2.32	0.64
1:J:25:ILE:HD12	1:J:70:ILE:HD13	1.80	0.64
1:K:28:LYS:HA	1:K:31:ARG:HB2	1.79	0.64
1:M:30:TYR:CE1	1:M:68:GLN:HG2	2.33	0.64
1:A:53:ILE:HG21	1:A:88:ARG:HH12	1.63	0.64
1:G:25:ILE:HD11	1:G:101:LEU:HD13	1.80	0.64
1:M:148:SER:HB2	1:N:154:ARG:CZ	2.28	0.64
1:A:127:PHE:CE1	1:A:138:ILE:HG23	2.33	0.64
1:E:8:PRO:HG3	1:E:134:ILE:CD1	2.28	0.64
1:G:16:ALA:HB2	1:G:101:LEU:HD12	1.79	0.64
1:H:34:TYR:HB2	1:H:67:CYS:HB2	1.80	0.64
1:I:167:GLU:OE1	1:I:167:GLU:HA	1.97	0.64
1:K:0:THR:HG22	1:L:2:VAL:HG12	1.79	0.64
1:M:80:HIS:CD2	1:M:102:ALA:HB2	2.33	0.64
1:N:104:ARG:HH22	1:O:75:ASP:HA	1.62	0.64
1:P:74:THR:HG21	1:P:120:GLY:O	1.98	0.64
1:P:119:ASP:HA	1:Q:105:LYS:HG2	1.79	0.64
1:B:60:GLU:HA	1:B:63:ASN:OD1	1.99	0.63
1:E:8:PRO:HG3	1:E:134:ILE:HD13	1.80	0.63
1:P:44:PHE:CD1	1:P:83:TRP:HD1	2.16	0.63
1:B:155:LEU:HB3	1:B:159:PHE:CE2	2.30	0.63
1:E:25:ILE:HD12	1:E:70:ILE:HD13	1.80	0.63
1:G:47:VAL:C	1:G:49:PRO:HD2	2.18	0.63
1:L:137:GLN:HB2	1:L:159:PHE:HE2	1.63	0.63
1:T:33:LYS:HG2	1:T:66:ASN:OD1	1.98	0.63
1:K:65:ARG:HB3	1:K:160:GLN:HE22	1.64	0.63
1:S:32:GLY:O	1:S:131:PRO:HB3	1.99	0.63
1:I:58:GLN:HB3	1:I:61:GLU:OE1	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:TYR:HB2	1:K:114:VAL:HG22	1.80	0.63
1:G:151:GLU:HG2	1:H:151:GLU:HG2	1.80	0.63
1:G:61:GLU:HB3	1:G:153:LEU:HD21	1.81	0.63
1:G:159:PHE:HE1	1:H:142:ASP:CB	2.12	0.63
1:Q:55:PHE:HZ	1:Q:148:SER:O	1.81	0.63
1:A:34:TYR:CE1	1:A:130:ASP:HA	2.34	0.63
1:O:132:ASN:HB2	1:O:134:ILE:HG12	1.81	0.63
1:I:140:ILE:HG22	1:J:138:ILE:HB	1.79	0.63
1:N:72:CYS:SG	1:N:73:SER:N	2.72	0.63
1:P:143:LYS:N	1:P:144:PRO:HD2	2.13	0.63
1:Q:28:LYS:HA	1:Q:31:ARG:HH21	1.64	0.63
1:I:165:HIS:CD2	1:I:165:HIS:H	2.16	0.63
1:J:71:ALA:O	1:J:101:LEU:HB3	1.99	0.63
1:L:38:PHE:HB2	1:L:147:ARG:HH12	1.64	0.63
1:O:7:ARG:HB3	1:O:8:PRO:HD2	1.79	0.63
1:Q:32:GLY:C	1:Q:131:PRO:HB3	2.19	0.63
1:T:106:GLN:HB3	1:T:110:LYS:HG3	1.80	0.63
2:D:30:TYR:CE1	2:D:68:GLN:HG2	2.34	0.62
1:L:60:GLU:HA	1:L:60:GLU:OE1	1.99	0.62
1:Q:115:PHE:CZ	1:Q:120:GLY:HA2	2.34	0.62
1:R:65:ARG:HE	1:R:156:LEU:HD23	1.64	0.62
1:S:41:PRO:HD2	1:S:124:ARG:NH1	2.14	0.62
1:A:123:PHE:CE2	1:B:4:LEU:HD23	2.34	0.62
1:A:62:PHE:CE2	1:A:69:VAL:HG21	2.33	0.62
1:C:116:ASP:OD2	1:C:119:ASP:HB2	1.99	0.62
1:H:56:SER:O	1:H:59:VAL:HG23	1.98	0.62
1:A:34:TYR:CD1	1:A:130:ASP:HA	2.35	0.62
1:E:40:TYR:HB2	1:E:41:PRO:CD	2.26	0.62
1:H:70:ILE:HG12	1:H:99:PRO:HG2	1.80	0.62
1:O:51:GLU:O	1:O:55:PHE:HD1	1.82	0.62
1:C:34:TYR:HA	1:C:129:ILE:O	1.98	0.62
2:D:15:GLN:OE1	2:D:22:PHE:HB3	1.98	0.62
2:D:43:ASP:HA	2:D:83:TRP:CZ3	2.34	0.62
1:R:149:VAL:O	1:R:153:LEU:HD13	2.00	0.62
1:R:104:ARG:HG3	1:S:120:GLY:O	2.00	0.62
2:D:143:LYS:N	2:D:144:PRO:HD2	2.14	0.62
1:F:80:HIS:CE1	1:F:102:ALA:HB2	2.33	0.62
1:I:34:TYR:CZ	1:I:160:GLN:HG2	2.34	0.62
1:J:18:ILE:HD12	1:J:23:LYS:HB2	1.81	0.62
1:L:124:ARG:HB3	1:L:147:ARG:HH21	1.64	0.62
1:O:13:LYS:NZ	1:O:26:CYS:HB2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:35:VAL:HB	1:R:129:ILE:HB	1.81	0.62
1:S:164:LYS:HD3	1:S:164:LYS:O	2.00	0.62
1:M:12:PHE:HB2	1:M:108:ILE:HD13	1.80	0.62
1:M:136:ARG:HB3	1:M:159:PHE:CD1	2.34	0.62
1:M:7:ARG:HB3	1:M:8:PRO:HD2	1.82	0.62
1:N:74:THR:HG21	1:N:121:ASN:HA	1.81	0.62
1:A:124:ARG:HB3	1:A:147:ARG:HD3	1.80	0.62
1:C:34:TYR:CD1	1:C:130:ASP:HA	2.33	0.62
1:O:30:TYR:CD2	1:O:68:GLN:HG2	2.34	0.62
1:Q:156:LEU:O	1:Q:160:GLN:HG3	2.00	0.62
1:A:123:PHE:HE2	1:B:4:LEU:HD23	1.64	0.62
1:J:112:TYR:HB3	1:J:127:PHE:CZ	2.35	0.62
1:L:43:ASP:HA	1:L:83:TRP:CZ3	2.35	0.62
1:R:41:PRO:HB2	1:R:46:PHE:CE2	2.35	0.62
1:S:107:GLU:HG2	1:S:108:ILE:N	2.15	0.62
1:B:40:TYR:HB2	1:B:41:PRO:HD2	1.82	0.62
2:D:15:GLN:CA	2:D:15:GLN:HE21	1.99	0.62
1:J:47:VAL:HG22	1:J:48:CYS:N	2.10	0.62
2:D:93:LEU:HB3	2:D:96:MET:HG2	1.82	0.62
1:N:148:SER:HB3	1:N:151:GLU:CB	2.30	0.62
1:Q:125:GLY:HA2	1:Q:140:ILE:HA	1.81	0.62
1:C:123:PHE:CD1	1:C:143:LYS:HG3	2.35	0.61
1:E:38:PHE:CZ	1:E:71:ALA:HB2	2.35	0.61
1:H:46:PHE:HZ	1:I:81:LEU:HD23	1.64	0.61
1:E:26:CYS:SG	1:E:28:LYS:HB2	2.40	0.61
1:O:83:TRP:CE2	1:O:93:LEU:HD21	2.35	0.61
1:P:105:LYS:HB2	1:P:107:GLU:HG2	1.82	0.61
1:Q:140:ILE:O	1:R:137:GLN:HG3	1.99	0.61
1:F:26:CYS:O	1:F:27:LEU:HB3	1.98	0.61
1:G:17:VAL:HG22	1:G:21:GLU:O	2.00	0.61
1:B:12:PHE:CE1	1:B:27:LEU:HB2	2.35	0.61
1:E:137:GLN:HB3	1:E:159:PHE:CZ	2.36	0.61
1:E:88:ARG:HA	1:E:91:GLY:O	2.00	0.61
1:G:172:ASN:ND2	1:H:146:GLY:HA3	2.15	0.61
1:K:37:LEU:HD12	1:K:70:ILE:O	2.01	0.61
1:N:56:SER:CB	1:N:96:MET:HG3	2.28	0.61
1:Q:86:LEU:HD11	1:Q:90:SER:HB3	1.82	0.61
1:B:130:ASP:OD2	1:B:134:ILE:HB	2.00	0.61
1:F:158:ALA:O	1:F:162:VAL:HG23	2.01	0.61
1:P:44:PHE:CE1	1:P:83:TRP:HD1	2.18	0.61
1:T:84:ASP:HA	1:T:93:LEU:HD12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:HG22	1:A:106:GLN:HG2	1.82	0.61
1:E:67:CYS:CB	1:E:156:LEU:HD21	2.31	0.61
1:F:106:GLN:O	1:F:110:LYS:HG3	2.01	0.61
1:J:124:ARG:CB	1:J:141:ASN:HB2	2.31	0.61
1:M:13:LYS:HG3	1:M:24:GLU:OE2	2.01	0.61
1:R:109:SER:HB3	1:R:114:VAL:HG23	1.83	0.61
1:F:80:HIS:HE1	1:F:102:ALA:CB	2.14	0.61
1:J:87:ASP:O	1:J:88:ARG:HB2	2.00	0.61
1:L:40:TYR:HB2	1:L:41:PRO:CD	2.28	0.61
1:R:30:TYR:CE1	1:R:68:GLN:HG2	2.36	0.61
1:T:35:VAL:HG22	1:T:68:GLN:HB3	1.81	0.61
1:H:124:ARG:HB3	1:H:147:ARG:CZ	2.31	0.61
1:Q:40:TYR:HB2	1:Q:41:PRO:HD2	1.82	0.61
1:S:47:VAL:CG2	1:S:51:GLU:CG	2.74	0.61
1:C:4:LEU:HB3	2:D:123:PHE:CD2	2.35	0.61
2:D:65:ARG:HB3	2:D:160:GLN:OE1	2.01	0.61
1:E:136:ARG:HD3	1:E:159:PHE:HD2	1.65	0.61
1:F:110:LYS:HE2	1:F:115:PHE:CE2	2.36	0.61
1:I:16:ALA:O	1:I:22:PHE:HA	2.01	0.61
1:K:105:LYS:O	1:K:106:GLN:HG3	2.01	0.61
1:P:21:GLU:HB2	1:P:23:LYS:HE3	1.82	0.61
1:L:39:PHE:CD2	1:L:72:CYS:HB3	2.36	0.61
1:M:126:LEU:HB3	1:M:139:THR:HB	1.82	0.61
1:Q:129:ILE:HG22	1:Q:130:ASP:O	2.01	0.61
1:C:143:LYS:N	1:C:144:PRO:HD2	2.15	0.60
1:A:130:ASP:OD2	1:A:136:ARG:NH1	2.33	0.60
1:L:38:PHE:HD2	1:L:147:ARG:NH2	2.00	0.60
1:H:129:ILE:HG23	1:H:134:ILE:O	2.01	0.60
1:I:15:GLN:O	1:I:101:LEU:HD12	2.02	0.60
1:I:13:LYS:HA	1:I:25:ILE:O	2.02	0.60
1:J:128:ILE:O	1:J:135:LEU:HD12	2.02	0.60
1:O:12:PHE:CE2	1:O:27:LEU:HD22	2.37	0.60
2:D:65:ARG:NH1	2:D:153:LEU:HD11	2.15	0.60
1:F:130:ASP:HB2	1:F:131:PRO:HD2	1.83	0.60
1:S:130:ASP:HB2	1:S:131:PRO:HD2	1.83	0.60
1:C:149:VAL:HA	1:C:152:THR:OG1	2.01	0.60
2:D:104:ARG:HG3	1:E:120:GLY:H	1.67	0.60
1:F:105:LYS:N	1:F:105:LYS:HD2	2.17	0.60
1:G:84:ASP:O	1:G:94:GLY:O	2.18	0.60
1:K:87:ASP:CG	1:K:90:SER:HB2	2.21	0.60
1:L:41:PRO:HG2	1:L:45:THR:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:GLN:O	1:O:80:HIS:HB2	2.02	0.60
1:T:124:ARG:HB3	1:T:147:ARG:HH22	1.65	0.60
1:T:109:SER:HB2	1:T:115:PHE:HB2	1.84	0.60
1:B:128:ILE:HB	1:B:137:GLN:HB3	1.84	0.60
1:O:84:ASP:HA	1:O:93:LEU:CB	2.30	0.60
1:T:9:ALA:CB	1:T:129:ILE:HD13	2.32	0.60
1:M:159:PHE:O	1:M:162:VAL:HG22	2.02	0.59
1:B:6:ASN:N	1:B:135:LEU:O	2.34	0.59
2:D:135:LEU:HD12	2:D:136:ARG:N	2.15	0.59
1:L:15:GLN:HG2	1:L:24:GLU:OE2	2.02	0.59
1:C:149:VAL:HB	1:C:153:LEU:CD1	2.32	0.59
1:E:83:TRP:HD1	1:E:92:GLY:HA2	1.67	0.59
1:O:128:ILE:HD12	1:O:137:GLN:HB3	1.84	0.59
1:H:124:ARG:HH11	1:H:147:ARG:NH2	1.98	0.59
1:S:164:LYS:HB3	1:S:165:HIS:HD2	1.67	0.59
1:T:60:GLU:CA	1:T:63:ASN:HB2	2.17	0.59
1:T:86:LEU:HB3	1:T:92:GLY:CA	2.31	0.59
1:B:38:PHE:HA	1:B:125:GLY:O	2.02	0.59
1:H:37:LEU:HD11	1:H:72:CYS:HB2	1.84	0.59
1:O:151:GLU:HG3	1:O:155:LEU:CD1	2.32	0.59
1:Q:105:LYS:O	1:Q:106:GLN:HB2	2.01	0.59
1:A:114:VAL:HB	1:A:123:PHE:HB2	1.85	0.59
1:H:127:PHE:CE2	1:H:138:ILE:HG23	2.38	0.59
1:L:65:ARG:NE	1:L:153:LEU:HD11	2.18	0.59
1:L:168:VAL:C	1:L:170:PRO:HD3	2.23	0.59
1:R:45:THR:HG21	1:S:78:TYR:CD1	2.37	0.59
1:A:132:ASN:HD22	1:A:132:ASN:N	1.98	0.59
1:N:83:TRP:CD2	1:N:93:LEU:HG	2.37	0.59
1:Q:116:ASP:HB2	1:Q:123:PHE:CZ	2.38	0.59
1:R:76:SER:HB3	1:R:79:SER:HB2	1.84	0.59
1:B:32:GLY:HA2	1:B:131:PRO:HB3	1.82	0.59
1:E:159:PHE:CD2	1:F:145:VAL:HG21	2.38	0.59
1:L:168:VAL:O	1:L:170:PRO:HD3	2.02	0.59
1:N:12:PHE:CE2	1:N:27:LEU:HD13	2.37	0.59
1:O:128:ILE:O	1:O:135:LEU:HD12	2.02	0.59
1:P:135:LEU:HD21	1:P:138:ILE:HD11	1.84	0.59
1:S:119:ASP:OD2	1:S:121:ASN:HB2	2.03	0.59
1:S:134:ILE:HG22	1:S:136:ARG:HD2	1.84	0.59
1:C:161:PHE:CD1	1:C:165:HIS:HE1	2.21	0.59
1:G:47:VAL:O	1:G:49:PRO:HD2	2.03	0.59
1:H:16:ALA:HB2	1:H:101:LEU:CD1	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:VAL:CA	1:J:1:MET:HA	2.26	0.59
1:M:36:VAL:HA	1:M:127:PHE:O	2.03	0.59
1:M:155:LEU:O	1:M:159:PHE:CD2	2.55	0.59
1:B:36:VAL:HB	1:B:69:VAL:HG22	1.85	0.58
2:D:116:ASP:OD2	2:D:119:ASP:HB2	2.03	0.58
1:R:137:GLN:HE22	1:R:155:LEU:HD22	1.67	0.58
1:A:125:GLY:HA2	1:A:139:THR:O	2.03	0.58
1:B:132:ASN:H	1:B:132:ASN:HD22	1.51	0.58
1:A:53:ILE:HD13	1:A:88:ARG:NH1	2.19	0.58
1:B:126:LEU:HB3	1:B:139:THR:HB	1.84	0.58
1:C:53:ILE:HA	1:C:56:SER:HB3	1.85	0.58
1:F:34:TYR:CD1	1:F:130:ASP:HA	2.38	0.58
1:G:16:ALA:HB2	1:G:101:LEU:CD1	2.34	0.58
1:J:34:TYR:CE2	1:J:160:GLN:HG3	2.38	0.58
1:L:69:VAL:O	1:L:98:ILE:HB	2.02	0.58
1:M:148:SER:H	1:N:154:ARG:NH2	2.01	0.58
1:T:76:SER:HB3	1:T:104:ARG:NH1	2.18	0.58
1:B:41:PRO:O	1:B:121:ASN:HB3	2.03	0.58
1:J:164:LYS:HE3	1:J:165:HIS:NE2	2.19	0.58
1:J:58:GLN:HA	1:J:58:GLN:NE2	2.12	0.58
1:J:83:TRP:HD1	1:J:92:GLY:HA2	1.65	0.58
1:M:96:MET:HG3	1:M:100:LEU:HD11	1.85	0.58
1:A:150:ASP:HA	1:A:153:LEU:CD1	2.34	0.58
1:B:12:PHE:CE1	1:B:27:LEU:HD13	2.38	0.58
1:B:45:THR:HA	1:C:78:TYR:CD2	2.38	0.58
1:B:30:TYR:HE1	1:B:68:GLN:OE1	1.86	0.58
2:D:53:ILE:HA	2:D:96:MET:HE1	1.85	0.58
1:F:87:ASP:OD2	1:F:89:LYS:HB2	2.03	0.58
1:G:130:ASP:HB2	1:G:131:PRO:HD2	1.84	0.58
1:G:65:ARG:NH2	1:G:153:LEU:HD23	2.13	0.58
1:J:5:PRO:O	1:J:7:ARG:HD3	2.03	0.58
1:K:124:ARG:HB3	1:K:147:ARG:NH1	2.19	0.58
1:C:53:ILE:HG22	1:C:57:ASP:OD2	2.04	0.58
2:D:4:LEU:HB2	2:D:7:ARG:CD	2.32	0.58
1:E:11:GLU:OE2	1:E:28:LYS:HE3	2.03	0.58
1:F:23:LYS:NZ	1:Q:23:LYS:HG2	2.19	0.58
1:I:109:SER:HB3	1:I:115:PHE:HB2	1.85	0.58
1:L:128:ILE:HD12	1:L:159:PHE:CD2	2.38	0.58
1:O:18:ILE:HD12	1:O:23:LYS:HE3	1.86	0.58
2:D:13:LYS:HD2	2:D:25:ILE:O	2.04	0.58
1:I:106:GLN:O	1:I:110:LYS:HG3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:VAL:HG21	1:J:167:GLU:HG2	1.84	0.58
1:K:75:ASP:HB2	1:K:80:HIS:HE2	1.68	0.58
1:M:48:CYS:HG	1:N:161:PHE:HE2	1.51	0.58
1:P:62:PHE:CD2	1:P:69:VAL:HG21	2.37	0.58
1:S:62:PHE:O	1:S:67:CYS:HB3	2.03	0.58
1:A:4:LEU:O	1:A:135:LEU:HD23	2.04	0.58
1:F:105:LYS:HB3	1:F:107:GLU:HG3	1.86	0.58
1:M:112:TYR:HB2	1:M:114:VAL:HG22	1.86	0.58
1:O:115:PHE:HA	1:O:122:ALA:HA	1.86	0.58
1:Q:39:PHE:N	1:Q:39:PHE:CD1	2.72	0.58
1:C:124:ARG:HB3	1:C:147:ARG:CZ	2.34	0.58
1:C:123:PHE:CE2	2:D:4:LEU:HD12	2.39	0.58
1:E:31:ARG:CZ	1:E:133:GLY:HA3	2.34	0.58
1:F:59:VAL:HG11	1:F:97:LYS:HB3	1.85	0.58
1:K:22:PHE:HE2	1:K:77:GLN:HB2	1.69	0.58
1:L:7:ARG:HG3	1:L:8:PRO:HD2	1.85	0.58
1:S:153:LEU:H	1:S:153:LEU:HD12	1.69	0.58
1:J:10:PRO:HB2	1:J:112:TYR:CE1	2.38	0.58
1:L:58:GLN:O	1:L:62:PHE:HD1	1.86	0.58
1:M:36:VAL:HG23	1:M:67:CYS:SG	2.43	0.58
1:H:124:ARG:NH1	1:H:147:ARG:HH21	1.99	0.57
1:O:109:SER:HB3	1:O:115:PHE:HB2	1.85	0.57
1:R:86:LEU:HD23	1:R:92:GLY:CA	2.34	0.57
1:T:28:LYS:HD2	1:T:31:ARG:HH21	1.69	0.57
1:A:34:TYR:HB2	1:A:67:CYS:CB	2.32	0.57
1:K:15:GLN:HE21	1:K:22:PHE:HB3	1.68	0.57
1:Q:56:SER:HA	1:Q:98:ILE:HG23	1.84	0.57
1:J:164:LYS:HG2	1:J:165:HIS:HD2	1.69	0.57
1:J:22:PHE:CD1	1:J:22:PHE:N	2.73	0.57
1:L:88:ARG:HA	1:L:92:GLY:O	2.04	0.57
1:P:11:GLU:HA	1:P:11:GLU:OE1	2.04	0.57
1:R:26:CYS:O	1:R:29:ASP:HB2	2.04	0.57
2:D:86:LEU:CG	2:D:92:GLY:HA3	2.32	0.57
1:G:61:GLU:O	1:G:65:ARG:HG3	2.04	0.57
1:P:36:VAL:HA	1:P:127:PHE:O	2.04	0.57
1:Q:14:GLY:HA3	1:Q:101:LEU:HD11	1.86	0.57
1:A:145:VAL:HG21	1:B:159:PHE:CE1	2.39	0.57
1:E:28:LYS:HA	1:E:31:ARG:HG2	1.84	0.57
1:J:42:ALA:HB3	1:J:45:THR:HG21	1.86	0.57
1:S:5:PRO:O	1:T:123:PHE:CZ	2.58	0.57
1:E:38:PHE:HB2	1:E:147:ARG:HH12	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:ASP:OD1	1:G:76:SER:HB3	2.04	0.57
1:K:65:ARG:CZ	1:K:153:LEU:HD11	2.34	0.57
1:N:34:TYR:CD1	1:N:130:ASP:HA	2.40	0.57
1:P:32:GLY:C	1:P:131:PRO:HB3	2.25	0.57
1:P:34:TYR:CD1	1:P:130:ASP:HA	2.39	0.57
1:Q:54:ALA:HB1	1:Q:58:GLN:OE1	2.05	0.57
1:Q:75:ASP:HB3	1:Q:79:SER:HB3	1.84	0.57
1:E:42:ALA:O	1:E:45:THR:HG22	2.04	0.57
1:F:34:TYR:CE2	1:F:160:GLN:HG2	2.39	0.57
1:T:3:LEU:O	1:T:4:LEU:HD12	2.04	0.57
1:C:101:LEU:HD12	1:C:102:ALA:H	1.70	0.57
1:H:105:LYS:HB2	1:H:107:GLU:HG2	1.87	0.57
1:J:117:GLU:HA	1:J:117:GLU:OE1	2.04	0.57
1:J:26:CYS:HB3	1:J:29:ASP:CG	2.25	0.57
1:M:75:ASP:HB2	1:M:80:HIS:NE2	2.20	0.57
1:C:124:ARG:HD2	1:C:145:VAL:O	2.04	0.57
2:D:18:ILE:HG12	2:D:99:PRO:HB3	1.86	0.57
1:K:47:VAL:HG23	1:K:49:PRO:O	2.05	0.57
1:Q:34:TYR:CD1	1:Q:131:PRO:HD3	2.39	0.57
1:R:104:ARG:HG2	1:S:121:ASN:ND2	2.20	0.57
1:S:56:SER:HA	1:S:59:VAL:HG23	1.86	0.57
1:H:105:LYS:HE2	1:H:107:GLU:OE1	2.05	0.57
1:G:144:PRO:HB2	1:H:162:VAL:HG11	1.87	0.57
1:M:116:ASP:HB2	1:M:123:PHE:CE2	2.40	0.57
1:O:128:ILE:HD12	1:O:137:GLN:CB	2.34	0.57
1:P:158:ALA:O	1:P:161:PHE:HB3	2.04	0.57
1:P:65:ARG:NH2	1:P:153:LEU:HD23	2.18	0.57
1:P:88:ARG:HG2	1:P:92:GLY:O	2.05	0.57
1:S:124:ARG:HB3	1:S:147:ARG:NH2	2.19	0.57
1:A:61:GLU:HA	1:A:61:GLU:OE1	2.05	0.56
1:C:86:LEU:HD23	1:C:92:GLY:CA	2.35	0.56
1:G:18:ILE:HG13	1:G:99:PRO:HA	1.86	0.56
1:I:7:ARG:O	1:I:134:ILE:HG23	2.05	0.56
1:N:75:ASP:HB2	1:N:80:HIS:HE2	1.69	0.56
1:R:4:LEU:HB2	1:R:7:ARG:CD	2.35	0.56
1:T:40:TYR:CZ	1:T:73:SER:HB2	2.40	0.56
1:T:86:LEU:C	1:T:92:GLY:HA3	2.25	0.56
2:D:104:ARG:NH1	1:E:74:THR:HG23	2.20	0.56
1:E:61:GLU:OE1	1:E:153:LEU:HD21	2.04	0.56
1:G:123:PHE:CD2	1:H:5:PRO:HD2	2.40	0.56
1:Q:56:SER:HA	1:Q:98:ILE:CG2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HD2	1:B:131:PRO:O	2.06	0.56
1:C:88:ARG:HG2	1:C:92:GLY:O	2.06	0.56
1:M:42:ALA:HA	1:M:75:ASP:OD1	2.06	0.56
1:M:46:PHE:HA	1:M:50:THR:OG1	2.05	0.56
1:N:22:PHE:CE1	1:N:77:GLN:HG2	2.40	0.56
1:O:35:VAL:HG22	1:O:68:GLN:HB3	1.86	0.56
1:A:36:VAL:HB	1:A:69:VAL:HG13	1.87	0.56
1:H:37:LEU:HD13	1:H:70:ILE:HG22	1.88	0.56
1:J:101:LEU:HD12	1:J:102:ALA:H	1.70	0.56
1:A:127:PHE:HE1	1:A:138:ILE:HG23	1.69	0.56
1:E:105:LYS:HE2	1:E:107:GLU:OE1	2.05	0.56
1:K:7:ARG:HG3	1:K:7:ARG:NH1	2.20	0.56
1:N:135:LEU:HD21	1:N:138:ILE:HD11	1.87	0.56
1:O:126:LEU:HD12	1:O:147:ARG:HD2	1.87	0.56
2:D:46:PHE:N	2:D:46:PHE:CD1	2.62	0.56
1:E:158:ALA:O	1:E:162:VAL:HG22	2.05	0.56
1:I:34:TYR:CD1	1:I:131:PRO:HD3	2.41	0.56
1:L:128:ILE:CG1	1:L:137:GLN:HB3	2.28	0.56
1:M:86:LEU:HG	1:M:92:GLY:HA3	1.86	0.56
1:S:137:GLN:HG2	1:S:155:LEU:HD13	1.87	0.56
1:S:80:HIS:HD2	1:S:100:LEU:HB2	1.71	0.56
1:T:25:ILE:HD12	1:T:30:TYR:CE1	2.40	0.56
1:B:159:PHE:HA	1:B:162:VAL:HG22	1.86	0.56
2:D:108:ILE:HD12	2:D:108:ILE:H	1.70	0.56
1:E:96:MET:HA	1:E:96:MET:CE	2.35	0.56
1:N:148:SER:HB3	1:N:151:GLU:HB3	1.87	0.56
1:A:14:GLY:HA3	1:A:101:LEU:HD11	1.87	0.56
1:C:41:PRO:O	1:C:74:THR:HG22	2.06	0.56
1:J:88:ARG:HA	1:J:92:GLY:N	2.20	0.56
1:K:106:GLN:NE2	1:K:115:PHE:CE2	2.74	0.56
1:K:128:ILE:HB	1:K:137:GLN:HB3	1.88	0.56
1:N:60:GLU:HA	1:N:63:ASN:OD1	2.05	0.56
1:P:30:TYR:HE2	1:P:68:GLN:HG2	1.67	0.56
1:S:1:MET:HG2	1:T:1:MET:O	2.06	0.56
1:J:126:LEU:HD12	1:J:147:ARG:NH1	2.20	0.56
1:M:128:ILE:HD12	1:M:159:PHE:CE2	2.41	0.56
1:R:143:LYS:HB2	1:R:144:PRO:HD3	1.86	0.56
1:F:157:ASP:O	1:F:161:PHE:HB2	2.06	0.56
1:J:48:CYS:CB	1:J:49:PRO:HD2	2.35	0.56
1:L:38:PHE:HB2	1:L:147:ARG:NH2	2.20	0.56
1:N:58:GLN:OE1	1:N:149:VAL:HG11	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:30:TYR:CD2	1:P:68:GLN:HG2	2.41	0.56
1:P:88:ARG:HG2	1:P:93:LEU:HA	1.86	0.56
1:S:105:LYS:O	1:S:106:GLN:HB2	2.04	0.56
1:T:81:LEU:HD12	1:T:85:ASN:HD21	1.69	0.56
1:A:83:TRP:O	1:A:83:TRP:CD1	2.59	0.56
2:D:86:LEU:HG	2:D:92:GLY:CA	2.35	0.56
1:H:105:LYS:HE3	1:I:118:GLU:O	2.06	0.56
1:N:26:CYS:SG	1:N:28:LYS:HB2	2.46	0.56
1:P:88:ARG:HA	1:P:92:GLY:O	2.06	0.56
1:S:38:PHE:CD1	1:S:38:PHE:N	2.74	0.56
1:A:136:ARG:HE	1:A:136:ARG:HA	1.71	0.55
1:A:116:ASP:HB3	1:A:119:ASP:HB2	1.88	0.55
1:A:132:ASN:ND2	1:A:132:ASN:H	1.97	0.55
1:B:45:THR:HG23	1:B:46:PHE:CE1	2.42	0.55
2:D:65:ARG:CD	2:D:156:LEU:HD23	2.35	0.55
1:G:47:VAL:HB	1:G:49:PRO:HD3	1.87	0.55
1:H:12:PHE:CE2	1:H:27:LEU:HD13	2.41	0.55
1:I:12:PHE:HB2	1:I:108:ILE:HG12	1.88	0.55
1:M:4:LEU:HD13	1:N:123:PHE:CE2	2.41	0.55
1:M:86:LEU:HD12	1:M:87:ASP:H	1.71	0.55
1:O:123:PHE:CE2	1:P:4:LEU:HB3	2.41	0.55
1:P:65:ARG:CZ	1:P:157:ASP:HB3	2.36	0.55
1:P:65:ARG:HD3	1:P:157:ASP:HA	1.87	0.55
1:R:71:ALA:HB3	1:R:100:LEU:HA	1.87	0.55
1:T:76:SER:OG	1:T:79:SER:HB2	2.06	0.55
1:I:35:VAL:HG13	1:I:68:GLN:O	2.05	0.55
1:L:72:CYS:HB2	1:L:101:LEU:HB3	1.88	0.55
1:O:137:GLN:HE22	1:P:139:THR:HG22	1.71	0.55
1:Q:72:CYS:HA	1:Q:101:LEU:O	2.06	0.55
1:S:126:LEU:HD12	1:S:147:ARG:HG2	1.87	0.55
1:A:28:LYS:CE	1:A:31:ARG:HE	2.14	0.55
1:L:40:TYR:CZ	1:L:73:SER:HB2	2.41	0.55
1:R:-2:GLY:O	1:R:-1:SER:HB3	2.05	0.55
1:G:43:ASP:HB3	1:G:44:PHE:CD2	2.42	0.55
1:R:150:ASP:HA	1:R:153:LEU:HD22	1.87	0.55
2:D:36:VAL:HG23	2:D:67:CYS:SG	2.47	0.55
1:J:141:ASN:ND2	1:J:147:ARG:HG3	2.22	0.55
1:J:70:ILE:HG12	1:J:99:PRO:HB2	1.87	0.55
1:J:78:TYR:CD1	1:J:78:TYR:N	2.74	0.55
1:M:40:TYR:O	1:M:122:ALA:HB3	2.07	0.55
1:M:39:PHE:HE2	1:M:72:CYS:HG	1.53	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:167:GLU:CD	1:S:167:GLU:H	2.10	0.55
1:G:18:ILE:HD12	1:G:18:ILE:N	2.22	0.55
1:G:38:PHE:O	1:G:38:PHE:CD1	2.60	0.55
1:G:65:ARG:CD	1:G:156:LEU:HD23	2.37	0.55
1:N:34:TYR:CE1	1:N:130:ASP:HA	2.42	0.55
1:P:37:LEU:HB3	1:P:127:PHE:HB2	1.88	0.55
1:S:15:GLN:HG2	1:S:24:GLU:CG	2.12	0.55
1:H:89:LYS:O	1:H:89:LYS:HD3	2.06	0.55
1:M:136:ARG:HB3	1:M:159:PHE:CE1	2.42	0.55
1:M:84:ASP:OD1	1:M:96:MET:HG2	2.06	0.55
1:Q:115:PHE:HE1	1:Q:117:GLU:HA	1.71	0.55
1:G:69:VAL:O	1:G:99:PRO:HD2	2.06	0.55
1:I:59:VAL:HG23	1:I:60:GLU:H	1.71	0.55
1:P:136:ARG:HB3	1:P:159:PHE:CE2	2.42	0.55
1:P:13:LYS:HG2	1:P:26:CYS:HB3	1.89	0.55
1:Q:16:ALA:O	1:Q:22:PHE:HA	2.07	0.55
1:R:84:ASP:O	1:R:94:GLY:O	2.25	0.55
1:T:54:ALA:O	1:T:57:ASP:HB2	2.07	0.55
1:C:103:ASP:HA	1:C:108:ILE:HD12	1.89	0.55
2:D:14:GLY:HA3	2:D:101:LEU:CD1	2.34	0.55
1:J:43:ASP:HA	1:J:83:TRP:CZ3	2.42	0.55
1:L:53:ILE:HD13	1:L:88:ARG:HG2	1.89	0.55
1:M:12:PHE:CZ	1:M:27:LEU:HD13	2.42	0.55
1:N:55:PHE:HZ	1:N:147:ARG:O	1.90	0.55
1:P:34:TYR:CE2	1:P:160:GLN:HG2	2.43	0.55
1:Q:142:ASP:OD2	1:Q:144:PRO:HD2	2.07	0.55
1:E:128:ILE:HG22	1:E:136:ARG:HB2	1.90	0.54
1:F:105:LYS:HD2	1:F:105:LYS:H	1.73	0.54
1:J:88:ARG:HG2	1:J:92:GLY:O	2.07	0.54
1:K:88:ARG:HA	1:K:92:GLY:O	2.07	0.54
1:M:130:ASP:OD2	1:M:132:ASN:HB2	2.07	0.54
1:A:83:TRP:O	1:A:83:TRP:HD1	1.89	0.54
1:C:13:LYS:NZ	1:C:24:GLU:HG2	2.21	0.54
1:F:164:LYS:HD3	1:F:165:HIS:CE1	2.42	0.54
1:H:151:GLU:OE2	1:H:155:LEU:HG	2.07	0.54
1:L:24:GLU:HA	1:L:24:GLU:OE1	2.07	0.54
1:Q:157:ASP:O	1:Q:160:GLN:HB2	2.07	0.54
1:Q:88:ARG:HA	1:Q:92:GLY:O	2.07	0.54
1:A:109:SER:OG	1:A:122:ALA:HB2	2.07	0.54
1:A:135:LEU:HD12	1:A:136:ARG:N	2.22	0.54
1:C:80:HIS:CD2	1:C:100:LEU:HB3	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:SER:CA	1:E:102:ALA:HB1	2.34	0.54
1:E:22:PHE:O	1:E:23:LYS:HD2	2.08	0.54
1:C:86:LEU:HD11	1:C:90:SER:CB	2.37	0.54
2:D:105:LYS:H	2:D:105:LYS:HD3	1.72	0.54
1:L:34:TYR:HA	1:L:129:ILE:O	2.06	0.54
1:O:86:LEU:O	1:O:92:GLY:HA3	2.08	0.54
1:Q:80:HIS:HD2	1:Q:100:LEU:HB3	1.72	0.54
1:B:26:CYS:HB3	1:B:29:ASP:OD1	2.07	0.54
1:B:74:THR:HG22	1:B:106:GLN:HG2	1.88	0.54
2:D:105:LYS:O	2:D:106:GLN:HB2	2.07	0.54
1:E:22:PHE:C	1:E:23:LYS:HD2	2.28	0.54
1:F:80:HIS:CE1	1:F:102:ALA:CB	2.90	0.54
1:I:55:PHE:HE2	1:I:147:ARG:HE	1.56	0.54
1:E:167:GLU:OE1	1:E:168:VAL:N	2.40	0.54
1:F:43:ASP:O	1:F:44:PHE:HB2	2.07	0.54
1:G:143:LYS:N	1:G:144:PRO:HD2	2.23	0.54
1:H:10:PRO:O	1:H:27:LEU:HD22	2.08	0.54
1:M:18:ILE:O	1:M:19:ASN:HB3	2.06	0.54
1:S:159:PHE:O	1:S:162:VAL:HG12	2.08	0.54
2:D:86:LEU:O	2:D:94:GLY:N	2.35	0.54
1:E:159:PHE:CE2	1:F:145:VAL:HG21	2.43	0.54
1:F:130:ASP:HB2	1:F:131:PRO:CD	2.38	0.54
1:H:160:GLN:O	1:H:163:GLU:HG2	2.08	0.54
1:H:22:PHE:HE1	1:H:77:GLN:HB2	1.70	0.54
1:K:119:ASP:HB3	1:K:121:ASN:ND2	2.22	0.54
1:L:104:ARG:HB3	1:M:120:GLY:HA3	1.88	0.54
1:C:34:TYR:HD1	1:C:130:ASP:HA	1.73	0.54
2:D:75:ASP:HB2	2:D:80:HIS:CE1	2.43	0.54
1:G:76:SER:O	1:G:79:SER:HB3	2.08	0.54
1:K:105:LYS:C	1:K:106:GLN:HG3	2.28	0.54
1:Q:18:ILE:HB	1:Q:23:LYS:HD3	1.89	0.54
1:S:74:THR:OG1	1:S:106:GLN:HG2	2.07	0.54
1:J:164:LYS:HG2	1:J:165:HIS:CD2	2.42	0.54
1:O:17:VAL:O	1:O:99:PRO:HA	2.08	0.54
1:O:4:LEU:HD12	1:O:4:LEU:N	2.22	0.54
1:P:107:GLU:HG3	1:P:108:ILE:HG13	1.90	0.54
1:Q:2:VAL:O	1:Q:4:LEU:HD23	2.07	0.54
1:Q:73:SER:OG	1:Q:80:HIS:HE1	1.91	0.54
1:A:157:ASP:HA	1:A:160:GLN:OE1	2.07	0.54
1:A:69:VAL:O	1:A:98:ILE:HD13	2.07	0.54
1:F:127:PHE:HE1	1:F:138:ILE:HG23	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:103:ASP:HB2	1:R:108:ILE:HD12	1.89	0.54
1:R:28:LYS:O	1:R:31:ARG:HG2	2.08	0.54
1:B:15:GLN:O	1:B:101:LEU:HD12	2.08	0.53
1:R:83:TRP:CE3	1:R:93:LEU:HD11	2.43	0.53
1:J:164:LYS:HD2	1:S:164:LYS:HG3	1.90	0.53
1:C:137:GLN:HG2	2:D:141:ASN:OD1	2.08	0.53
1:J:106:GLN:HA	1:J:109:SER:OG	2.07	0.53
1:J:36:VAL:HG12	1:J:69:VAL:HG13	1.91	0.53
1:K:72:CYS:HA	1:K:101:LEU:O	2.08	0.53
1:K:40:TYR:HB2	1:K:41:PRO:CD	2.38	0.53
1:P:38:PHE:HA	1:P:125:GLY:O	2.08	0.53
1:R:115:PHE:HA	1:R:122:ALA:HA	1.89	0.53
1:R:6:ASN:HB3	1:R:7:ARG:HD2	1.89	0.53
1:J:112:TYR:HD2	1:J:127:PHE:CD2	2.26	0.53
1:Q:38:PHE:HB3	1:Q:126:LEU:HD12	1.90	0.53
1:T:16:ALA:HB3	1:T:23:LYS:O	2.09	0.53
1:A:98:ILE:HG23	1:A:99:PRO:HD2	1.90	0.53
1:F:105:LYS:O	1:F:106:GLN:HB2	2.08	0.53
1:I:59:VAL:HG11	1:I:97:LYS:HB3	1.91	0.53
1:J:48:CYS:CB	1:J:49:PRO:CD	2.86	0.53
1:P:17:VAL:HB	1:P:100:LEU:HB2	1.89	0.53
1:P:128:ILE:HG21	1:P:159:PHE:CD2	2.43	0.53
1:B:26:CYS:O	1:B:29:ASP:HB2	2.09	0.53
2:D:130:ASP:HB3	2:D:136:ARG:HD3	1.89	0.53
2:D:39:PHE:O	2:D:124:ARG:HG3	2.08	0.53
1:E:145:VAL:HG21	1:F:159:PHE:CZ	2.44	0.53
1:G:71:ALA:HB3	1:G:100:LEU:HD23	1.89	0.53
1:H:4:LEU:HD12	1:H:7:ARG:CZ	2.38	0.53
1:H:53:ILE:HA	1:H:96:MET:SD	2.49	0.53
1:K:51:GLU:O	1:K:54:ALA:HB3	2.09	0.53
1:M:18:ILE:HG12	1:M:99:PRO:HA	1.91	0.53
1:O:17:VAL:HB	1:O:100:LEU:HB2	1.90	0.53
1:O:56:SER:HB3	1:O:96:MET:HE1	1.89	0.53
1:R:86:LEU:HD23	1:R:92:GLY:N	2.23	0.53
1:S:168:VAL:O	1:S:168:VAL:HG12	2.08	0.53
1:T:75:ASP:HB2	1:T:80:HIS:CE1	2.41	0.53
1:C:141:ASN:HD22	1:C:145:VAL:HG12	1.72	0.53
1:F:139:THR:HG22	1:F:141:ASN:HD21	1.73	0.53
1:O:141:ASN:ND2	1:O:147:ARG:HG3	2.23	0.53
1:S:72:CYS:HA	1:S:101:LEU:O	2.09	0.53
1:A:59:VAL:O	1:A:62:PHE:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:VAL:HG21	1:L:97:LYS:CG	2.39	0.53
1:P:42:ALA:O	1:P:45:THR:HG23	2.08	0.53
1:R:13:LYS:HG3	1:R:24:GLU:OE2	2.09	0.53
1:A:75:ASP:CB	1:A:80:HIS:HE1	2.19	0.53
1:G:54:ALA:O	1:G:58:GLN:HG3	2.08	0.53
1:I:51:GLU:OE2	1:I:146:GLY:HA2	2.09	0.53
1:R:71:ALA:O	1:R:101:LEU:HB3	2.09	0.53
1:T:2:VAL:HG12	1:T:4:LEU:HD13	1.91	0.53
1:A:103:ASP:HB2	1:A:108:ILE:HD12	1.90	0.53
1:E:53:ILE:O	1:E:56:SER:HB3	2.09	0.53
1:F:151:GLU:OE1	1:F:151:GLU:HA	2.09	0.53
1:G:108:ILE:O	1:G:112:TYR:HD1	1.91	0.53
1:J:125:GLY:CA	1:J:140:ILE:HA	2.31	0.53
1:R:59:VAL:HA	1:R:62:PHE:CD2	2.38	0.53
1:G:159:PHE:CE1	1:H:142:ASP:HB2	2.42	0.53
1:J:40:TYR:HE1	1:J:71:ALA:HB1	1.74	0.53
1:L:40:TYR:CE1	1:L:73:SER:HB2	2.44	0.53
1:O:116:ASP:HB2	1:P:7:ARG:HH12	1.74	0.53
1:P:124:ARG:HB3	1:P:147:ARG:NH1	2.24	0.53
1:R:4:LEU:HD12	1:R:7:ARG:NE	2.16	0.53
1:E:123:PHE:HE2	1:F:4:LEU:CD2	2.19	0.52
1:F:68:GLN:OE1	1:F:99:PRO:HD3	2.10	0.52
1:H:80:HIS:CE1	1:H:102:ALA:HB2	2.44	0.52
1:I:74:THR:HA	1:I:103:ASP:O	2.08	0.52
1:P:69:VAL:HG12	1:P:98:ILE:HD12	1.91	0.52
1:S:44:PHE:CD1	1:S:83:TRP:CD1	2.96	0.52
1:B:40:TYR:HB2	1:B:46:PHE:HZ	1.75	0.52
1:F:161:PHE:CE1	1:F:165:HIS:HB2	2.44	0.52
1:G:123:PHE:CE2	1:H:5:PRO:HD2	2.45	0.52
1:L:130:ASP:OD2	1:L:134:ILE:HB	2.09	0.52
1:O:60:GLU:OE1	1:O:60:GLU:HA	2.09	0.52
1:Q:34:TYR:OH	1:Q:160:GLN:HG2	2.09	0.52
1:S:41:PRO:HD2	1:S:124:ARG:HH11	1.73	0.52
1:S:125:GLY:O	1:S:147:ARG:NH1	2.42	0.52
1:T:31:ARG:HH12	1:T:133:GLY:CA	2.22	0.52
1:E:116:ASP:O	1:E:119:ASP:O	2.26	0.52
1:F:34:TYR:CZ	1:F:131:PRO:HD3	2.45	0.52
1:F:80:HIS:N	1:F:80:HIS:CD2	2.76	0.52
1:G:151:GLU:OE1	1:H:151:GLU:HB2	2.10	0.52
1:J:126:LEU:N	1:J:139:THR:O	2.37	0.52
1:L:115:PHE:CZ	1:L:120:GLY:HA2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:68:GLN:HA	1:P:68:GLN:OE1	2.10	0.52
1:R:55:PHE:CD1	1:R:149:VAL:HG22	2.44	0.52
2:D:101:LEU:HD12	2:D:102:ALA:N	2.24	0.52
2:D:161:PHE:O	2:D:165:HIS:HB2	2.10	0.52
1:G:87:ASP:OD1	1:G:90:SER:HB2	2.09	0.52
1:H:15:GLN:O	1:H:101:LEU:HD12	2.09	0.52
1:O:40:TYR:HB2	1:O:41:PRO:HD2	1.91	0.52
1:R:3:LEU:CD2	1:R:10:PRO:HG2	2.40	0.52
1:C:103:ASP:OD2	1:C:109:SER:HB2	2.10	0.52
1:C:43:ASP:O	1:C:44:PHE:HB2	2.09	0.52
1:G:6:ASN:O	1:G:7:ARG:HD2	2.10	0.52
1:M:4:LEU:HB3	1:M:5:PRO:HD2	1.91	0.52
1:M:9:ALA:HB2	1:M:135:LEU:HB2	1.91	0.52
1:O:155:LEU:O	1:O:158:ALA:HB3	2.10	0.52
1:Q:68:GLN:HA	1:Q:68:GLN:OE1	2.10	0.52
1:B:149:VAL:O	1:B:153:LEU:HD13	2.10	0.52
1:K:55:PHE:HE2	1:K:152:THR:OG1	1.93	0.52
1:L:86:LEU:HD23	1:L:92:GLY:N	2.24	0.52
1:B:80:HIS:CE1	1:B:101:LEU:O	2.62	0.52
1:C:87:ASP:OD2	1:C:89:LYS:HB2	2.10	0.52
1:K:154:ARG:NH2	1:L:148:SER:HB2	2.24	0.52
1:L:58:GLN:OE1	1:L:58:GLN:HA	2.10	0.52
1:M:108:ILE:O	1:M:111:ALA:HB3	2.10	0.52
1:N:38:PHE:CE1	1:N:71:ALA:HB2	2.44	0.52
1:R:48:CYS:HB3	1:R:50:THR:HA	1.92	0.52
1:B:39:PHE:HE1	1:B:127:PHE:CE2	2.27	0.52
1:C:155:LEU:O	1:C:159:PHE:CD1	2.61	0.52
2:D:43:ASP:HB3	2:D:83:TRP:CE3	2.45	0.52
1:E:83:TRP:CD1	1:E:92:GLY:HA2	2.44	0.52
1:K:68:GLN:NE2	1:K:68:GLN:HA	2.24	0.52
1:O:76:SER:O	1:O:80:HIS:HD2	1.92	0.52
1:Q:75:ASP:HB3	1:Q:79:SER:HB2	1.91	0.52
1:S:3:LEU:O	1:S:138:ILE:HD13	2.09	0.52
1:T:137:GLN:HB2	1:T:159:PHE:CE2	2.45	0.52
1:I:143:LYS:HB2	1:I:144:PRO:HD3	1.90	0.52
1:I:55:PHE:HE1	1:I:149:VAL:HG22	1.71	0.52
1:I:66:ASN:O	1:I:66:ASN:CG	2.48	0.52
1:J:55:PHE:HD1	1:J:62:PHE:HZ	1.58	0.52
1:N:39:PHE:CE2	1:N:72:CYS:HB3	2.45	0.52
1:N:5:PRO:HG3	1:N:138:ILE:HD12	1.91	0.52
1:O:167:GLU:OE1	1:P:47:VAL:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:126:LEU:HD22	1:T:147:ARG:HD2	1.92	0.52
1:T:33:LYS:HA	1:T:66:ASN:ND2	2.25	0.52
1:T:84:ASP:HA	1:T:93:LEU:HB2	1.91	0.52
1:A:135:LEU:HD12	1:A:136:ARG:H	1.74	0.52
2:D:10:PRO:HD2	2:D:112:TYR:CZ	2.45	0.52
1:E:171:VAL:HG12	1:E:172:ASN:H	1.74	0.52
1:G:72:CYS:HA	1:G:101:LEU:O	2.10	0.52
1:L:72:CYS:CB	1:L:101:LEU:HB3	2.40	0.52
1:T:136:ARG:HD2	1:T:159:PHE:CG	2.44	0.52
1:B:155:LEU:O	1:B:159:PHE:CD2	2.63	0.51
1:B:38:PHE:HB2	1:B:147:ARG:HH22	1.76	0.51
1:F:86:LEU:HG	1:F:92:GLY:HA3	1.91	0.51
1:G:16:ALA:HB2	1:G:101:LEU:HA	1.92	0.51
1:G:69:VAL:HG11	1:G:98:ILE:HD13	1.92	0.51
1:K:124:ARG:HH11	1:K:147:ARG:HH22	1.58	0.51
1:M:151:GLU:O	1:M:154:ARG:HB3	2.10	0.51
1:M:48:CYS:N	1:M:49:PRO:CD	2.73	0.51
1:O:18:ILE:HD12	1:O:23:LYS:CE	2.40	0.51
1:T:2:VAL:CG1	1:T:4:LEU:HD13	2.41	0.51
1:T:69:VAL:HG11	1:T:98:ILE:HD13	1.91	0.51
1:F:18:ILE:HG13	1:F:23:LYS:CB	2.40	0.51
1:I:134:ILE:CG2	1:I:136:ARG:HH12	2.23	0.51
1:J:130:ASP:HB2	1:J:131:PRO:HD2	1.90	0.51
1:J:151:GLU:O	1:J:155:LEU:HG	2.10	0.51
1:M:18:ILE:HD11	1:M:99:PRO:HB3	1.91	0.51
1:Q:39:PHE:O	1:Q:147:ARG:NH1	2.44	0.51
1:B:158:ALA:O	1:B:162:VAL:HG13	2.10	0.51
1:C:124:ARG:HH11	1:C:147:ARG:HH21	1.53	0.51
1:M:141:ASN:HD22	1:M:145:VAL:HG12	1.74	0.51
1:R:38:PHE:HE2	1:R:69:VAL:HG12	1.75	0.51
1:R:68:GLN:NE2	1:R:68:GLN:HA	2.25	0.51
1:B:45:THR:HG23	1:B:46:PHE:CD1	2.45	0.51
1:E:171:VAL:HG12	1:E:172:ASN:N	2.26	0.51
1:E:123:PHE:HZ	1:F:6:ASN:HB2	1.74	0.51
1:G:49:PRO:HB3	1:G:52:ILE:HB	1.93	0.51
1:K:142:ASP:OD1	1:K:143:LYS:N	2.44	0.51
1:Q:50:THR:HG23	1:Q:51:GLU:N	2.25	0.51
1:S:25:ILE:HD11	1:S:101:LEU:HD13	1.92	0.51
1:S:9:ALA:HB2	1:S:135:LEU:HB2	1.91	0.51
1:T:136:ARG:HD2	1:T:159:PHE:CD1	2.45	0.51
1:A:119:ASP:HB3	1:A:143:LYS:NZ	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:HB2	1:B:108:ILE:HD12	1.93	0.51
1:B:128:ILE:HD11	1:B:152:THR:HG23	1.92	0.51
1:B:143:LYS:HD3	1:B:143:LYS:H	1.76	0.51
1:C:130:ASP:HB2	1:C:131:PRO:HD2	1.91	0.51
2:D:71:ALA:HB3	2:D:100:LEU:HD23	1.93	0.51
1:G:158:ALA:O	1:G:162:VAL:HG23	2.10	0.51
1:S:12:PHE:CD1	1:S:12:PHE:O	2.63	0.51
1:T:151:GLU:O	1:T:155:LEU:HG	2.11	0.51
1:T:84:ASP:CA	1:T:93:LEU:HD12	2.41	0.51
1:A:142:ASP:HB2	1:A:145:VAL:HG23	1.93	0.51
1:A:83:TRP:NE1	1:A:93:LEU:HG	2.26	0.51
2:D:47:VAL:HG12	2:D:48:CYS:N	2.17	0.51
1:E:32:GLY:HA2	1:E:131:PRO:HB3	1.92	0.51
1:J:132:ASN:HB2	1:J:134:ILE:HG12	1.92	0.51
1:K:26:CYS:O	1:K:29:ASP:HB2	2.10	0.51
1:L:65:ARG:CG	1:L:160:GLN:HE22	2.14	0.51
1:A:130:ASP:HB2	1:A:131:PRO:HD2	1.93	0.51
1:B:39:PHE:CE1	1:B:127:PHE:HE2	2.28	0.51
1:I:134:ILE:HG21	1:I:136:ARG:HH12	1.76	0.51
1:M:151:GLU:HG2	1:N:151:GLU:OE1	2.10	0.51
1:P:75:ASP:HB2	1:P:80:HIS:CE1	2.46	0.51
1:Q:124:ARG:HB2	1:Q:141:ASN:O	2.10	0.51
1:R:83:TRP:CD1	1:R:92:GLY:HA2	2.46	0.51
1:T:40:TYR:CZ	1:T:73:SER:CB	2.94	0.51
1:A:55:PHE:CD1	1:A:149:VAL:HG22	2.46	0.51
1:B:17:VAL:HB	1:B:100:LEU:HB2	1.93	0.51
1:C:123:PHE:HD1	1:C:143:LYS:HG3	1.76	0.51
1:C:53:ILE:HG12	1:C:96:MET:CE	2.41	0.51
2:D:124:ARG:HG2	2:D:147:ARG:NH1	2.18	0.51
1:E:96:MET:O	1:E:97:LYS:HB2	2.10	0.51
1:F:110:LYS:HG2	1:F:115:PHE:CG	2.46	0.51
1:I:56:SER:HA	1:I:98:ILE:HG23	1.93	0.51
1:J:150:ASP:HA	1:J:153:LEU:CD2	2.37	0.51
1:K:151:GLU:OE1	1:K:151:GLU:HA	2.11	0.51
1:L:56:SER:O	1:L:59:VAL:HG22	2.11	0.51
1:O:55:PHE:HB3	1:O:98:ILE:CD1	2.40	0.51
1:P:160:GLN:HA	1:P:163:GLU:HB3	1.91	0.51
1:B:143:LYS:N	1:B:143:LYS:HD3	2.26	0.51
1:L:6:ASN:HA	1:L:135:LEU:O	2.11	0.51
1:N:124:ARG:HB3	1:N:147:ARG:NH1	2.25	0.51
1:O:4:LEU:HD23	1:P:123:PHE:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:158:ALA:HA	1:P:161:PHE:HB3	1.92	0.51
1:R:116:ASP:OD2	1:R:119:ASP:HB2	2.11	0.51
1:B:75:ASP:HB3	1:B:79:SER:HB3	1.92	0.51
1:B:83:TRP:HD1	1:B:92:GLY:HA2	1.72	0.51
1:E:53:ILE:CD1	1:E:88:ARG:HD2	2.41	0.51
1:K:72:CYS:SG	1:K:101:LEU:HG	2.51	0.51
1:M:126:LEU:HD11	1:M:152:THR:OG1	2.11	0.51
1:R:34:TYR:HB2	1:R:67:CYS:HA	1.93	0.51
1:C:86:LEU:HD23	1:C:92:GLY:HA2	1.93	0.50
1:H:168:VAL:CG1	1:H:169:CYS:H	2.22	0.50
1:L:116:ASP:N	1:L:121:ASN:O	2.44	0.50
1:L:73:SER:HB3	1:L:80:HIS:CE1	2.46	0.50
1:Q:112:TYR:HB2	1:Q:114:VAL:HG22	1.93	0.50
1:T:43:ASP:HA	1:T:83:TRP:CZ3	2.46	0.50
1:G:105:LYS:O	1:G:106:GLN:HB2	2.11	0.50
1:N:15:GLN:HG2	1:N:77:GLN:OE1	2.11	0.50
1:N:76:SER:O	1:N:80:HIS:HD2	1.95	0.50
1:R:38:PHE:O	1:R:72:CYS:HB3	2.11	0.50
1:H:23:LYS:HG3	1:S:23:LYS:HG3	1.93	0.50
1:T:11:GLU:OE1	1:T:11:GLU:HA	2.10	0.50
1:T:42:ALA:HB3	1:T:45:THR:CG2	2.41	0.50
1:A:13:LYS:NZ	1:A:26:CYS:HB2	2.26	0.50
2:D:39:PHE:HE1	2:D:127:PHE:CE1	2.30	0.50
1:F:51:GLU:HB3	1:F:147:ARG:HH21	1.75	0.50
1:L:104:ARG:O	1:M:120:GLY:HA3	2.12	0.50
1:Q:76:SER:H	1:Q:104:ARG:HH11	1.59	0.50
1:R:109:SER:O	1:R:114:VAL:HG22	2.11	0.50
1:T:124:ARG:HB3	1:T:147:ARG:NH2	2.26	0.50
2:D:128:ILE:HG22	2:D:136:ARG:HB2	1.93	0.50
1:G:45:THR:HG23	1:G:47:VAL:HG22	1.93	0.50
1:I:36:VAL:HG22	1:I:128:ILE:HG23	1.93	0.50
1:L:143:LYS:HB2	1:L:144:PRO:HD3	1.94	0.50
1:L:65:ARG:CD	1:L:153:LEU:HD11	2.41	0.50
1:L:39:PHE:HB2	1:L:123:PHE:O	2.12	0.50
1:M:18:ILE:HD12	1:M:23:LYS:HD3	1.94	0.50
1:M:18:ILE:HD12	1:M:23:LYS:CD	2.41	0.50
1:O:162:VAL:O	1:O:166:GLY:CA	2.59	0.50
1:O:26:CYS:O	1:O:29:ASP:HB2	2.12	0.50
1:O:32:GLY:O	1:O:33:LYS:CG	2.60	0.50
1:S:145:VAL:HG21	1:T:159:PHE:CD1	2.45	0.50
1:S:38:PHE:HB2	1:S:125:GLY:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:81:LEU:CD1	1:T:85:ASN:HD21	2.24	0.50
1:F:109:SER:HB3	1:F:114:VAL:HG23	1.93	0.50
1:F:104:ARG:HH22	1:G:75:ASP:HA	1.76	0.50
1:M:30:TYR:O	1:M:31:ARG:HD3	2.10	0.50
1:N:154:ARG:NH2	1:N:155:LEU:HD21	2.27	0.50
1:Q:38:PHE:HA	1:Q:126:LEU:HA	1.93	0.50
1:Q:50:THR:O	1:Q:53:ILE:HG13	2.12	0.50
1:R:38:PHE:HB2	1:R:125:GLY:O	2.11	0.50
1:S:150:ASP:N	1:S:150:ASP:OD1	2.45	0.50
1:S:42:ALA:HA	1:S:75:ASP:OD2	2.11	0.50
1:A:84:ASP:OD1	1:A:96:MET:HB2	2.11	0.50
1:B:105:LYS:HD2	1:C:118:GLU:O	2.11	0.50
2:D:55:PHE:HD2	2:D:62:PHE:CZ	2.29	0.50
1:E:8:PRO:HA	1:E:134:ILE:HA	1.94	0.50
1:G:171:VAL:HB	1:H:48:CYS:SG	2.51	0.50
1:I:2:VAL:HG23	1:J:1:MET:H1	1.77	0.50
1:J:83:TRP:CG	1:J:93:LEU:HG	2.47	0.50
1:M:35:VAL:HB	1:M:129:ILE:HB	1.94	0.50
1:T:40:TYR:CD2	1:T:42:ALA:O	2.64	0.50
2:D:108:ILE:HD12	2:D:108:ILE:N	2.27	0.50
1:K:123:PHE:CZ	1:K:143:LYS:HE2	2.47	0.50
1:O:141:ASN:HD22	1:O:147:ARG:HG3	1.77	0.50
1:O:137:GLN:NE2	1:P:139:THR:HG22	2.26	0.50
1:Q:124:ARG:HG2	1:Q:143:LYS:HA	1.93	0.50
1:Q:16:ALA:HB2	1:Q:101:LEU:HA	1.94	0.50
1:R:4:LEU:CD1	1:R:7:ARG:HE	2.20	0.50
1:A:68:GLN:OE1	1:A:98:ILE:HG12	2.12	0.50
1:B:77:GLN:H	1:B:77:GLN:CD	2.15	0.50
1:C:86:LEU:HD11	1:C:90:SER:HB2	1.93	0.50
1:C:97:LYS:HD3	1:C:97:LYS:N	2.26	0.50
2:D:128:ILE:O	2:D:136:ARG:N	2.43	0.50
2:D:37:LEU:HD13	2:D:70:ILE:HB	1.93	0.50
1:E:128:ILE:HB	1:E:137:GLN:HG3	1.93	0.50
1:J:76:SER:HB3	1:J:104:ARG:HE	1.76	0.50
1:L:38:PHE:HB2	1:L:147:ARG:NH1	2.26	0.50
1:M:76:SER:O	1:M:80:HIS:HD2	1.95	0.50
1:N:34:TYR:HB3	1:N:67:CYS:SG	2.52	0.50
1:Q:153:LEU:H	1:Q:153:LEU:HD12	1.76	0.50
1:T:51:GLU:OE2	1:T:147:ARG:NE	2.45	0.50
2:D:126:LEU:HB3	2:D:139:THR:HG22	1.94	0.50
1:F:20:GLY:O	1:F:21:GLU:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ILE:HA	1:G:134:ILE:O	2.12	0.50
1:H:7:ARG:CD	1:H:7:ARG:N	2.75	0.50
1:I:161:PHE:CD2	1:I:166:GLY:HA2	2.47	0.50
1:M:86:LEU:HD11	1:M:90:SER:HB2	1.93	0.50
1:Q:17:VAL:HG12	1:Q:21:GLU:N	2.27	0.50
1:F:23:LYS:HZ1	1:Q:23:LYS:HG2	1.77	0.50
1:S:58:GLN:HA	1:S:58:GLN:OE1	2.12	0.50
1:S:96:MET:HE2	1:S:96:MET:HA	1.92	0.50
1:C:117:GLU:HA	1:C:117:GLU:OE1	2.12	0.49
1:C:153:LEU:O	1:C:156:LEU:HB3	2.12	0.49
1:H:7:ARG:HD2	1:H:7:ARG:N	2.27	0.49
1:I:40:TYR:CE1	1:I:71:ALA:HB1	2.47	0.49
1:I:87:ASP:HB2	1:I:90:SER:OG	2.11	0.49
1:J:97:LYS:HA	1:J:97:LYS:HE2	1.94	0.49
1:P:40:TYR:CG	1:P:52:ILE:HD11	2.47	0.49
1:P:44:PHE:CD1	1:P:83:TRP:CD1	2.99	0.49
1:S:38:PHE:N	1:S:38:PHE:HD1	2.08	0.49
1:S:86:LEU:HB3	1:S:92:GLY:CA	2.42	0.49
1:T:106:GLN:HG2	1:T:115:PHE:CE1	2.47	0.49
1:A:15:GLN:HG2	1:A:77:GLN:CD	2.32	0.49
1:A:37:LEU:HA	1:A:70:ILE:O	2.12	0.49
1:E:130:ASP:HB2	1:E:131:PRO:HD2	1.94	0.49
1:F:41:PRO:HA	1:F:122:ALA:HB3	1.93	0.49
1:G:37:LEU:HD11	1:G:72:CYS:HB3	1.94	0.49
1:G:83:TRP:CE3	1:G:93:LEU:HD11	2.46	0.49
1:H:116:ASP:N	1:H:121:ASN:O	2.35	0.49
1:L:128:ILE:HD12	1:L:159:PHE:HD2	1.77	0.49
1:M:6:ASN:HB2	1:N:123:PHE:HZ	1.76	0.49
1:S:105:LYS:HB2	1:S:107:GLU:OE1	2.12	0.49
2:D:75:ASP:HB2	2:D:80:HIS:HE1	1.76	0.49
1:G:124:ARG:HE	1:G:143:LYS:HA	1.77	0.49
1:J:78:TYR:HD1	1:J:78:TYR:H	1.57	0.49
1:K:46:PHE:HA	1:K:51:GLU:OE2	2.13	0.49
1:M:34:TYR:CE1	1:M:131:PRO:HD2	2.47	0.49
1:N:32:GLY:C	1:N:131:PRO:HB3	2.33	0.49
1:Q:141:ASN:HD22	1:Q:147:ARG:HG2	1.77	0.49
1:R:87:ASP:HB3	1:R:90:SER:HB2	1.94	0.49
1:A:55:PHE:CE1	1:A:149:VAL:HG22	2.47	0.49
1:C:10:PRO:HD2	1:C:112:TYR:CE1	2.48	0.49
1:C:161:PHE:CE1	1:C:165:HIS:HE1	2.29	0.49
1:C:168:VAL:O	1:C:170:PRO:HD3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:CYS:SG	1:F:28:LYS:HB3	2.52	0.49
1:N:120:GLY:O	1:O:104:ARG:HG3	2.13	0.49
1:N:56:SER:HA	1:N:98:ILE:HG13	1.93	0.49
1:R:38:PHE:CE1	1:R:71:ALA:HA	2.48	0.49
1:C:27:LEU:HD11	1:C:129:ILE:HG21	1.93	0.49
2:D:155:LEU:O	2:D:159:PHE:CD1	2.64	0.49
1:E:38:PHE:HE2	1:E:52:ILE:HD12	1.78	0.49
1:E:3:LEU:HD12	1:E:4:LEU:N	2.28	0.49
1:F:51:GLU:OE1	1:F:146:GLY:HA2	2.11	0.49
1:G:103:ASP:O	1:G:106:GLN:N	2.44	0.49
1:I:12:PHE:HB2	1:I:108:ILE:CD1	2.43	0.49
1:N:148:SER:HB3	1:N:151:GLU:HB2	1.92	0.49
1:A:17:VAL:HA	1:A:21:GLU:O	2.13	0.49
1:G:40:TYR:CE2	1:G:83:TRP:CZ3	3.00	0.49
1:K:51:GLU:HG3	1:K:52:ILE:N	2.24	0.49
1:L:59:VAL:HG21	1:L:97:LYS:CB	2.43	0.49
1:O:136:ARG:HH21	1:O:159:PHE:HD2	1.60	0.49
1:S:40:TYR:CZ	1:S:73:SER:HB3	2.46	0.49
1:A:137:GLN:HG2	1:B:140:ILE:O	2.12	0.49
1:C:49:PRO:O	1:C:52:ILE:N	2.44	0.49
1:C:98:ILE:HG13	1:C:99:PRO:CD	2.41	0.49
2:D:105:LYS:HD3	2:D:105:LYS:N	2.28	0.49
1:E:86:LEU:HB2	1:E:92:GLY:HA3	1.95	0.49
1:K:51:GLU:OE1	1:K:124:ARG:NH1	2.45	0.49
1:M:143:LYS:HD3	1:M:143:LYS:H	1.77	0.49
1:R:5:PRO:CA	1:R:135:LEU:HD23	2.39	0.49
1:S:104:ARG:O	1:S:106:GLN:HG3	2.13	0.49
2:D:4:LEU:HB2	2:D:7:ARG:NE	2.27	0.49
1:E:50:THR:O	1:E:54:ALA:HB2	2.13	0.49
1:E:36:VAL:HG23	1:E:67:CYS:SG	2.52	0.49
1:H:158:ALA:O	1:H:162:VAL:HG13	2.13	0.49
1:J:127:PHE:CE2	1:J:138:ILE:HG23	2.48	0.49
1:J:124:ARG:HB2	1:J:141:ASN:O	2.13	0.49
1:K:53:ILE:HA	1:K:56:SER:CB	2.35	0.49
1:L:127:PHE:CE1	1:L:138:ILE:HG23	2.48	0.49
1:L:38:PHE:HA	1:L:125:GLY:O	2.12	0.49
1:M:12:PHE:HB3	1:M:108:ILE:HG23	1.94	0.49
1:Q:141:ASN:ND2	1:Q:147:ARG:HG2	2.27	0.49
1:S:5:PRO:HB3	1:S:136:ARG:O	2.12	0.49
1:A:124:ARG:CB	1:A:147:ARG:HD3	2.42	0.49
1:B:72:CYS:SG	1:B:101:LEU:HB3	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ILE:HD12	1:E:137:GLN:CG	2.43	0.49
1:F:130:ASP:OD2	1:F:132:ASN:HB2	2.13	0.49
1:I:8:PRO:CA	1:I:134:ILE:HD13	2.42	0.49
1:J:50:THR:O	1:J:54:ALA:HB2	2.13	0.49
1:M:10:PRO:HD2	1:M:112:TYR:CE2	2.48	0.49
1:O:31:ARG:HG3	1:O:131:PRO:O	2.12	0.49
1:O:86:LEU:HG	1:O:92:GLY:CA	2.43	0.49
1:S:16:ALA:HB2	1:S:101:LEU:HA	1.94	0.49
1:C:72:CYS:HB2	1:C:101:LEU:HB3	1.94	0.49
1:F:110:LYS:HE2	1:F:115:PHE:CZ	2.48	0.49
1:L:142:ASP:CG	1:L:144:PRO:HD2	2.32	0.49
1:N:105:LYS:HB2	1:N:107:GLU:HG3	1.94	0.49
1:S:130:ASP:HB2	1:S:131:PRO:CD	2.43	0.49
1:C:143:LYS:HB2	1:C:143:LYS:NZ	2.28	0.48
1:C:77:GLN:O	1:C:80:HIS:HB2	2.13	0.48
2:D:65:ARG:HD2	2:D:156:LEU:HD23	1.95	0.48
1:F:168:VAL:O	1:F:169:CYS:HB2	2.13	0.48
1:G:49:PRO:CB	1:G:52:ILE:HB	2.43	0.48
1:J:40:TYR:CZ	1:J:73:SER:HB2	2.48	0.48
1:K:34:TYR:CE1	1:K:130:ASP:HA	2.48	0.48
1:K:44:PHE:HA	1:K:83:TRP:NE1	2.28	0.48
1:N:83:TRP:O	1:N:93:LEU:HB2	2.12	0.48
1:O:149:VAL:O	1:O:153:LEU:HD13	2.12	0.48
1:R:34:TYR:O	1:R:68:GLN:N	2.41	0.48
1:K:104:ARG:HH22	1:T:75:ASP:CG	2.16	0.48
1:A:132:ASN:ND2	1:A:132:ASN:N	2.57	0.48
1:F:1:MET:HG2	1:F:2:VAL:HG23	1.94	0.48
1:F:80:HIS:H	1:F:80:HIS:CD2	2.31	0.48
1:F:68:GLN:OE1	1:F:99:PRO:CD	2.61	0.48
1:G:48:CYS:HB2	1:G:124:ARG:CZ	2.43	0.48
1:I:16:ALA:CB	1:I:25:ILE:HD13	2.43	0.48
1:K:12:PHE:HB2	1:K:108:ILE:HD13	1.95	0.48
1:B:86:LEU:HD23	1:B:91:GLY:O	2.13	0.48
1:C:142:ASP:C	1:C:144:PRO:HD2	2.33	0.48
2:D:34:TYR:CD1	2:D:131:PRO:HD3	2.47	0.48
1:J:124:ARG:HB2	1:J:141:ASN:CB	2.40	0.48
1:O:116:ASP:CB	1:P:7:ARG:HH12	2.26	0.48
1:Q:45:THR:O	1:Q:46:PHE:C	2.51	0.48
1:T:33:LYS:HA	1:T:66:ASN:HD21	1.78	0.48
1:A:40:TYR:HH	1:A:80:HIS:CD2	2.31	0.48
1:E:149:VAL:O	1:E:153:LEU:HD13	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PHE:CD2	1:F:72:CYS:HB3	2.48	0.48
1:G:108:ILE:O	1:G:111:ALA:HB3	2.12	0.48
1:G:2:VAL:O	1:G:4:LEU:HD13	2.12	0.48
1:K:34:TYR:HA	1:K:129:ILE:O	2.14	0.48
1:M:77:GLN:HG3	1:M:78:TYR:N	2.29	0.48
1:Q:26:CYS:O	1:Q:29:ASP:HB2	2.14	0.48
1:S:86:LEU:O	1:S:92:GLY:HA3	2.13	0.48
1:C:41:PRO:HB3	1:C:121:ASN:HB2	1.95	0.48
1:C:35:VAL:HB	1:C:129:ILE:HD12	1.95	0.48
2:D:46:PHE:N	2:D:46:PHE:HD1	2.07	0.48
1:E:28:LYS:O	1:E:31:ARG:HG2	2.14	0.48
1:F:34:TYR:CE1	1:F:130:ASP:HA	2.47	0.48
1:H:4:LEU:HB2	1:H:7:ARG:CD	2.38	0.48
1:H:61:GLU:O	1:H:65:ARG:N	2.43	0.48
1:J:59:VAL:HG11	1:J:97:LYS:HG3	1.96	0.48
1:L:126:LEU:C	1:L:126:LEU:HD23	2.34	0.48
1:S:37:LEU:O	1:S:127:PHE:HB2	2.13	0.48
1:B:68:GLN:HE21	1:B:99:PRO:HG3	1.77	0.48
1:C:151:GLU:OE2	2:D:151:GLU:HG2	2.13	0.48
2:D:104:ARG:HG3	1:E:120:GLY:N	2.28	0.48
1:C:159:PHE:CE1	2:D:145:VAL:HG21	2.49	0.48
2:D:16:ALA:HA	2:D:101:LEU:HA	1.95	0.48
2:D:23:LYS:HE3	1:O:23:LYS:CB	2.42	0.48
1:G:17:VAL:HA	1:G:21:GLU:O	2.13	0.48
1:I:44:PHE:CE1	1:I:83:TRP:CG	3.02	0.48
1:J:101:LEU:HD12	1:J:102:ALA:N	2.27	0.48
1:J:28:LYS:O	1:J:31:ARG:HB2	2.13	0.48
1:L:127:PHE:CD1	1:L:138:ILE:HG12	2.48	0.48
1:O:32:GLY:O	1:O:33:LYS:HG2	2.14	0.48
1:Q:15:GLN:HG3	1:Q:77:GLN:HE21	1.78	0.48
1:S:103:ASP:OD2	1:S:108:ILE:HB	2.13	0.48
1:B:62:PHE:HB3	1:B:67:CYS:O	2.14	0.48
1:E:136:ARG:HA	1:E:136:ARG:NE	2.29	0.48
1:I:39:PHE:HE2	1:I:127:PHE:CD1	2.32	0.48
1:I:142:ASP:HB3	1:I:144:PRO:HD2	1.96	0.48
1:I:60:GLU:O	1:I:63:ASN:HB2	2.14	0.48
1:K:34:TYR:CD1	1:K:129:ILE:O	2.67	0.48
1:K:47:VAL:HG22	1:K:51:GLU:CG	2.43	0.48
1:M:39:PHE:CE2	1:M:72:CYS:SG	3.07	0.48
1:M:86:LEU:HD11	1:M:90:SER:CB	2.43	0.48
1:O:39:PHE:HE1	1:O:127:PHE:CE2	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:59:VAL:HG21	1:P:97:LYS:HB2	1.94	0.48
1:R:18:ILE:HG12	1:R:99:PRO:HB3	1.96	0.48
1:R:86:LEU:HG	1:R:87:ASP:N	2.28	0.48
1:S:153:LEU:N	1:S:153:LEU:HD12	2.28	0.48
1:S:59:VAL:HG21	1:S:97:LYS:HB2	1.95	0.48
1:B:39:PHE:HE1	1:B:127:PHE:HE2	1.62	0.48
1:H:84:ASP:HA	1:H:93:LEU:HB2	1.95	0.48
1:N:31:ARG:HD2	1:N:132:ASN:HA	1.96	0.48
1:O:17:VAL:HA	1:O:21:GLU:O	2.14	0.48
1:O:48:CYS:N	1:O:49:PRO:CD	2.76	0.48
1:P:34:TYR:CE1	1:P:130:ASP:HA	2.49	0.48
1:Q:51:GLU:C	1:Q:52:ILE:HG13	2.33	0.48
1:B:124:ARG:HD2	1:B:142:ASP:O	2.13	0.48
1:H:12:PHE:HE2	1:H:27:LEU:HD13	1.78	0.48
1:J:47:VAL:HG13	1:J:48:CYS:O	2.14	0.48
1:K:127:PHE:CE1	1:K:138:ILE:HG23	2.48	0.48
1:K:164:LYS:HD3	1:K:165:HIS:CE1	2.49	0.48
1:L:105:LYS:C	1:L:107:GLU:H	2.17	0.48
1:O:36:VAL:HA	1:O:127:PHE:O	2.13	0.48
1:S:143:LYS:HB3	1:S:144:PRO:HD3	1.96	0.48
1:T:60:GLU:HA	1:T:63:ASN:CB	2.18	0.48
1:F:40:TYR:HE1	1:F:43:ASP:OD1	1.97	0.48
1:G:48:CYS:HB2	1:G:124:ARG:NH1	2.29	0.48
1:M:112:TYR:CB	1:M:114:VAL:HG22	2.44	0.48
1:M:48:CYS:HB2	1:M:49:PRO:HD3	1.96	0.48
1:N:36:VAL:HB	1:N:69:VAL:HG22	1.95	0.48
1:P:2:VAL:HG12	1:P:4:LEU:HD22	1.96	0.48
1:Q:16:ALA:CB	1:Q:101:LEU:HA	2.44	0.48
1:Q:87:ASP:HA	1:Q:94:GLY:HA2	1.96	0.48
1:R:15:GLN:OE1	1:R:24:GLU:HB2	2.13	0.48
1:R:65:ARG:NE	1:R:156:LEU:HD23	2.26	0.48
1:T:40:TYR:HD2	1:T:42:ALA:O	1.97	0.48
1:T:86:LEU:CB	1:T:92:GLY:HA3	2.43	0.48
1:A:140:ILE:HB	1:B:138:ILE:HB	1.95	0.47
1:E:14:GLY:O	1:E:24:GLU:HA	2.14	0.47
1:H:38:PHE:HB2	1:H:147:ARG:NH1	2.29	0.47
1:H:4:LEU:HB3	1:H:5:PRO:HD2	1.95	0.47
1:I:150:ASP:OD1	1:I:150:ASP:N	2.45	0.47
1:N:16:ALA:HB2	1:N:25:ILE:HD11	1.95	0.47
1:P:15:GLN:OE1	1:P:15:GLN:HA	2.13	0.47
1:S:126:LEU:HD12	1:S:147:ARG:CG	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:86:LEU:C	1:S:92:GLY:HA3	2.34	0.47
1:S:96:MET:CE	1:S:96:MET:HA	2.44	0.47
1:T:137:GLN:HB2	1:T:159:PHE:HE2	1.78	0.47
1:C:62:PHE:O	1:C:67:CYS:N	2.46	0.47
1:E:136:ARG:HD3	1:E:159:PHE:CD2	2.48	0.47
1:J:48:CYS:HB3	1:J:49:PRO:HD2	1.96	0.47
1:P:54:ALA:O	1:P:58:GLN:HG2	2.15	0.47
1:S:41:PRO:HG3	1:S:143:LYS:HD2	1.96	0.47
1:S:149:VAL:O	1:S:152:THR:HB	2.14	0.47
1:C:54:ALA:O	1:C:58:GLN:HB2	2.15	0.47
1:E:72:CYS:HB2	1:E:101:LEU:HB3	1.96	0.47
1:F:78:TYR:CB	1:G:45:THR:HB	2.43	0.47
1:K:25:ILE:HG22	1:K:29:ASP:OD2	2.13	0.47
1:M:44:PHE:N	1:M:83:TRP:CZ3	2.83	0.47
1:P:105:LYS:HD3	1:P:107:GLU:CD	2.35	0.47
1:P:13:LYS:HG2	1:P:26:CYS:CB	2.44	0.47
1:A:18:ILE:HD12	1:A:18:ILE:N	2.29	0.47
1:G:127:PHE:HD2	1:G:135:LEU:HD11	1.79	0.47
1:H:74:THR:HA	1:H:103:ASP:O	2.14	0.47
1:K:155:LEU:O	1:K:158:ALA:HB3	2.14	0.47
1:O:151:GLU:O	1:O:155:LEU:HD12	2.14	0.47
1:P:2:VAL:HG12	1:P:4:LEU:CD2	2.44	0.47
1:T:30:TYR:CE2	1:T:68:GLN:HG2	2.49	0.47
1:A:15:GLN:OE1	1:A:24:GLU:HB2	2.14	0.47
1:B:104:ARG:NH1	1:C:104:ARG:HH12	2.12	0.47
1:C:42:ALA:HB3	1:C:45:THR:HG21	1.96	0.47
1:I:8:PRO:HA	1:I:134:ILE:HD13	1.96	0.47
1:I:161:PHE:O	1:I:166:GLY:N	2.46	0.47
1:Q:145:VAL:HG21	1:R:159:PHE:CE1	2.50	0.47
1:T:41:PRO:O	1:T:121:ASN:HB3	2.14	0.47
1:B:49:PRO:O	1:B:53:ILE:HG13	2.13	0.47
1:B:51:GLU:OE1	1:B:124:ARG:NH1	2.48	0.47
1:C:38:PHE:CZ	1:C:71:ALA:HB2	2.50	0.47
1:F:47:VAL:HG11	1:F:144:PRO:O	2.15	0.47
1:L:12:PHE:CD1	1:L:108:ILE:HD13	2.50	0.47
1:L:115:PHE:CE1	1:L:121:ASN:N	2.78	0.47
1:L:127:PHE:HA	1:L:137:GLN:O	2.13	0.47
1:L:143:LYS:N	1:L:144:PRO:HD2	2.30	0.47
1:L:46:PHE:HB2	1:L:49:PRO:HG2	1.96	0.47
1:O:128:ILE:HB	1:O:137:GLN:H	1.78	0.47
1:O:88:ARG:HA	1:O:92:GLY:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:5:PRO:HB3	1:T:136:ARG:O	2.15	0.47
1:B:132:ASN:ND2	1:B:132:ASN:N	2.63	0.47
1:B:142:ASP:OD1	1:B:144:PRO:HD2	2.15	0.47
1:H:127:PHE:HE2	1:H:138:ILE:HG23	1.77	0.47
1:K:127:PHE:CD1	1:K:138:ILE:HG23	2.49	0.47
1:L:65:ARG:HD2	1:L:153:LEU:HD11	1.96	0.47
1:R:6:ASN:HB3	1:R:7:ARG:CD	2.44	0.47
2:D:151:GLU:O	2:D:155:LEU:HG	2.15	0.47
1:E:96:MET:HB3	1:E:98:ILE:HG13	1.97	0.47
1:G:149:VAL:O	1:G:152:THR:HB	2.14	0.47
1:I:106:GLN:HB2	1:I:110:LYS:HE3	1.96	0.47
1:I:109:SER:OG	1:I:114:VAL:HG23	2.15	0.47
1:J:154:ARG:NH2	1:J:155:LEU:HD21	2.30	0.47
1:J:22:PHE:HD1	1:J:22:PHE:N	2.12	0.47
1:M:18:ILE:O	1:M:19:ASN:CB	2.62	0.47
1:B:50:THR:HG23	1:B:51:GLU:N	2.30	0.47
2:D:104:ARG:HG3	1:E:120:GLY:CA	2.45	0.47
2:D:47:VAL:CG1	2:D:48:CYS:H	2.17	0.47
1:E:25:ILE:HD11	1:E:101:LEU:HD22	1.96	0.47
1:G:59:VAL:HG11	1:G:97:LYS:HB2	1.96	0.47
1:H:40:TYR:CE1	1:H:71:ALA:HB1	2.50	0.47
1:K:35:VAL:HB	1:K:129:ILE:HB	1.97	0.47
1:M:157:ASP:O	1:M:161:PHE:N	2.46	0.47
1:P:74:THR:HG23	1:Q:104:ARG:HH21	1.80	0.47
1:S:32:GLY:C	1:S:131:PRO:HB3	2.34	0.47
1:A:13:LYS:HZ3	1:A:26:CYS:HB2	1.79	0.47
1:A:41:PRO:HB3	1:A:121:ASN:HD22	1.80	0.47
2:D:105:LYS:O	2:D:106:GLN:CB	2.63	0.47
2:D:34:TYR:CE1	2:D:130:ASP:HA	2.50	0.47
1:G:40:TYR:CE2	1:G:83:TRP:HZ3	2.33	0.47
1:K:12:PHE:CE1	1:K:27:LEU:HB2	2.50	0.47
1:L:115:PHE:CD1	1:L:121:ASN:O	2.68	0.47
1:P:148:SER:CB	1:P:151:GLU:HB3	2.42	0.47
1:P:18:ILE:HB	1:P:23:LYS:HD3	1.96	0.47
1:Q:40:TYR:CD2	1:Q:42:ALA:O	2.68	0.47
2:D:104:ARG:HG3	1:E:120:GLY:HA3	1.97	0.47
1:E:126:LEU:HB3	1:E:139:THR:HB	1.97	0.47
1:H:55:PHE:CE1	1:H:149:VAL:HG12	2.49	0.47
1:H:36:VAL:HB	1:H:69:VAL:HG22	1.96	0.47
1:I:12:PHE:CB	1:I:108:ILE:HG12	2.46	0.47
1:I:25:ILE:HD11	1:I:101:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:VAL:C	1:N:47:VAL:HG11	2.35	0.47
1:P:86:LEU:HD23	1:P:91:GLY:O	2.15	0.47
1:Q:17:VAL:HG22	1:Q:22:PHE:CD1	2.50	0.47
1:Q:36:VAL:HG23	1:Q:67:CYS:SG	2.54	0.47
1:R:34:TYR:CB	1:R:67:CYS:HA	2.45	0.47
1:B:36:VAL:HG12	1:B:69:VAL:HG13	1.98	0.46
1:B:22:PHE:HE1	1:B:77:GLN:CG	2.28	0.46
2:D:65:ARG:HD3	2:D:156:LEU:HD23	1.96	0.46
1:I:123:PHE:CB	1:I:140:ILE:HD11	2.45	0.46
1:J:126:LEU:HD23	1:J:127:PHE:N	2.30	0.46
1:J:31:ARG:HD3	1:J:131:PRO:O	2.14	0.46
1:J:18:ILE:HG12	1:J:99:PRO:HA	1.96	0.46
1:J:69:VAL:HG12	1:J:70:ILE:N	2.30	0.46
1:J:6:ASN:C	1:J:7:ARG:HD2	2.35	0.46
1:K:27:LEU:CD2	1:K:31:ARG:HH21	2.27	0.46
1:F:131:PRO:HG2	1:O:163:GLU:HG2	1.96	0.46
1:P:59:VAL:HG21	1:P:97:LYS:CB	2.44	0.46
1:Q:39:PHE:HD1	1:Q:39:PHE:N	2.11	0.46
1:S:5:PRO:HD3	1:S:138:ILE:HD11	1.97	0.46
1:G:40:TYR:HE2	1:G:83:TRP:CZ3	2.34	0.46
1:I:83:TRP:CD1	1:I:92:GLY:HA2	2.50	0.46
1:J:71:ALA:HB3	1:J:100:LEU:HA	1.97	0.46
1:K:124:ARG:HD2	1:K:145:VAL:O	2.15	0.46
1:K:55:PHE:CE1	1:K:149:VAL:HG22	2.50	0.46
1:K:80:HIS:ND1	1:K:100:LEU:HB3	2.30	0.46
1:N:83:TRP:CE3	1:N:93:LEU:HG	2.50	0.46
1:O:39:PHE:CE1	1:O:127:PHE:HE2	2.33	0.46
1:P:128:ILE:HG21	1:P:159:PHE:CE2	2.50	0.46
1:Q:38:PHE:HD2	1:Q:147:ARG:NH2	2.12	0.46
1:Q:96:MET:SD	1:Q:98:ILE:HG12	2.56	0.46
1:S:59:VAL:HG21	1:S:97:LYS:CB	2.46	0.46
1:T:54:ALA:HA	1:T:57:ASP:OD2	2.15	0.46
1:A:60:GLU:HA	1:A:60:GLU:OE1	2.16	0.46
1:G:86:LEU:CG	1:G:92:GLY:HA3	2.40	0.46
1:I:148:SER:HB3	1:I:151:GLU:HB3	1.97	0.46
1:K:38:PHE:HA	1:K:125:GLY:O	2.16	0.46
1:M:134:ILE:HG21	1:M:136:ARG:HH22	1.80	0.46
1:M:69:VAL:HB	1:M:98:ILE:HG21	1.97	0.46
1:M:38:PHE:CZ	1:M:71:ALA:HA	2.50	0.46
1:N:30:TYR:CE2	1:N:68:GLN:HG2	2.51	0.46
1:O:68:GLN:HE21	1:O:70:ILE:HG12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:136:ARG:HB3	1:P:159:PHE:CZ	2.50	0.46
1:Q:34:TYR:CE1	1:Q:130:ASP:HA	2.49	0.46
1:T:30:TYR:C	1:T:31:ARG:HD2	2.35	0.46
1:H:56:SER:OG	1:H:97:LYS:HD3	2.15	0.46
1:I:80:HIS:HD2	1:I:100:LEU:HB3	1.80	0.46
1:I:106:GLN:CB	1:I:110:LYS:HE3	2.46	0.46
1:I:40:TYR:O	1:I:73:SER:HB3	2.15	0.46
1:J:116:ASP:HB3	1:J:121:ASN:O	2.15	0.46
1:L:127:PHE:O	1:L:128:ILE:HG12	2.15	0.46
1:M:40:TYR:HB2	1:M:41:PRO:HD2	1.97	0.46
1:N:76:SER:HB3	1:N:104:ARG:CD	2.45	0.46
1:S:153:LEU:H	1:S:153:LEU:CD1	2.26	0.46
1:A:83:TRP:CD1	1:A:93:LEU:HG	2.51	0.46
1:A:148:SER:HB2	1:B:154:ARG:NH2	2.31	0.46
1:B:22:PHE:HE1	1:B:77:GLN:HG2	1.80	0.46
1:E:27:LEU:HD11	1:E:129:ILE:HG21	1.96	0.46
1:F:39:PHE:HE2	1:F:72:CYS:HG	1.63	0.46
1:G:47:VAL:C	1:G:49:PRO:CD	2.84	0.46
1:H:96:MET:HA	1:H:96:MET:HE2	1.97	0.46
1:K:44:PHE:CD2	1:K:83:TRP:CD1	3.04	0.46
1:M:12:PHE:HB3	1:M:108:ILE:CG2	2.46	0.46
1:M:124:ARG:HB3	1:M:147:ARG:CZ	2.46	0.46
1:O:56:SER:HB3	1:O:96:MET:CE	2.44	0.46
1:P:71:ALA:HB2	1:P:98:ILE:HD11	1.97	0.46
1:Q:55:PHE:CE2	1:Q:149:VAL:HG13	2.51	0.46
1:R:55:PHE:CE1	1:R:149:VAL:HG22	2.51	0.46
1:C:14:GLY:C	1:C:24:GLU:HG3	2.36	0.46
1:C:40:TYR:HE2	1:C:43:ASP:OD1	1.98	0.46
2:D:53:ILE:CA	2:D:96:MET:HE1	2.45	0.46
1:E:82:ALA:O	1:E:85:ASN:N	2.49	0.46
1:J:164:LYS:CG	1:J:165:HIS:HD2	2.28	0.46
1:J:16:ALA:HB2	1:J:25:ILE:HD13	1.98	0.46
1:L:6:ASN:HD22	1:L:134:ILE:CG2	2.28	0.46
1:M:143:LYS:N	1:M:144:PRO:CD	2.77	0.46
1:N:13:LYS:HD3	1:N:26:CYS:HB2	1.98	0.46
1:Q:38:PHE:HB2	1:Q:147:ARG:NH1	2.31	0.46
1:R:3:LEU:HD23	1:R:10:PRO:HG2	1.97	0.46
1:R:18:ILE:HG12	1:R:99:PRO:CB	2.46	0.46
1:S:5:PRO:HD2	1:T:123:PHE:CD2	2.51	0.46
1:T:34:TYR:CD1	1:T:131:PRO:HD3	2.50	0.46
1:C:126:LEU:N	1:C:139:THR:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:CYS:O	1:C:29:ASP:HB2	2.15	0.46
1:F:55:PHE:O	1:F:59:VAL:N	2.49	0.46
1:F:17:VAL:HG21	1:F:80:HIS:HB2	1.98	0.46
1:H:123:PHE:CB	1:H:140:ILE:HD11	2.45	0.46
1:K:35:VAL:HB	1:K:129:ILE:HD12	1.97	0.46
1:N:143:LYS:N	1:N:144:PRO:HD2	2.31	0.46
1:O:13:LYS:HZ2	1:O:26:CYS:HB2	1.79	0.46
1:P:104:ARG:HA	1:P:104:ARG:HD3	1.84	0.46
1:P:34:TYR:HA	1:P:129:ILE:O	2.16	0.46
1:P:46:PHE:O	1:P:47:VAL:HG12	2.15	0.46
1:T:65:ARG:NH1	1:T:153:LEU:HB3	2.31	0.46
1:A:76:SER:HA	1:A:104:ARG:HD3	1.97	0.46
1:B:132:ASN:HD22	1:B:132:ASN:N	2.13	0.46
1:F:13:LYS:HB2	1:F:13:LYS:HE3	1.78	0.46
1:F:52:ILE:CG2	1:F:53:ILE:N	2.79	0.46
1:L:65:ARG:HD2	1:L:156:LEU:HD12	1.97	0.46
1:R:48:CYS:HA	1:R:50:THR:HB	1.98	0.46
1:S:109:SER:CB	1:S:115:PHE:HB2	2.45	0.46
1:S:167:GLU:CD	1:S:167:GLU:N	2.69	0.46
1:S:151:GLU:HB2	1:T:151:GLU:CD	2.37	0.46
1:B:154:ARG:NH2	1:B:155:LEU:HD21	2.31	0.46
1:C:84:ASP:OD1	1:C:96:MET:HG2	2.16	0.46
1:F:154:ARG:NH2	1:F:155:LEU:HD21	2.30	0.46
1:I:130:ASP:HB3	1:I:136:ARG:HG2	1.97	0.46
1:I:16:ALA:HB2	1:I:25:ILE:HD13	1.97	0.46
1:P:65:ARG:HD2	1:P:160:GLN:NE2	2.29	0.46
1:A:39:PHE:N	1:A:39:PHE:CD1	2.84	0.46
1:C:70:ILE:HG12	1:C:99:PRO:HB2	1.97	0.46
2:D:78:TYR:N	2:D:78:TYR:CD1	2.84	0.46
1:F:116:ASP:OD2	1:F:119:ASP:HB2	2.16	0.46
1:F:56:SER:O	1:F:59:VAL:HB	2.16	0.46
1:G:71:ALA:O	1:G:101:LEU:N	2.48	0.46
1:G:35:VAL:HG22	1:G:68:GLN:HB3	1.98	0.46
1:H:136:ARG:HB3	1:H:159:PHE:CE1	2.51	0.46
1:J:76:SER:HB2	1:J:78:TYR:HD1	1.81	0.46
1:K:154:ARG:CZ	1:L:148:SER:HB2	2.46	0.46
1:K:51:GLU:CG	1:K:52:ILE:H	2.24	0.46
1:K:53:ILE:CA	1:K:56:SER:HB3	2.33	0.46
1:M:89:LYS:O	1:M:89:LYS:HD3	2.16	0.46
1:P:143:LYS:N	1:P:144:PRO:CD	2.79	0.46
1:R:105:LYS:O	1:R:106:GLN:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:108:ILE:O	1:T:111:ALA:HB3	2.15	0.46
1:T:162:VAL:HA	1:T:166:GLY:N	2.27	0.46
1:A:128:ILE:HD12	1:A:137:GLN:HB3	1.98	0.45
1:G:144:PRO:HB2	1:H:162:VAL:CG1	2.46	0.45
1:G:125:GLY:C	1:G:147:ARG:HH12	2.19	0.45
1:L:69:VAL:HB	1:L:98:ILE:CG2	2.42	0.45
1:M:65:ARG:HD2	1:M:156:LEU:HD22	1.97	0.45
1:O:139:THR:HG23	1:P:139:THR:HG23	1.97	0.45
1:Q:16:ALA:HB2	1:Q:101:LEU:HD12	1.98	0.45
1:T:168:VAL:O	1:T:169:CYS:C	2.55	0.45
2:D:126:LEU:HD22	2:D:137:GLN:OE1	2.16	0.45
1:F:51:GLU:HB3	1:F:147:ARG:NH2	2.32	0.45
1:H:40:TYR:HE1	1:H:71:ALA:HB1	1.81	0.45
1:J:38:PHE:HE1	1:J:40:TYR:HB3	1.81	0.45
1:J:17:VAL:HG21	1:J:80:HIS:HB2	1.97	0.45
1:K:33:LYS:O	1:K:131:PRO:HA	2.16	0.45
1:S:99:PRO:C	1:S:100:LEU:HD23	2.36	0.45
1:T:87:ASP:OD1	1:T:90:SER:HB3	2.17	0.45
1:A:140:ILE:HD12	1:B:138:ILE:HB	1.97	0.45
1:C:82:ALA:HA	1:C:85:ASN:ND2	2.28	0.45
2:D:17:VAL:N	2:D:100:LEU:O	2.45	0.45
1:H:104:ARG:HB3	1:I:120:GLY:HA3	1.98	0.45
1:J:168:VAL:HG22	1:J:169:CYS:N	2.32	0.45
1:K:47:VAL:HG22	1:K:51:GLU:HG2	1.96	0.45
1:L:86:LEU:HB3	1:L:92:GLY:HA3	1.98	0.45
1:M:11:GLU:HA	1:M:11:GLU:OE1	2.16	0.45
1:S:15:GLN:HA	1:S:24:GLU:HA	1.97	0.45
1:T:65:ARG:HD3	1:T:156:LEU:HD23	1.99	0.45
1:A:41:PRO:HB3	1:A:121:ASN:ND2	2.31	0.45
1:A:75:ASP:HB2	1:A:80:HIS:CE1	2.36	0.45
1:A:145:VAL:HG21	1:B:159:PHE:HE1	1.79	0.45
1:C:126:LEU:HD13	1:C:139:THR:OG1	2.16	0.45
1:J:26:CYS:HB3	1:J:29:ASP:OD1	2.15	0.45
1:J:40:TYR:CE1	1:J:71:ALA:HB1	2.51	0.45
1:K:140:ILE:HG22	1:L:5:PRO:HG3	1.98	0.45
1:L:72:CYS:SG	1:L:101:LEU:HD23	2.57	0.45
1:M:137:GLN:NE2	1:M:139:THR:OG1	2.49	0.45
1:M:143:LYS:HB2	1:M:143:LYS:HZ2	1.82	0.45
1:O:86:LEU:HD11	1:O:90:SER:CB	2.34	0.45
1:P:106:GLN:NE2	1:P:115:PHE:CZ	2.85	0.45
1:R:15:GLN:C	1:R:101:LEU:HD12	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:136:ARG:HB3	1:S:159:PHE:CZ	2.51	0.45
1:A:138:ILE:HB	1:B:140:ILE:HB	1.98	0.45
1:E:151:GLU:CD	1:F:151:GLU:HG2	2.36	0.45
1:F:43:ASP:HA	1:F:83:TRP:CZ3	2.52	0.45
1:I:22:PHE:C	1:I:23:LYS:HD2	2.37	0.45
1:J:96:MET:HG2	1:J:100:LEU:HG	1.98	0.45
1:K:141:ASN:HD21	1:L:155:LEU:HD21	1.80	0.45
1:N:22:PHE:CZ	1:N:81:LEU:HD22	2.52	0.45
1:R:151:GLU:HG3	1:R:155:LEU:HD11	1.98	0.45
1:S:157:ASP:HA	1:S:160:GLN:HB2	1.97	0.45
1:S:53:ILE:HA	1:S:96:MET:HE1	1.98	0.45
1:A:96:MET:CG	1:A:100:LEU:HD21	2.46	0.45
1:F:116:ASP:HB3	1:F:123:PHE:HE1	1.82	0.45
1:I:18:ILE:O	1:I:19:ASN:HB2	2.16	0.45
1:J:74:THR:HA	1:J:103:ASP:O	2.17	0.45
1:K:44:PHE:HA	1:K:83:TRP:CE2	2.51	0.45
1:L:95:HIS:ND1	1:L:95:HIS:N	2.65	0.45
1:M:148:SER:N	1:N:154:ARG:NH2	2.65	0.45
1:O:140:ILE:O	1:P:137:GLN:HB2	2.17	0.45
1:S:34:TYR:HB2	1:S:66:ASN:O	2.17	0.45
1:T:39:PHE:CE2	1:T:114:VAL:HG21	2.51	0.45
1:A:119:ASP:O	1:A:121:ASN:OD1	2.35	0.45
1:A:53:ILE:HG13	1:A:93:LEU:HD22	1.98	0.45
1:E:69:VAL:O	1:E:99:PRO:HD2	2.17	0.45
1:H:67:CYS:SG	1:H:68:GLN:N	2.90	0.45
1:H:22:PHE:CZ	1:H:77:GLN:HB2	2.50	0.45
1:M:40:TYR:HB2	1:M:41:PRO:CD	2.47	0.45
1:O:40:TYR:HB2	1:O:41:PRO:CD	2.46	0.45
1:O:50:THR:OG1	1:O:53:ILE:HB	2.17	0.45
1:Q:39:PHE:HZ	1:Q:112:TYR:CD2	2.34	0.45
1:Q:68:GLN:CG	1:Q:70:ILE:HD11	2.46	0.45
1:R:16:ALA:HB2	1:R:101:LEU:CD1	2.47	0.45
1:R:39:PHE:HB2	1:R:123:PHE:O	2.17	0.45
1:S:86:LEU:HB3	1:S:92:GLY:HA3	1.98	0.45
1:C:149:VAL:HA	1:C:152:THR:HG1	1.82	0.45
1:F:14:GLY:O	1:F:24:GLU:OE1	2.34	0.45
1:F:18:ILE:HG13	1:F:23:LYS:HB2	1.97	0.45
1:H:128:ILE:O	1:H:135:LEU:HD12	2.16	0.45
1:H:134:ILE:HG22	1:H:135:LEU:N	2.31	0.45
1:J:35:VAL:HG12	1:J:36:VAL:N	2.32	0.45
1:K:124:ARG:HH11	1:K:147:ARG:NH2	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:PRO:HA	1:M:122:ALA:N	2.25	0.45
1:R:57:ASP:HB2	1:R:58:GLN:OE1	2.16	0.45
2:D:110:LYS:C	2:D:113:GLY:H	2.20	0.45
2:D:124:ARG:CG	2:D:147:ARG:HH12	2.20	0.45
2:D:78:TYR:N	2:D:78:TYR:HD1	2.13	0.45
1:F:105:LYS:HE2	1:G:118:GLU:O	2.17	0.45
1:J:47:VAL:CG2	1:J:48:CYS:H	2.12	0.45
1:K:55:PHE:CE1	1:K:147:ARG:O	2.70	0.45
1:N:147:ARG:N	1:N:147:ARG:NE	2.62	0.45
1:O:59:VAL:O	1:O:62:PHE:HB2	2.17	0.45
1:O:78:TYR:CD1	1:O:78:TYR:N	2.84	0.45
1:P:58:GLN:O	1:P:61:GLU:HB2	2.17	0.45
1:R:41:PRO:HB3	1:R:143:LYS:HZ2	1.81	0.45
1:B:34:TYR:HA	1:B:129:ILE:O	2.16	0.45
1:B:34:TYR:CE1	1:B:131:PRO:HD3	2.52	0.45
1:C:84:ASP:HB2	1:C:93:LEU:HD12	1.98	0.45
1:F:86:LEU:HD12	1:F:87:ASP:H	1.82	0.45
1:G:39:PHE:HA	1:G:72:CYS:O	2.18	0.45
1:I:39:PHE:O	1:I:124:ARG:HA	2.17	0.45
1:J:4:LEU:O	1:J:7:ARG:HB2	2.17	0.45
1:J:84:ASP:HA	1:J:93:LEU:HB2	1.99	0.45
1:M:128:ILE:O	1:M:135:LEU:HD12	2.16	0.45
1:O:55:PHE:CZ	1:O:149:VAL:HG22	2.52	0.45
1:P:35:VAL:HA	1:P:68:GLN:O	2.17	0.45
1:P:7:ARG:HD2	1:P:7:ARG:N	2.32	0.45
1:Q:25:ILE:HD12	1:Q:30:TYR:CE2	2.52	0.45
1:Q:73:SER:OG	1:Q:80:HIS:CE1	2.70	0.45
1:R:86:LEU:HB3	1:R:92:GLY:HA3	1.98	0.45
1:C:1:MET:HB3	1:C:2:VAL:H	1.55	0.44
1:C:82:ALA:O	1:C:85:ASN:HB2	2.17	0.44
1:F:136:ARG:HA	1:F:136:ARG:HD2	1.82	0.44
1:F:155:LEU:O	1:F:158:ALA:HB3	2.16	0.44
1:G:40:TYR:CE1	1:G:73:SER:HB3	2.52	0.44
1:G:43:ASP:CB	1:G:44:PHE:CD2	3.01	0.44
1:I:40:TYR:HE1	1:I:71:ALA:HB1	1.79	0.44
1:J:143:LYS:HB2	1:J:144:PRO:HD3	1.99	0.44
1:L:143:LYS:N	1:L:144:PRO:CD	2.79	0.44
1:N:135:LEU:HD21	1:N:138:ILE:CD1	2.46	0.44
1:N:56:SER:HA	1:N:98:ILE:CD1	2.48	0.44
1:P:130:ASP:OD2	1:P:132:ASN:HB2	2.16	0.44
1:T:126:LEU:HD23	1:T:139:THR:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:VAL:O	1:B:99:PRO:HD2	2.17	0.44
1:G:141:ASN:HD21	1:H:155:LEU:CD2	2.30	0.44
1:H:145:VAL:HG12	1:H:146:GLY:O	2.17	0.44
1:K:30:TYR:CD1	1:K:68:GLN:HG2	2.51	0.44
1:L:126:LEU:HB2	1:L:147:ARG:NH1	2.29	0.44
1:L:129:ILE:HA	1:L:134:ILE:O	2.17	0.44
1:L:37:LEU:HD12	1:L:38:PHE:H	1.80	0.44
1:L:94:GLY:O	1:L:96:MET:HE2	2.17	0.44
1:N:17:VAL:O	1:N:99:PRO:HA	2.17	0.44
1:O:41:PRO:HB3	1:O:143:LYS:HE2	1.98	0.44
1:O:124:ARG:HB3	1:O:147:ARG:NH1	2.32	0.44
1:F:24:GLU:HB3	1:Q:24:GLU:HB3	1.98	0.44
1:Q:68:GLN:HG3	1:Q:70:ILE:HD11	1.97	0.44
1:T:71:ALA:O	1:T:101:LEU:HB3	2.17	0.44
1:A:5:PRO:HA	1:A:135:LEU:HG	2.00	0.44
1:B:160:GLN:O	1:B:164:LYS:HB2	2.16	0.44
1:C:101:LEU:HD12	1:C:102:ALA:N	2.33	0.44
1:C:142:ASP:HB3	1:C:145:VAL:HG23	1.99	0.44
1:C:141:ASN:HD22	1:C:145:VAL:CG1	2.30	0.44
2:D:135:LEU:O	2:D:136:ARG:HD2	2.17	0.44
1:G:96:MET:SD	1:G:100:LEU:HD21	2.58	0.44
1:H:58:GLN:NE2	1:H:61:GLU:OE1	2.51	0.44
1:H:86:LEU:HD11	1:H:90:SER:OG	2.16	0.44
1:I:25:ILE:CD1	1:I:101:LEU:HD13	2.42	0.44
1:K:134:ILE:HG22	1:K:135:LEU:N	2.32	0.44
1:K:147:ARG:HE	1:K:147:ARG:N	2.15	0.44
1:L:126:LEU:HD22	1:L:139:THR:OG1	2.17	0.44
1:B:36:VAL:HG13	1:B:126:LEU:HD21	1.98	0.44
2:D:54:ALA:O	2:D:57:ASP:HB2	2.17	0.44
1:J:112:TYR:HD2	1:J:127:PHE:CE2	2.35	0.44
1:O:62:PHE:HE1	1:O:152:THR:HG21	1.82	0.44
1:P:22:PHE:C	1:P:23:LYS:HD2	2.38	0.44
1:Q:34:TYR:CZ	1:Q:160:GLN:HG2	2.53	0.44
1:F:143:LYS:N	1:F:144:PRO:CD	2.81	0.44
1:G:141:ASN:HD21	1:H:155:LEU:HD22	1.83	0.44
1:F:78:TYR:CG	1:G:45:THR:HB	2.52	0.44
1:G:42:ALA:HA	1:G:75:ASP:OD2	2.18	0.44
1:I:59:VAL:HG23	1:I:60:GLU:N	2.32	0.44
1:I:83:TRP:NE1	1:I:92:GLY:HA2	2.33	0.44
1:K:3:LEU:HD11	1:K:112:TYR:HA	1.98	0.44
1:K:116:ASP:HB2	1:K:123:PHE:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASN:HB2	1:K:166:GLY:HA3	1.99	0.44
1:L:84:ASP:OD1	1:L:95:HIS:HA	2.18	0.44
1:N:76:SER:OG	1:N:79:SER:HB2	2.17	0.44
1:N:7:ARG:CD	1:N:7:ARG:N	2.78	0.44
1:P:135:LEU:HD12	1:P:136:ARG:N	2.29	0.44
1:P:54:ALA:O	1:P:58:GLN:CG	2.66	0.44
1:S:48:CYS:SG	1:S:49:PRO:HD2	2.58	0.44
1:T:115:PHE:HE2	1:T:117:GLU:OE2	2.00	0.44
1:B:129:ILE:CG2	1:B:133:GLY:HA2	2.47	0.44
1:B:44:PHE:CZ	1:B:83:TRP:HB2	2.53	0.44
1:B:71:ALA:HB2	1:B:98:ILE:HD11	2.00	0.44
1:C:53:ILE:HG23	1:C:96:MET:HE1	1.99	0.44
1:C:96:MET:HG3	1:C:96:MET:O	2.18	0.44
1:F:127:PHE:CD1	1:F:138:ILE:HA	2.53	0.44
1:F:44:PHE:N	1:F:83:TRP:CZ2	2.81	0.44
1:G:37:LEU:HD11	1:G:72:CYS:CB	2.48	0.44
1:J:38:PHE:HE2	1:J:55:PHE:CE2	2.36	0.44
1:N:36:VAL:HG23	1:N:67:CYS:SG	2.57	0.44
1:Q:28:LYS:CA	1:Q:31:ARG:HH21	2.29	0.44
1:S:55:PHE:CE2	1:S:149:VAL:HG22	2.53	0.44
1:A:40:TYR:HA	1:A:41:PRO:HD3	1.82	0.44
1:B:143:LYS:HB2	1:B:144:PRO:CD	2.48	0.44
1:C:159:PHE:CZ	2:D:145:VAL:HG21	2.52	0.44
2:D:32:GLY:C	2:D:131:PRO:HB3	2.38	0.44
1:G:145:VAL:HG21	1:H:159:PHE:CD1	2.53	0.44
1:I:13:LYS:HG2	1:I:14:GLY:H	1.83	0.44
1:J:65:ARG:NE	1:J:153:LEU:HD12	2.33	0.44
1:J:77:GLN:HG2	1:J:78:TYR:CE1	2.52	0.44
1:K:55:PHE:CD2	1:K:149:VAL:HG13	2.53	0.44
1:L:105:LYS:O	1:L:106:GLN:HB2	2.18	0.44
1:M:47:VAL:HG12	1:M:48:CYS:H	1.82	0.44
1:O:74:THR:O	1:O:103:ASP:O	2.35	0.44
1:S:38:PHE:HD1	1:S:38:PHE:H	1.63	0.44
1:A:134:ILE:HG22	1:A:136:ARG:NH2	2.33	0.44
1:B:32:GLY:C	1:B:131:PRO:HB3	2.38	0.44
1:E:21:GLU:HB3	1:E:23:LYS:NZ	2.32	0.44
1:F:154:ARG:HH22	1:F:155:LEU:HD21	1.83	0.44
1:I:55:PHE:HE2	1:I:147:ARG:HH21	1.66	0.44
1:J:37:LEU:HG	1:J:39:PHE:CE1	2.53	0.44
1:K:34:TYR:CE2	1:K:131:PRO:HD3	2.53	0.44
1:L:120:GLY:H	1:M:105:LYS:HG3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:12:PHE:CE2	1:M:27:LEU:HD13	2.52	0.44
1:M:38:PHE:HB2	1:M:147:ARG:NH1	2.32	0.44
1:N:143:LYS:HB2	1:N:144:PRO:HD3	1.99	0.44
1:T:12:PHE:CE1	1:T:27:LEU:HB2	2.53	0.44
1:A:124:ARG:HB3	1:A:147:ARG:NH1	2.33	0.44
1:B:38:PHE:HB2	1:B:147:ARG:HH12	1.83	0.44
1:F:14:GLY:O	1:F:101:LEU:CD1	2.66	0.44
1:J:87:ASP:OD2	1:J:89:LYS:HE3	2.18	0.44
1:M:65:ARG:HE	1:M:153:LEU:HD12	1.83	0.44
1:B:24:GLU:HB2	1:M:24:GLU:HB3	2.00	0.44
1:M:4:LEU:HD13	1:N:123:PHE:HE2	1.83	0.44
1:M:94:GLY:O	1:M:96:MET:HE3	2.18	0.44
1:R:41:PRO:O	1:R:42:ALA:HB2	2.17	0.44
1:S:73:SER:OG	1:S:80:HIS:CE1	2.71	0.44
2:D:12:PHE:HB2	2:D:108:ILE:HG23	2.00	0.43
1:G:36:VAL:HG22	1:G:128:ILE:HG12	2.00	0.43
1:H:40:TYR:CE2	1:H:83:TRP:HZ3	2.36	0.43
1:H:68:GLN:OE1	1:H:68:GLN:HA	2.17	0.43
1:K:39:PHE:CE1	1:K:114:VAL:HG21	2.53	0.43
1:N:34:TYR:HD1	1:N:129:ILE:O	1.99	0.43
1:O:9:ALA:HA	1:O:10:PRO:HD3	1.86	0.43
1:R:86:LEU:HG	1:R:90:SER:HB3	2.00	0.43
1:R:83:TRP:CG	1:R:93:LEU:HG	2.52	0.43
1:T:97:LYS:N	1:T:97:LYS:HD2	2.33	0.43
1:B:37:LEU:HD12	1:B:38:PHE:N	2.33	0.43
1:C:58:GLN:HG3	1:C:61:GLU:HG3	1.99	0.43
2:D:149:VAL:O	2:D:153:LEU:HB2	2.18	0.43
2:D:4:LEU:HA	2:D:5:PRO:HD3	1.93	0.43
1:E:8:PRO:HA	1:E:135:LEU:H	1.83	0.43
1:G:62:PHE:CD2	1:G:69:VAL:HG21	2.54	0.43
1:I:119:ASP:OD2	1:I:121:ASN:HB2	2.18	0.43
1:I:5:PRO:HD3	1:I:138:ILE:HD12	1.98	0.43
1:J:25:ILE:HB	1:J:30:TYR:HE1	1.83	0.43
1:J:53:ILE:HG23	1:J:88:ARG:NH2	2.33	0.43
1:K:126:LEU:HD23	1:K:126:LEU:C	2.38	0.43
1:L:35:VAL:HB	1:L:129:ILE:HD12	1.99	0.43
1:P:38:PHE:HD2	1:P:147:ARG:NH2	2.16	0.43
1:T:38:PHE:CD1	1:T:38:PHE:C	2.91	0.43
1:C:11:GLU:CD	1:C:27:LEU:HB3	2.38	0.43
2:D:158:ALA:O	2:D:162:VAL:HG23	2.18	0.43
1:F:76:SER:HB3	1:F:104:ARG:NH1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:PRO:C	1:J:7:ARG:H	2.21	0.43
1:K:55:PHE:CD1	1:K:149:VAL:HG22	2.53	0.43
1:L:51:GLU:O	1:L:54:ALA:HB3	2.18	0.43
1:P:15:GLN:NE2	1:P:24:GLU:OE2	2.52	0.43
1:P:104:ARG:HH22	1:Q:104:ARG:NH1	2.15	0.43
1:Q:59:VAL:HA	1:Q:62:PHE:HD2	1.82	0.43
1:Q:159:PHE:CG	1:R:145:VAL:HG21	2.53	0.43
1:S:49:PRO:C	1:S:50:THR:HG1	2.21	0.43
1:T:143:LYS:N	1:T:144:PRO:CD	2.81	0.43
1:A:154:ARG:NH2	1:B:148:SER:H	2.16	0.43
1:C:149:VAL:O	1:C:152:THR:N	2.51	0.43
1:I:145:VAL:HG21	1:J:159:PHE:HE1	1.78	0.43
1:K:126:LEU:N	1:K:139:THR:O	2.47	0.43
1:L:31:ARG:HA	1:L:31:ARG:HD3	1.89	0.43
1:L:34:TYR:CD1	1:L:130:ASP:HA	2.54	0.43
1:P:80:HIS:HB3	1:P:100:LEU:HD12	2.00	0.43
1:Q:16:ALA:HB1	1:Q:100:LEU:O	2.18	0.43
1:R:119:ASP:OD2	1:R:143:LYS:HE2	2.18	0.43
1:R:16:ALA:HA	1:R:101:LEU:HA	1.99	0.43
1:K:104:ARG:HG3	1:T:120:GLY:C	2.39	0.43
1:A:88:ARG:HA	1:A:92:GLY:O	2.18	0.43
1:B:53:ILE:HG12	1:B:93:LEU:HD22	2.00	0.43
1:C:136:ARG:HB3	1:C:159:PHE:CE2	2.54	0.43
1:E:43:ASP:HB2	1:E:75:ASP:CG	2.39	0.43
1:F:16:ALA:HB2	1:F:101:LEU:CD1	2.49	0.43
1:B:160:GLN:OE1	1:K:164:LYS:O	2.36	0.43
1:L:162:VAL:O	1:L:166:GLY:HA2	2.17	0.43
1:P:75:ASP:HA	1:Q:104:ARG:NH2	2.33	0.43
1:Q:50:THR:HG23	1:Q:52:ILE:H	1.84	0.43
1:T:42:ALA:HB3	1:T:45:THR:HG21	2.01	0.43
1:A:145:VAL:HG11	1:B:159:PHE:CE1	2.53	0.43
1:A:160:GLN:O	1:A:164:LYS:HB3	2.19	0.43
1:A:38:PHE:CD1	1:A:38:PHE:O	2.72	0.43
1:E:105:LYS:HB2	1:E:107:GLU:HG2	2.01	0.43
1:G:151:GLU:OE2	1:G:154:ARG:NH2	2.52	0.43
1:J:112:TYR:HB2	1:J:114:VAL:HG22	1.99	0.43
1:I:2:VAL:HG23	1:J:1:MET:N	2.34	0.43
1:J:38:PHE:O	1:J:72:CYS:N	2.52	0.43
1:M:11:GLU:OE1	1:M:27:LEU:HB3	2.19	0.43
1:P:137:GLN:HG2	1:P:155:LEU:HD13	2.01	0.43
1:P:88:ARG:HA	1:P:92:GLY:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:LEU:HG	1:R:3:LEU:H	1.62	0.43
1:A:50:THR:O	1:A:54:ALA:HB2	2.19	0.43
1:B:43:ASP:O	1:B:44:PHE:HB2	2.18	0.43
2:D:110:LYS:HG2	2:D:115:PHE:HB2	1.99	0.43
1:C:5:PRO:HD2	2:D:123:PHE:CD1	2.54	0.43
1:G:136:ARG:HB3	1:G:159:PHE:CE1	2.54	0.43
1:H:130:ASP:OD1	1:H:132:ASN:N	2.52	0.43
1:H:89:LYS:C	1:H:89:LYS:HD3	2.39	0.43
1:J:75:ASP:HB2	1:J:80:HIS:HE1	1.83	0.43
1:K:96:MET:HA	1:K:96:MET:HE2	1.99	0.43
1:L:16:ALA:O	1:L:22:PHE:HA	2.18	0.43
1:M:58:GLN:HA	1:M:58:GLN:NE2	2.32	0.43
1:Q:105:LYS:HE3	1:Q:107:GLU:OE1	2.19	0.43
1:Q:137:GLN:HG3	1:Q:155:LEU:HD22	2.00	0.43
1:F:40:TYR:HA	1:F:124:ARG:HG2	2.01	0.43
1:G:168:VAL:CG2	1:G:170:PRO:HD2	2.49	0.43
1:H:30:TYR:O	1:H:33:LYS:HB2	2.19	0.43
1:H:34:TYR:HB2	1:H:66:ASN:O	2.19	0.43
1:I:48:CYS:SG	1:J:169:CYS:HA	2.58	0.43
1:M:48:CYS:N	1:M:49:PRO:HD3	2.34	0.43
1:O:126:LEU:HD23	1:O:127:PHE:N	2.33	0.43
1:O:162:VAL:HG21	1:P:145:VAL:CG2	2.44	0.43
1:A:137:GLN:HB2	1:A:159:PHE:HZ	1.84	0.43
1:B:35:VAL:HB	1:B:129:ILE:HB	2.00	0.43
2:D:49:PRO:O	2:D:53:ILE:HB	2.19	0.43
1:E:58:GLN:HB2	1:E:149:VAL:HG11	2.00	0.43
1:E:82:ALA:O	1:E:85:ASN:HB2	2.19	0.43
1:F:105:LYS:CB	1:F:107:GLU:HG3	2.49	0.43
1:G:2:VAL:HG12	1:G:4:LEU:CD1	2.48	0.43
1:I:25:ILE:HD11	1:I:101:LEU:CD1	2.43	0.43
1:K:18:ILE:O	1:K:21:GLU:N	2.52	0.43
1:L:39:PHE:CD1	1:L:114:VAL:HG21	2.54	0.43
1:L:117:GLU:HA	1:L:117:GLU:OE1	2.18	0.43
1:M:143:LYS:H	1:M:143:LYS:CD	2.31	0.43
1:O:116:ASP:O	1:O:116:ASP:OD1	2.36	0.43
1:O:53:ILE:H	1:O:53:ILE:HG13	1.54	0.43
1:Q:76:SER:HB3	1:Q:104:ARG:HB2	2.00	0.43
1:R:153:LEU:O	1:R:157:ASP:CG	2.57	0.43
1:T:124:ARG:HB3	1:T:147:ARG:CZ	2.48	0.43
1:B:41:PRO:HD2	1:B:46:PHE:HZ	1.84	0.43
1:C:4:LEU:HB3	2:D:123:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ILE:HG22	1:E:130:ASP:O	2.19	0.43
1:E:128:ILE:O	1:E:135:LEU:HD12	2.18	0.43
1:G:168:VAL:HG23	1:G:170:PRO:HD2	2.00	0.43
1:G:40:TYR:CD1	1:G:73:SER:HB3	2.54	0.43
1:I:89:LYS:HG3	1:I:89:LYS:O	2.19	0.43
1:J:149:VAL:O	1:J:153:LEU:HD22	2.19	0.43
1:J:15:GLN:HE22	1:J:24:GLU:CB	2.30	0.43
1:A:44:PHE:CD2	1:J:79:SER:HA	2.54	0.43
1:K:23:LYS:HE2	1:K:23:LYS:HB3	1.91	0.43
1:M:2:VAL:O	1:M:4:LEU:HG	2.19	0.43
1:P:53:ILE:HG23	1:P:88:ARG:CZ	2.49	0.43
1:S:43:ASP:O	1:S:44:PHE:HB2	2.19	0.43
1:T:51:GLU:HG2	1:T:55:PHE:HE2	1.83	0.43
1:B:50:THR:CG2	1:B:51:GLU:N	2.82	0.42
1:C:58:GLN:HG3	1:C:61:GLU:CG	2.49	0.42
1:C:68:GLN:HA	1:C:68:GLN:OE1	2.18	0.42
1:E:130:ASP:CB	1:E:131:PRO:HD2	2.47	0.42
1:E:157:ASP:O	1:E:160:GLN:HB2	2.19	0.42
1:H:154:ARG:NH2	1:H:155:LEU:HD21	2.34	0.42
1:I:130:ASP:HB3	1:I:136:ARG:CG	2.49	0.42
1:J:106:GLN:HA	1:J:109:SER:HG	1.83	0.42
1:K:80:HIS:O	1:K:84:ASP:HB2	2.18	0.42
1:M:55:PHE:CZ	1:M:149:VAL:HG22	2.52	0.42
1:P:36:VAL:HG23	1:P:67:CYS:SG	2.59	0.42
1:Q:145:VAL:HG21	1:R:159:PHE:CD1	2.54	0.42
1:R:17:VAL:C	1:R:18:ILE:HG13	2.39	0.42
1:R:5:PRO:HB3	1:R:136:ARG:O	2.19	0.42
1:S:69:VAL:HG12	1:S:98:ILE:HD13	2.02	0.42
1:A:38:PHE:HE1	1:A:52:ILE:HG23	1.84	0.42
1:C:164:LYS:HB3	1:C:165:HIS:CD2	2.54	0.42
1:E:4:LEU:HD22	1:E:4:LEU:N	2.33	0.42
1:E:62:PHE:CE2	1:E:69:VAL:HG21	2.55	0.42
1:F:164:LYS:CD	1:F:165:HIS:CE1	3.02	0.42
1:F:37:LEU:O	1:F:126:LEU:HA	2.19	0.42
1:G:142:ASP:CG	1:G:144:PRO:HD2	2.40	0.42
1:G:151:GLU:OE2	1:G:154:ARG:NE	2.51	0.42
1:G:98:ILE:HG23	1:G:99:PRO:HD2	2.01	0.42
1:I:58:GLN:OE1	1:I:58:GLN:HA	2.19	0.42
1:J:130:ASP:OD1	1:J:134:ILE:HG12	2.19	0.42
1:K:100:LEU:HA	1:K:100:LEU:HD23	1.80	0.42
1:K:55:PHE:CE2	1:K:149:VAL:HA	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:LYS:HG3	1:M:160:GLN:OE1	2.20	0.42
1:O:134:ILE:N	1:O:134:ILE:HD13	2.33	0.42
1:R:153:LEU:H	1:R:153:LEU:CD1	2.32	0.42
1:S:44:PHE:CE1	1:S:83:TRP:HA	2.54	0.42
1:A:116:ASP:CB	1:A:119:ASP:HB2	2.49	0.42
1:A:18:ILE:O	1:A:21:GLU:HB2	2.19	0.42
1:C:134:ILE:HG22	1:C:135:LEU:N	2.34	0.42
1:C:162:VAL:O	1:C:167:GLU:HA	2.20	0.42
1:G:38:PHE:CE1	1:G:71:ALA:HA	2.54	0.42
1:I:44:PHE:HE1	1:I:83:TRP:CD1	2.36	0.42
1:I:96:MET:HA	1:I:96:MET:CE	2.50	0.42
1:J:15:GLN:NE2	1:J:24:GLU:HB2	2.31	0.42
1:J:40:TYR:HE2	1:J:43:ASP:OD1	2.03	0.42
1:L:44:PHE:N	1:L:83:TRP:CE2	2.78	0.42
1:O:143:LYS:N	1:O:144:PRO:HD2	2.35	0.42
1:S:109:SER:HB2	1:S:115:PHE:HB2	2.01	0.42
1:S:154:ARG:NH1	1:T:148:SER:HB2	2.35	0.42
1:A:36:VAL:HB	1:A:69:VAL:HA	2.00	0.42
1:C:143:LYS:N	1:C:144:PRO:CD	2.82	0.42
1:E:16:ALA:O	1:E:22:PHE:HA	2.19	0.42
1:F:149:VAL:O	1:F:153:LEU:HD13	2.19	0.42
1:H:130:ASP:HB2	1:H:131:PRO:CD	2.45	0.42
1:H:32:GLY:N	1:H:131:PRO:O	2.50	0.42
1:M:43:ASP:HB3	1:M:83:TRP:CE3	2.53	0.42
1:N:135:LEU:HD12	1:N:136:ARG:N	2.35	0.42
1:O:101:LEU:HD12	1:O:102:ALA:H	1.84	0.42
1:Q:38:PHE:HB3	1:Q:126:LEU:CG	2.50	0.42
1:R:128:ILE:HG22	1:R:136:ARG:CG	2.50	0.42
1:S:34:TYR:CE1	1:S:131:PRO:HD3	2.54	0.42
1:B:105:LYS:O	1:B:107:GLU:N	2.53	0.42
2:D:105:LYS:HD2	1:E:118:GLU:O	2.20	0.42
1:G:126:LEU:HD23	1:G:127:PHE:N	2.34	0.42
1:H:9:ALA:HA	1:H:10:PRO:HD3	1.81	0.42
1:J:159:PHE:O	1:J:163:GLU:HG3	2.19	0.42
1:L:115:PHE:HE1	1:L:121:ASN:H	1.61	0.42
1:O:86:LEU:CD1	1:O:90:SER:HB3	2.34	0.42
1:P:112:TYR:CD1	1:P:127:PHE:CZ	3.08	0.42
1:Q:137:GLN:HB2	1:Q:159:PHE:CE2	2.54	0.42
1:Q:18:ILE:CG1	1:Q:23:LYS:HD3	2.49	0.42
1:C:13:LYS:HA	1:C:13:LYS:HD2	1.84	0.42
1:E:5:PRO:CB	1:E:136:ARG:O	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ARG:NH1	1:E:133:GLY:HA3	2.34	0.42
1:F:121:ASN:CG	1:G:104:ARG:HE	2.23	0.42
1:J:52:ILE:HG13	1:J:52:ILE:H	1.25	0.42
1:J:69:VAL:HB	1:J:98:ILE:HD12	2.02	0.42
1:M:87:ASP:OD1	1:M:89:LYS:HB3	2.20	0.42
1:M:83:TRP:HE1	1:M:92:GLY:HA2	1.83	0.42
1:R:58:GLN:OE1	1:R:58:GLN:N	2.51	0.42
1:S:143:LYS:HB3	1:S:144:PRO:CD	2.50	0.42
1:T:142:ASP:CG	1:T:143:LYS:H	2.23	0.42
1:B:3:LEU:C	1:B:4:LEU:HD12	2.39	0.42
1:C:36:VAL:HG22	1:C:128:ILE:HG12	2.01	0.42
1:C:62:PHE:HB3	1:C:67:CYS:O	2.18	0.42
1:C:8:PRO:HA	1:C:134:ILE:HA	2.02	0.42
1:G:103:ASP:OD1	1:G:106:GLN:HA	2.18	0.42
1:H:103:ASP:HB2	1:H:108:ILE:CD1	2.43	0.42
1:I:43:ASP:HA	1:I:83:TRP:CZ3	2.55	0.42
1:K:123:PHE:CE2	1:K:143:LYS:HE2	2.55	0.42
1:K:136:ARG:HG3	1:K:159:PHE:CD1	2.55	0.42
1:M:74:THR:HA	1:M:103:ASP:O	2.19	0.42
1:O:5:PRO:HD2	1:P:123:PHE:CE2	2.54	0.42
1:P:129:ILE:HG22	1:P:130:ASP:O	2.20	0.42
1:Q:145:VAL:HG13	1:R:158:ALA:HB1	2.01	0.42
1:B:68:GLN:NE2	1:B:99:PRO:HG3	2.35	0.42
1:K:55:PHE:HE1	1:K:147:ARG:O	2.01	0.42
1:N:39:PHE:CD2	1:N:72:CYS:HB3	2.55	0.42
1:N:51:GLU:O	1:N:54:ALA:N	2.53	0.42
1:N:44:PHE:N	1:N:83:TRP:CE2	2.88	0.42
1:P:19:ASN:O	1:P:21:GLU:HG3	2.20	0.42
1:P:24:GLU:OE1	1:P:24:GLU:HA	2.20	0.42
1:P:93:LEU:HD13	1:P:96:MET:CE	2.49	0.42
1:T:51:GLU:OE2	1:T:147:ARG:CZ	2.67	0.42
1:A:143:LYS:N	1:A:144:PRO:HD2	2.35	0.42
1:A:98:ILE:HA	1:A:99:PRO:HD3	1.88	0.42
1:C:108:ILE:O	1:C:111:ALA:HB3	2.20	0.42
1:C:126:LEU:HB3	1:C:139:THR:CB	2.46	0.42
2:D:135:LEU:HD21	2:D:138:ILE:HD11	2.01	0.42
2:D:105:LYS:HD2	1:E:119:ASP:HA	2.02	0.42
1:F:14:GLY:O	1:F:101:LEU:HD11	2.20	0.42
1:I:165:HIS:CD2	1:I:165:HIS:N	2.85	0.42
1:J:25:ILE:HB	1:J:30:TYR:CE1	2.55	0.42
1:J:83:TRP:NE1	1:J:92:GLY:HA2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:ASN:HA	1:L:137:GLN:OE1	2.20	0.42
1:M:50:THR:HG22	1:M:50:THR:O	2.19	0.42
1:N:147:ARG:NE	1:N:147:ARG:H	1.99	0.42
1:O:114:VAL:HG11	1:O:125:GLY:HA3	2.02	0.42
1:P:105:LYS:HD3	1:P:107:GLU:OE1	2.19	0.42
1:P:138:ILE:HD12	1:P:138:ILE:N	2.34	0.42
1:P:4:LEU:HD22	1:P:4:LEU:N	2.35	0.42
1:Q:80:HIS:CD2	1:Q:100:LEU:HB3	2.54	0.42
1:S:35:VAL:CG1	1:S:70:ILE:HD12	2.50	0.42
1:T:84:ASP:OD1	1:T:96:MET:HB2	2.19	0.42
1:C:142:ASP:CG	1:C:144:PRO:HD2	2.41	0.42
1:C:60:GLU:HA	1:C:63:ASN:ND2	2.35	0.42
1:I:30:TYR:CE1	1:I:68:GLN:HG2	2.55	0.42
1:J:34:TYR:CD2	1:J:156:LEU:HD21	2.55	0.42
1:L:72:CYS:SG	1:L:73:SER:N	2.93	0.42
1:M:130:ASP:OD1	1:M:134:ILE:O	2.38	0.42
1:N:6:ASN:HB3	1:N:7:ARG:HD2	2.02	0.42
1:N:78:TYR:O	1:N:81:LEU:HB3	2.20	0.42
1:P:158:ALA:HA	1:P:161:PHE:CB	2.49	0.42
1:R:38:PHE:HE2	1:R:69:VAL:CG1	2.33	0.42
1:R:76:SER:OG	1:R:78:TYR:N	2.53	0.42
1:S:105:LYS:HB3	1:S:105:LYS:HE2	1.67	0.42
1:S:37:LEU:HD23	1:S:112:TYR:CZ	2.55	0.42
1:A:36:VAL:O	1:A:70:ILE:N	2.53	0.41
1:A:5:PRO:O	1:A:6:ASN:CB	2.67	0.41
1:B:75:ASP:O	1:B:102:ALA:HB1	2.20	0.41
1:L:105:LYS:HE3	1:M:117:GLU:O	2.20	0.41
1:L:127:PHE:HD1	1:L:138:ILE:HG12	1.85	0.41
1:P:65:ARG:CD	1:P:160:GLN:HE22	2.31	0.41
1:P:38:PHE:HB2	1:P:147:ARG:NH1	2.35	0.41
1:Q:88:ARG:HG3	1:Q:94:GLY:N	2.35	0.41
1:T:65:ARG:HB3	1:T:65:ARG:HE	1.53	0.41
1:B:127:PHE:HE1	1:B:138:ILE:HG23	1.85	0.41
1:B:143:LYS:N	1:B:144:PRO:HD2	2.34	0.41
1:E:51:GLU:O	1:E:54:ALA:HB3	2.20	0.41
1:E:87:ASP:O	1:E:88:ARG:HG2	2.20	0.41
1:F:135:LEU:HD12	1:F:136:ARG:H	1.84	0.41
1:I:62:PHE:O	1:I:67:CYS:N	2.50	0.41
1:I:75:ASP:O	1:I:102:ALA:HB1	2.20	0.41
1:J:71:ALA:CB	1:J:100:LEU:HD22	2.51	0.41
1:N:87:ASP:HA	1:N:95:HIS:NE2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:LEU:HD23	1:Q:127:PHE:N	2.35	0.41
1:Q:158:ALA:O	1:Q:161:PHE:HB3	2.20	0.41
1:T:126:LEU:CB	1:T:139:THR:HB	2.41	0.41
1:T:40:TYR:CE1	1:T:73:SER:HB2	2.55	0.41
1:B:58:GLN:NE2	1:B:149:VAL:HG21	2.35	0.41
1:C:53:ILE:HG23	1:C:96:MET:CE	2.51	0.41
1:E:22:PHE:CZ	1:E:81:LEU:HD22	2.55	0.41
1:G:34:TYR:CD1	1:G:130:ASP:HA	2.55	0.41
1:G:96:MET:SD	1:G:100:LEU:HD11	2.60	0.41
1:G:1:MET:HB3	1:H:1:MET:SD	2.60	0.41
1:I:56:SER:O	1:I:97:LYS:HB2	2.20	0.41
1:L:125:GLY:O	1:L:147:ARG:NH1	2.53	0.41
1:M:71:ALA:HB3	1:M:100:LEU:HA	2.01	0.41
1:P:130:ASP:HB3	1:P:136:ARG:HH11	1.85	0.41
1:Q:76:SER:HA	1:Q:102:ALA:HB1	2.02	0.41
1:S:34:TYR:CD1	1:S:131:PRO:HD3	2.55	0.41
1:T:62:PHE:HB3	1:T:67:CYS:CB	2.35	0.41
1:T:86:LEU:HG	1:T:92:GLY:N	2.35	0.41
1:A:34:TYR:CE1	1:A:131:PRO:HD3	2.56	0.41
2:D:51:GLU:HG3	2:D:147:ARG:H	1.85	0.41
2:D:93:LEU:HD13	2:D:96:MET:HG3	2.01	0.41
1:E:143:LYS:N	1:E:144:PRO:HD2	2.35	0.41
1:F:7:ARG:HB3	1:F:8:PRO:HD2	2.02	0.41
1:H:154:ARG:HH22	1:H:155:LEU:HD21	1.85	0.41
1:I:44:PHE:HE1	1:I:83:TRP:CG	2.38	0.41
1:J:169:CYS:HA	1:J:170:PRO:HD3	1.83	0.41
1:M:18:ILE:CD1	1:M:99:PRO:HB3	2.50	0.41
1:M:76:SER:O	1:M:80:HIS:CD2	2.73	0.41
1:N:132:ASN:HB2	1:N:134:ILE:HG13	2.01	0.41
1:N:68:GLN:OE1	1:N:68:GLN:HA	2.19	0.41
1:O:74:THR:HA	1:O:103:ASP:HB2	2.02	0.41
1:P:23:LYS:HD2	1:P:23:LYS:N	2.35	0.41
2:D:110:LYS:HG2	2:D:115:PHE:CB	2.50	0.41
2:D:130:ASP:OD2	2:D:134:ILE:HB	2.20	0.41
1:E:159:PHE:CE1	1:F:145:VAL:HG11	2.54	0.41
1:E:34:TYR:O	1:E:67:CYS:HA	2.21	0.41
1:G:75:ASP:O	1:G:80:HIS:HE1	2.03	0.41
1:I:65:ARG:NE	1:I:153:LEU:HD12	2.35	0.41
1:J:75:ASP:HB3	1:J:79:SER:HB2	2.02	0.41
1:N:94:GLY:C	1:N:95:HIS:HD2	2.24	0.41
1:O:26:CYS:SG	1:O:27:LEU:N	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2:VAL:HG22	1:P:113:GLY:HA3	2.02	0.41
1:S:150:ASP:O	1:S:154:ARG:HB2	2.21	0.41
1:B:116:ASP:HB2	1:B:123:PHE:CE2	2.56	0.41
1:E:51:GLU:OE2	1:E:147:ARG:HB2	2.21	0.41
1:F:146:GLY:O	1:F:147:ARG:HG3	2.21	0.41
1:J:60:GLU:OE1	1:J:60:GLU:CA	2.64	0.41
1:M:37:LEU:HG	1:M:39:PHE:CE1	2.55	0.41
1:Q:115:PHE:CE1	1:Q:117:GLU:HA	2.54	0.41
1:Q:124:ARG:HG3	1:Q:142:ASP:O	2.21	0.41
1:R:36:VAL:CG2	1:R:128:ILE:HG12	2.44	0.41
1:R:43:ASP:OD1	1:R:80:HIS:CE1	2.74	0.41
1:A:12:PHE:CE1	1:A:27:LEU:HD22	2.55	0.41
1:B:137:GLN:OE1	1:B:137:GLN:HA	2.20	0.41
1:C:149:VAL:O	1:C:150:ASP:C	2.57	0.41
1:C:93:LEU:HD13	1:C:96:MET:SD	2.61	0.41
1:F:54:ALA:O	1:F:58:GLN:HG3	2.20	0.41
1:G:34:TYR:CE1	1:G:131:PRO:HD3	2.56	0.41
1:I:126:LEU:C	1:I:127:PHE:CD1	2.94	0.41
1:I:154:ARG:HH21	1:I:155:LEU:HD21	1.85	0.41
1:L:21:GLU:HB2	1:L:23:LYS:HE3	2.02	0.41
1:M:47:VAL:HB	1:M:49:PRO:HD2	2.03	0.41
1:M:77:GLN:O	1:M:81:LEU:N	2.54	0.41
1:O:123:PHE:CD2	1:P:4:LEU:HD12	2.56	0.41
1:Q:59:VAL:HA	1:Q:62:PHE:CD2	2.55	0.41
1:Q:138:ILE:HB	1:R:140:ILE:HB	2.03	0.41
1:B:3:LEU:HD21	1:B:111:ALA:O	2.21	0.41
1:B:36:VAL:O	1:B:69:VAL:HA	2.21	0.41
1:C:58:GLN:HG2	1:C:149:VAL:HG21	2.01	0.41
1:C:61:GLU:CB	1:C:153:LEU:HD21	2.50	0.41
2:D:123:PHE:HA	2:D:143:LYS:HE2	2.02	0.41
1:E:103:ASP:HB2	1:E:108:ILE:CD1	2.46	0.41
1:G:2:VAL:H	1:H:1:MET:HB2	1.86	0.41
1:H:13:LYS:O	1:H:101:LEU:HD11	2.20	0.41
1:H:42:ALA:O	1:H:45:THR:HG23	2.21	0.41
1:K:46:PHE:CE2	1:K:83:TRP:HZ2	2.39	0.41
1:P:84:ASP:O	1:P:94:GLY:N	2.54	0.41
1:P:53:ILE:HG12	1:P:93:LEU:HD23	2.01	0.41
1:T:68:GLN:OE1	1:T:68:GLN:HA	2.19	0.41
2:D:16:ALA:HA	2:D:100:LEU:O	2.21	0.41
2:D:66:ASN:HB2	1:M:166:GLY:HA2	2.03	0.41
1:E:155:LEU:O	1:E:159:PHE:HD1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ASP:OD1	1:F:83:TRP:CZ3	2.74	0.41
1:G:163:GLU:O	1:G:163:GLU:HG2	2.20	0.41
1:G:76:SER:O	1:G:80:HIS:CE1	2.74	0.41
1:I:33:LYS:HD2	1:I:66:ASN:OD1	2.21	0.41
1:L:38:PHE:CD2	1:L:147:ARG:NH2	2.85	0.41
1:L:25:ILE:HD11	1:L:101:LEU:HD13	2.02	0.41
1:N:104:ARG:HH22	1:O:75:ASP:CA	2.32	0.41
1:N:9:ALA:HB2	1:N:135:LEU:HB2	2.03	0.41
1:N:77:GLN:HE21	1:N:77:GLN:HB3	1.71	0.41
1:N:98:ILE:HA	1:N:99:PRO:HD3	1.88	0.41
1:O:12:PHE:CE2	1:O:27:LEU:HD13	2.56	0.41
1:R:3:LEU:HD12	1:R:3:LEU:O	2.20	0.41
1:S:126:LEU:HD23	1:S:127:PHE:N	2.36	0.41
1:K:104:ARG:HG2	1:T:121:ASN:ND2	2.35	0.41
1:T:126:LEU:HB2	1:T:147:ARG:HD3	2.03	0.41
1:A:165:HIS:N	1:A:165:HIS:ND1	2.69	0.41
1:A:61:GLU:CG	1:A:65:ARG:HH21	2.34	0.41
1:B:104:ARG:NH2	1:C:75:ASP:HA	2.36	0.41
1:B:36:VAL:HG23	1:B:67:CYS:SG	2.61	0.41
2:D:17:VAL:O	2:D:99:PRO:HA	2.21	0.41
2:D:120:GLY:HA3	1:E:104:ARG:HB3	2.03	0.41
1:H:123:PHE:HB3	1:H:140:ILE:HD11	2.02	0.41
1:K:31:ARG:CZ	1:K:133:GLY:HA3	2.51	0.41
1:K:65:ARG:HG2	1:K:156:LEU:HG	2.01	0.41
1:L:87:ASP:O	1:L:90:SER:N	2.54	0.41
1:N:80:HIS:CD2	1:N:102:ALA:HB2	2.56	0.41
1:O:68:GLN:HG3	1:O:70:ILE:HG13	2.03	0.41
1:R:68:GLN:HE21	1:R:68:GLN:HA	1.84	0.41
1:S:41:PRO:CD	1:S:124:ARG:HG2	2.42	0.41
1:T:130:ASP:CG	1:T:131:PRO:HD2	2.40	0.41
1:A:69:VAL:C	1:A:70:ILE:HG13	2.41	0.41
1:A:76:SER:HB3	1:A:104:ARG:CZ	2.51	0.41
2:D:34:TYR:CD1	2:D:130:ASP:HA	2.55	0.41
2:D:7:ARG:C	2:D:134:ILE:HG23	2.42	0.41
1:E:4:LEU:HA	1:E:5:PRO:HD3	1.82	0.41
1:G:112:TYR:HB3	1:G:127:PHE:CZ	2.56	0.41
1:I:105:LYS:O	1:I:106:GLN:HB2	2.20	0.41
1:J:139:THR:HG22	1:J:139:THR:O	2.21	0.41
1:J:81:LEU:O	1:J:84:ASP:HB3	2.21	0.41
1:K:39:PHE:O	1:K:40:TYR:HB3	2.21	0.41
1:O:124:ARG:HB3	1:O:147:ARG:CZ	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:116:ASP:HB2	1:P:7:ARG:HH22	1.85	0.41
1:R:39:PHE:N	1:R:39:PHE:CD1	2.89	0.41
1:R:47:VAL:O	1:R:47:VAL:HG23	2.20	0.41
1:T:115:PHE:HA	1:T:122:ALA:HB2	2.03	0.41
1:A:150:ASP:O	1:A:153:LEU:HB2	2.21	0.40
2:D:126:LEU:HB3	2:D:139:THR:CG2	2.52	0.40
2:D:34:TYR:HA	2:D:129:ILE:O	2.20	0.40
1:G:98:ILE:HA	1:G:99:PRO:HD3	1.85	0.40
1:H:40:TYR:CG	1:H:52:ILE:HD11	2.56	0.40
1:J:127:PHE:N	1:J:127:PHE:CD1	2.88	0.40
1:N:105:LYS:HD2	1:N:107:GLU:OE2	2.21	0.40
1:N:18:ILE:HD12	1:N:23:LYS:CB	2.39	0.40
1:O:71:ALA:O	1:O:101:LEU:HB3	2.21	0.40
1:O:130:ASP:HB2	1:O:131:PRO:HD2	2.02	0.40
1:O:48:CYS:SG	1:O:48:CYS:O	2.79	0.40
1:O:51:GLU:O	1:O:54:ALA:HB3	2.20	0.40
1:P:16:ALA:HA	1:P:100:LEU:O	2.20	0.40
1:Q:4:LEU:HA	1:Q:5:PRO:HD3	1.73	0.40
1:S:22:PHE:C	1:S:23:LYS:HD2	2.42	0.40
1:T:126:LEU:HB3	1:T:139:THR:CB	2.41	0.40
1:T:164:LYS:HB2	1:T:164:LYS:HE3	1.89	0.40
1:C:105:LYS:HD3	1:C:107:GLU:OE1	2.22	0.40
2:D:10:PRO:HD2	2:D:112:TYR:OH	2.20	0.40
2:D:127:PHE:CE2	2:D:138:ILE:HG23	2.55	0.40
1:E:128:ILE:HD12	1:E:137:GLN:HG3	2.03	0.40
1:E:156:LEU:HD12	1:E:156:LEU:HA	1.84	0.40
1:I:3:LEU:C	1:I:4:LEU:HD12	2.41	0.40
1:K:124:ARG:HD3	1:K:147:ARG:NH2	2.36	0.40
1:K:61:GLU:O	1:K:65:ARG:HD3	2.21	0.40
1:L:105:LYS:C	1:L:107:GLU:N	2.74	0.40
1:L:137:GLN:HG2	1:L:155:LEU:HD13	2.03	0.40
1:Q:35:VAL:HB	1:Q:129:ILE:HD12	2.02	0.40
1:Q:4:LEU:O	1:Q:135:LEU:HD23	2.22	0.40
1:S:142:ASP:HB2	1:T:136:ARG:HG2	2.04	0.40
1:T:105:LYS:C	1:T:107:GLU:H	2.23	0.40
1:T:71:ALA:HB3	1:T:100:LEU:CD2	2.52	0.40
1:C:2:VAL:CG2	2:D:3:LEU:HB3	2.51	0.40
1:C:61:GLU:HB3	1:C:153:LEU:HD21	2.04	0.40
2:D:142:ASP:C	2:D:144:PRO:HD2	2.42	0.40
2:D:69:VAL:HG12	2:D:70:ILE:N	2.37	0.40
2:D:53:ILE:HG13	2:D:96:MET:CE	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ALA:CB	1:G:101:LEU:HA	2.52	0.40
1:G:34:TYR:CE1	1:G:130:ASP:HA	2.56	0.40
1:G:40:TYR:OH	1:G:80:HIS:HD2	2.04	0.40
1:H:4:LEU:HB3	1:H:5:PRO:CD	2.51	0.40
1:H:86:LEU:HD12	1:H:86:LEU:HA	1.89	0.40
1:L:116:ASP:CG	1:L:123:PHE:CZ	2.95	0.40
1:M:108:ILE:O	1:M:112:TYR:HD1	2.05	0.40
1:N:123:PHE:CE1	1:N:143:LYS:HG2	2.57	0.40
1:N:141:ASN:ND2	1:N:145:VAL:HG12	2.36	0.40
1:P:157:ASP:OD1	1:P:158:ALA:N	2.54	0.40
1:Q:40:TYR:CE2	1:Q:42:ALA:O	2.75	0.40
1:Q:93:LEU:HD13	1:Q:96:MET:CE	2.52	0.40
1:T:124:ARG:HD2	1:T:145:VAL:O	2.21	0.40
1:A:74:THR:CG2	1:A:106:GLN:HG2	2.49	0.40
1:A:28:LYS:HE3	1:A:31:ARG:NE	2.23	0.40
1:A:43:ASP:OD1	1:A:83:TRP:CZ3	2.74	0.40
1:C:126:LEU:HD23	1:C:127:PHE:N	2.37	0.40
1:C:161:PHE:CE1	1:C:165:HIS:CE1	3.10	0.40
1:E:4:LEU:O	1:E:135:LEU:HD23	2.21	0.40
1:E:32:GLY:HA2	1:E:131:PRO:CB	2.51	0.40
1:G:121:ASN:N	1:G:121:ASN:OD1	2.55	0.40
1:I:12:PHE:HB2	1:I:108:ILE:CG1	2.51	0.40
1:I:4:LEU:CD1	1:J:1:MET:H2	2.34	0.40
1:L:168:VAL:O	1:L:168:VAL:HG12	2.20	0.40
1:L:44:PHE:HA	1:L:83:TRP:NE1	2.37	0.40
1:Q:145:VAL:HG13	1:R:158:ALA:CB	2.50	0.40
1:T:38:PHE:HB2	1:T:125:GLY:O	2.21	0.40
1:T:59:VAL:HG13	1:T:63:ASN:OD1	2.21	0.40
1:A:5:PRO:HD3	1:B:140:ILE:HG21	2.04	0.40
1:B:155:LEU:O	1:B:158:ALA:N	2.55	0.40
1:C:35:VAL:CG1	1:C:129:ILE:HD12	2.52	0.40
1:C:84:ASP:CB	1:C:93:LEU:HD12	2.52	0.40
2:D:162:VAL:O	2:D:166:GLY:N	2.54	0.40
1:E:159:PHE:CG	1:F:145:VAL:HG21	2.56	0.40
1:G:25:ILE:CD1	1:G:101:LEU:HD13	2.49	0.40
1:G:116:ASP:OD1	1:G:118:GLU:HB3	2.21	0.40
1:H:74:THR:HG22	1:H:74:THR:O	2.22	0.40
1:H:84:ASP:O	1:H:94:GLY:N	2.54	0.40
1:I:25:ILE:O	1:I:25:ILE:HG13	2.21	0.40
1:I:86:LEU:HD23	1:I:91:GLY:O	2.22	0.40
1:M:38:PHE:HA	1:M:125:GLY:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:12:PHE:CZ	1:N:27:LEU:HD13	2.57	0.40
1:R:109:SER:HB3	1:R:114:VAL:CG2	2.51	0.40
1:R:36:VAL:HG23	1:R:67:CYS:SG	2.62	0.40
1:R:98:ILE:HA	1:R:99:PRO:HD3	1.97	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	163/219 (74%)	154 (94%)	9 (6%)	0	100	100
1	B	164/219 (75%)	154 (94%)	10 (6%)	0	100	100
1	C	172/219 (78%)	157 (91%)	15 (9%)	0	100	100
1	E	165/219 (75%)	155 (94%)	8 (5%)	2 (1%)	13	48
1	F	170/219 (78%)	149 (88%)	21 (12%)	0	100	100
1	G	170/219 (78%)	157 (92%)	11 (6%)	2 (1%)	13	48
1	H	169/219 (77%)	151 (89%)	18 (11%)	0	100	100
1	I	165/219 (75%)	154 (93%)	11 (7%)	0	100	100
1	J	169/219 (77%)	155 (92%)	12 (7%)	2 (1%)	13	48
1	K	168/219 (77%)	156 (93%)	12 (7%)	0	100	100
1	L	169/219 (77%)	155 (92%)	13 (8%)	1 (1%)	25	64
1	M	169/219 (77%)	156 (92%)	12 (7%)	1 (1%)	25	64
1	N	163/219 (74%)	147 (90%)	16 (10%)	0	100	100
1	O	163/219 (74%)	153 (94%)	10 (6%)	0	100	100
1	P	165/219 (75%)	152 (92%)	12 (7%)	1 (1%)	25	64
1	Q	159/219 (73%)	145 (91%)	14 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	R	164/219 (75%)	147 (90%)	17 (10%)	0	100 100
1	S	170/219 (78%)	150 (88%)	19 (11%)	1 (1%)	25 64
1	T	168/219 (77%)	151 (90%)	17 (10%)	0	100 100
2	D	166/219 (76%)	156 (94%)	10 (6%)	0	100 100
All	All	3331/4380 (76%)	3054 (92%)	267 (8%)	10 (0%)	41 76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	47	VAL
1	M	47	VAL
1	E	171	VAL
1	J	47	VAL
1	J	48	CYS
1	E	168	VAL
1	G	2	VAL
1	L	168	VAL
1	G	49	PRO
1	S	168	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	144/188 (77%)	130 (90%)	14 (10%)	8 31
1	B	145/188 (77%)	134 (92%)	11 (8%)	13 43
1	C	152/188 (81%)	140 (92%)	12 (8%)	12 41
1	E	147/188 (78%)	133 (90%)	14 (10%)	8 32
1	F	149/188 (79%)	137 (92%)	12 (8%)	11 40
1	G	150/188 (80%)	139 (93%)	11 (7%)	14 44
1	H	149/188 (79%)	142 (95%)	7 (5%)	26 63
1	I	145/188 (77%)	132 (91%)	13 (9%)	9 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	149/188 (79%)	136 (91%)	13 (9%)	10 37
1	K	148/188 (79%)	137 (93%)	11 (7%)	13 44
1	L	149/188 (79%)	134 (90%)	15 (10%)	7 29
1	M	148/188 (79%)	141 (95%)	7 (5%)	26 63
1	N	143/188 (76%)	135 (94%)	8 (6%)	21 56
1	O	145/188 (77%)	134 (92%)	11 (8%)	13 43
1	P	145/188 (77%)	133 (92%)	12 (8%)	11 39
1	Q	142/188 (76%)	128 (90%)	14 (10%)	8 30
1	R	145/188 (77%)	135 (93%)	10 (7%)	15 48
1	S	149/188 (79%)	133 (89%)	16 (11%)	6 26
1	T	148/188 (79%)	139 (94%)	9 (6%)	18 53
2	D	146/188 (78%)	134 (92%)	12 (8%)	11 39
All	All	2938/3760 (78%)	2706 (92%)	232 (8%)	12 41

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	45	THR
1	A	53	ILE
1	A	74	THR
1	A	77	GLN
1	A	84	ASP
1	A	107	GLU
1	A	129	ILE
1	A	132	ASN
1	A	136	ARG
1	A	145	VAL
1	A	150	ASP
1	A	156	LEU
1	A	165	HIS
1	B	26	CYS
1	B	29	ASP
1	B	37	LEU
1	B	56	SER
1	B	74	THR
1	B	77	GLN
1	B	87	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	97	LYS
1	B	132	ASN
1	B	143	LYS
1	B	145	VAL
1	C	52	ILE
1	C	53	ILE
1	C	67	CYS
1	C	76	SER
1	C	80	HIS
1	C	98	ILE
1	C	104	ARG
1	C	109	SER
1	C	139	THR
1	C	165	HIS
1	C	169	CYS
1	C	171	VAL
2	D	7	ARG
2	D	15	GLN
2	D	26	CYS
2	D	28	LYS
2	D	43	ASP
2	D	46	PHE
2	D	74	THR
2	D	78	TYR
2	D	80	HIS
2	D	105	LYS
2	D	132	ASN
2	D	139	THR
1	E	17	VAL
1	E	37	LEU
1	E	45	THR
1	E	46	PHE
1	E	90	SER
1	E	114	VAL
1	E	126	LEU
1	E	130	ASP
1	E	137	GLN
1	E	148	SER
1	E	155	LEU
1	E	165	HIS
1	E	167	GLU
1	E	169	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	0	THR
1	F	25	ILE
1	F	52	ILE
1	F	53	ILE
1	F	59	VAL
1	F	77	GLN
1	F	84	ASP
1	F	90	SER
1	F	105	LYS
1	F	121	ASN
1	F	129	ILE
1	F	143	LYS
1	G	38	PHE
1	G	47	VAL
1	G	48	CYS
1	G	58	GLN
1	G	67	CYS
1	G	75	ASP
1	G	83	TRP
1	G	90	SER
1	G	104	ARG
1	G	109	SER
1	G	116	ASP
1	H	84	ASP
1	H	97	LYS
1	H	103	ASP
1	H	104	ARG
1	H	114	VAL
1	H	138	ILE
1	H	153	LEU
1	I	47	VAL
1	I	51	GLU
1	I	66	ASN
1	I	74	THR
1	I	97	LYS
1	I	109	SER
1	I	114	VAL
1	I	126	LEU
1	I	130	ASP
1	I	142	ASP
1	I	148	SER
1	I	150	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	165	HIS
1	J	1	MET
1	J	18	ILE
1	J	22	PHE
1	J	36	VAL
1	J	48	CYS
1	J	52	ILE
1	J	58	GLN
1	J	60	GLU
1	J	78	TYR
1	J	114	VAL
1	J	130	ASP
1	J	134	ILE
1	J	140	ILE
1	K	45	THR
1	K	74	THR
1	K	75	ASP
1	K	76	SER
1	K	84	ASP
1	K	90	SER
1	K	93	LEU
1	K	106	GLN
1	K	143	LYS
1	K	145	VAL
1	K	147	ARG
1	L	3	LEU
1	L	6	ASN
1	L	7	ARG
1	L	19	ASN
1	L	23	LYS
1	L	26	CYS
1	L	29	ASP
1	L	43	ASP
1	L	95	HIS
1	L	97	LYS
1	L	119	ASP
1	L	121	ASN
1	L	156	LEU
1	L	162	VAL
1	L	167	GLU
1	M	50	THR
1	M	57	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	64	SER
1	M	97	LYS
1	M	104	ARG
1	M	109	SER
1	M	143	LYS
1	N	7	ARG
1	N	26	CYS
1	N	50	THR
1	N	93	LEU
1	N	96	MET
1	N	119	ASP
1	N	147	ARG
1	N	150	ASP
1	O	31	ARG
1	O	40	TYR
1	O	53	ILE
1	O	59	VAL
1	O	64	SER
1	O	74	THR
1	O	86	LEU
1	O	104	ARG
1	O	114	VAL
1	O	139	THR
1	O	156	LEU
1	P	23	LYS
1	P	40	TYR
1	P	47	VAL
1	P	48	CYS
1	P	50	THR
1	P	74	THR
1	P	76	SER
1	P	93	LEU
1	P	98	ILE
1	P	139	THR
1	P	150	ASP
1	P	162	VAL
1	Q	3	LEU
1	Q	4	LEU
1	Q	17	VAL
1	Q	31	ARG
1	Q	39	PHE
1	Q	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	52	ILE
1	Q	57	ASP
1	Q	74	THR
1	Q	86	LEU
1	Q	95	HIS
1	Q	109	SER
1	Q	154	ARG
1	Q	157	ASP
1	R	3	LEU
1	R	43	ASP
1	R	50	THR
1	R	59	VAL
1	R	74	THR
1	R	75	ASP
1	R	80	HIS
1	R	90	SER
1	R	119	ASP
1	R	153	LEU
1	S	2	VAL
1	S	18	ILE
1	S	38	PHE
1	S	48	CYS
1	S	50	THR
1	S	51	GLU
1	S	52	ILE
1	S	74	THR
1	S	90	SER
1	S	97	LYS
1	S	100	LEU
1	S	104	ARG
1	S	119	ASP
1	S	140	ILE
1	S	150	ASP
1	S	167	GLU
1	T	31	ARG
1	T	37	LEU
1	T	47	VAL
1	T	64	SER
1	T	65	ARG
1	T	80	HIS
1	T	83	TRP
1	T	109	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	114	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	B	58	GLN
1	B	77	GLN
1	B	132	ASN
1	C	63	ASN
1	C	85	ASN
1	C	121	ASN
1	C	132	ASN
1	C	141	ASN
1	C	165	HIS
2	D	15	GLN
2	D	68	GLN
1	E	15	GLN
1	E	68	GLN
1	E	80	HIS
1	E	137	GLN
1	F	15	GLN
1	F	80	HIS
1	F	141	ASN
1	F	165	HIS
1	G	6	ASN
1	G	15	GLN
1	G	58	GLN
1	G	80	HIS
1	G	132	ASN
1	G	141	ASN
1	G	160	GLN
1	H	19	ASN
1	H	58	GLN
1	I	80	HIS
1	I	141	ASN
1	I	165	HIS
1	J	58	GLN
1	J	80	HIS
1	J	132	ASN
1	J	165	HIS
1	K	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	68	GLN
1	K	77	GLN
1	K	85	ASN
1	K	106	GLN
1	K	165	HIS
1	L	6	ASN
1	L	19	ASN
1	L	160	GLN
1	M	15	GLN
1	M	58	GLN
1	M	66	ASN
1	M	80	HIS
1	N	141	ASN
1	O	68	GLN
1	O	121	ASN
1	O	137	GLN
1	O	141	ASN
1	P	66	ASN
1	P	80	HIS
1	P	106	GLN
1	Q	15	GLN
1	Q	77	GLN
1	Q	80	HIS
1	R	68	GLN
1	R	121	ASN
1	R	141	ASN
1	S	19	ASN
1	S	77	GLN
1	S	80	HIS
1	S	85	ASN
1	S	121	ASN
1	S	165	HIS
1	T	63	ASN
1	T	85	ASN
1	T	121	ASN
1	T	160	GLN
1	T	165	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 carbohydrates 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	165/219 (75%)	-0.28	0	100	100	32, 41, 45, 47	0
1	B	166/219 (75%)	-0.28	0	100	100	34, 41, 45, 49	0
1	C	174/219 (79%)	-0.30	0	100	100	34, 41, 46, 49	0
1	E	169/219 (77%)	-0.34	0	100	100	32, 39, 44, 48	0
1	F	172/219 (78%)	-0.36	0	100	100	32, 40, 45, 46	0
1	G	172/219 (78%)	-0.26	0	100	100	34, 41, 45, 47	0
1	H	171/219 (78%)	-0.26	0	100	100	31, 40, 45, 50	0
1	I	167/219 (76%)	-0.29	0	100	100	30, 40, 46, 49	0
1	J	171/219 (78%)	-0.37	0	100	100	30, 40, 44, 49	0
1	K	170/219 (77%)	-0.37	0	100	100	27, 39, 42, 45	0
1	L	171/219 (78%)	-0.30	0	100	100	31, 40, 44, 48	0
1	M	171/219 (78%)	-0.20	1 (0%)	89	72	32, 41, 46, 49	0
1	N	165/219 (75%)	-0.27	0	100	100	31, 40, 47, 50	0
1	O	167/219 (76%)	-0.32	0	100	100	27, 41, 44, 46	0
1	P	167/219 (76%)	-0.27	0	100	100	33, 42, 45, 49	0
1	Q	163/219 (74%)	-0.33	0	100	100	31, 40, 45, 46	0
1	R	168/219 (76%)	-0.20	0	100	100	31, 42, 46, 50	0
1	S	172/219 (78%)	-0.31	0	100	100	31, 41, 45, 49	0
1	T	170/219 (77%)	-0.27	0	100	100	35, 41, 47, 57	0
2	D	168/219 (76%)	-0.34	0	100	100	32, 40, 45, 50	0
All	All	3379/4380 (77%)	-0.29	1 (0%)	100	100	27, 40, 45, 57	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	168	VAL	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.