



Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 06:58 AM JST

PDB ID : 8IBD / pdb_00008ibd
EMDB ID : EMD-35340
Title : Respiratory complex CI:CIII2, type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

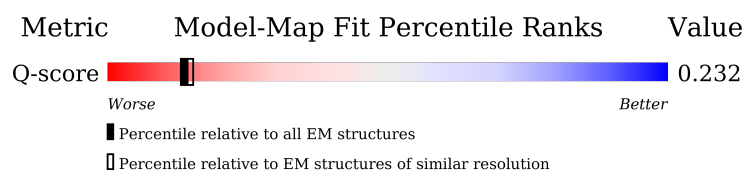
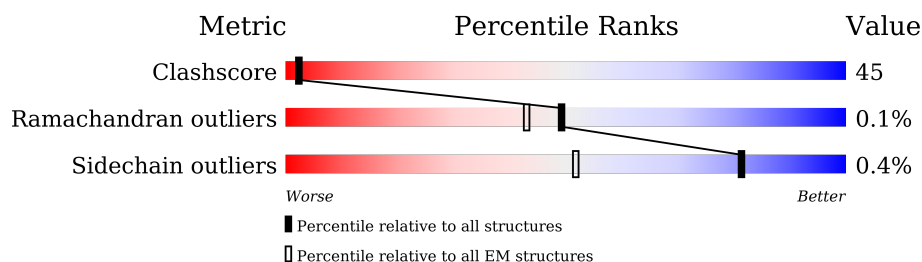
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	224	
3	C	263	
4	D	463	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	AI	274	
49	Ae	274	
49	Ai	274	
50	AF	111	
50	Af	111	
51	AG	82	
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	B	301	-	-	X	-
56	SF4	F	502	-	-	X	-
56	SF4	G	802	-	-	X	-
56	SF4	I	302	-	-	X	-
56	SF4	I	303	-	-	X	-
57	UQ1	B	302	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
63	ADP	O	401	-	-	X	-
69	HEC	AD	401	X	-	-	-
69	HEC	Ad	401	X	-	-	-
71	3PH	Ad	402	-	-	X	-

2 Entry composition [i](#)

There are 71 unique types of molecules in this entry. The entry contains 96599 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			799	552	112	130	5		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1643	1061	279	300	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	427	Total	C	N	O	S	0	0
			3438	2197	591	626	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total	C	N	O	S	0	0
			3288	2073	588	605	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total	C	N	O	S	0	0
			2532	1702	383	425	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total	C	N	O	S	0	0
			1380	869	237	262	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	163	Total	C	N	O	S	0	0
			1229	828	175	211	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	116	LEU	ASN	conflict	UNP P03925
J	117	GLY	LEU	conflict	UNP P03925

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	116	Total	C	N	O	S	0	0
			940	598	161	177	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	89	Total	C	N	O	S	0	0
			718	462	105	146	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total	C	N	O	S	0	0
			1145	736	203	198	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	95	Total	C	N	O	S	0	0
			802	523	140	136	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	73	Total	C	N	O	S	0	0
			582	383	102	95	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	123	Total	C	N	O	S	0	0
			1025	658	181	182	4		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	84	Total	C	N	O	S	0	0
			686	435	128	121	2		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	23	Total	C	N	O	0	0
			193	126	30	37		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	395	Total	C	N	O	S	0	0
			3077	1918	545	598	16		
45	Aa	394	Total	C	N	O	S	0	0
			3076	1923	545	592	16		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
46	Ab	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
47	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	236	Total	C	N	O	S	0	0
			1878	1200	323	341	14		
48	Ad	239	Total	C	N	O	S	0	0
			1903	1215	326	348	14		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	109	Total	C	N	O	S	0	0
			830	525	152	147	6		
49	AI	28	Total	C	N	O		0	0
			200	129	37	34			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	Ai	28	Total	C	N	O		0	0
			204	130	40	34			

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	97	Total	C	N	O	S	0	0
			855	546	152	154	3		
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	74	Total	C	N	O	S	0	0
			622	404	114	103	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
52	Ah	62	Total	C	N	O	S	0	0
			512	316	93	98	5		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	21	Total	C	N	O	0	0
			165	109	27	29		
53	Aj	43	Total	C	N	O	0	0
			345	223	59	63		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

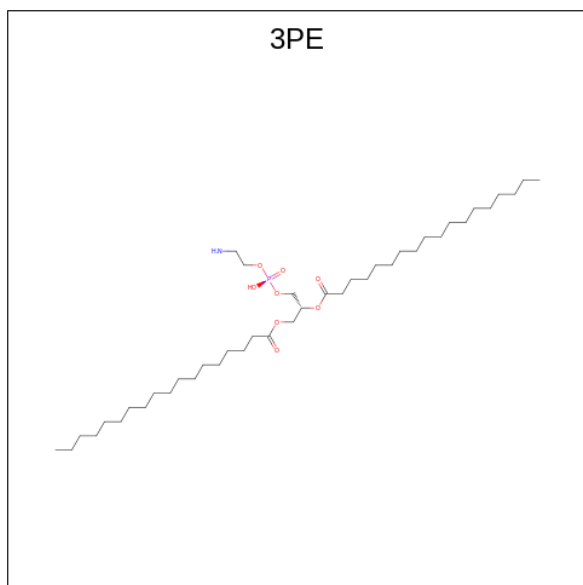
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	17	Total	C	N	O	S	0	0
			118	77	19	21	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ak	38	Total	C	N	O	S	0	0
			309	202	58	48	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



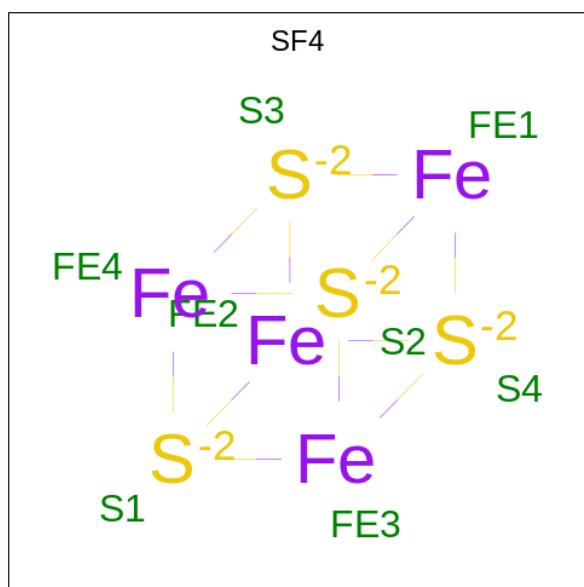
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
55	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
55	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	d	1	Total	C	N	O	P	0
			31	21	1	8	1	
55	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	m	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



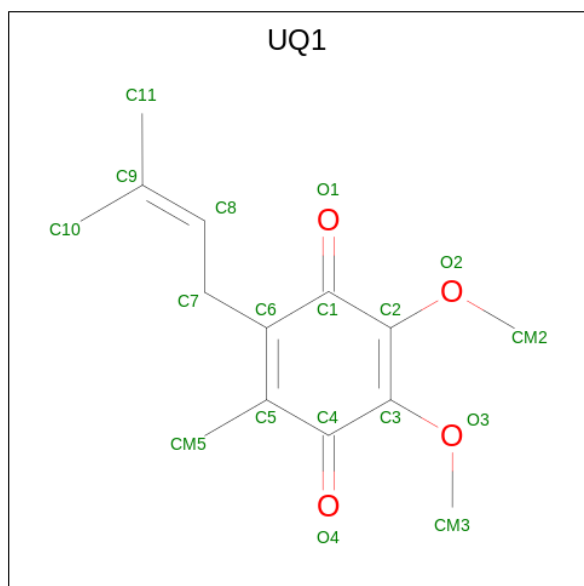
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

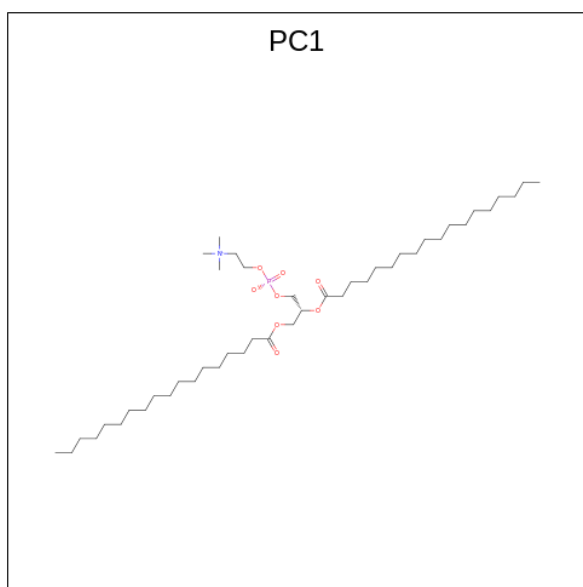
Mol	Chain	Residues	Atoms			AltConf
56	F	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 57 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



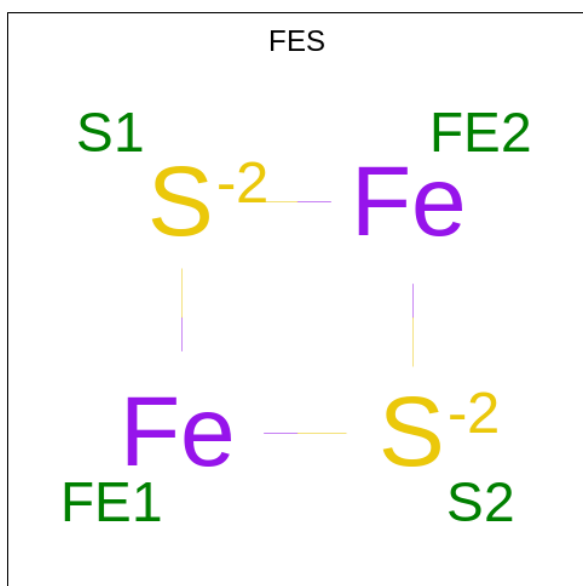
Mol	Chain	Residues	Atoms			AltConf
57	B	1	Total	C	O	0
			18	14	4	

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



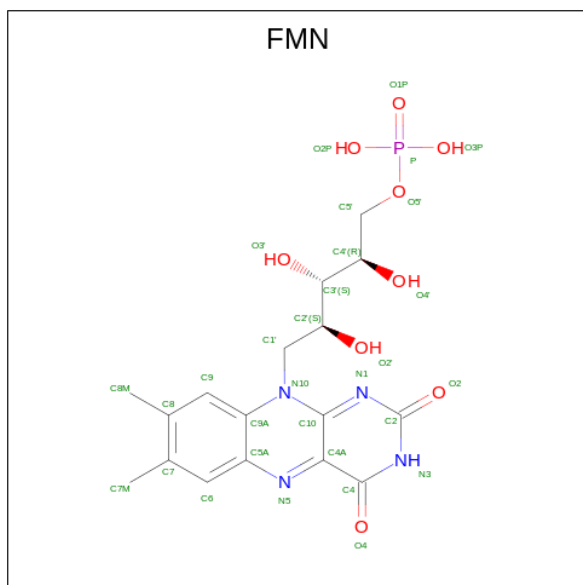
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

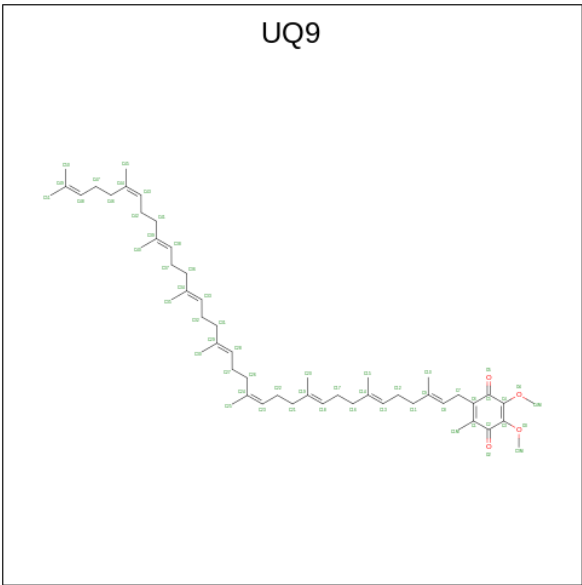
Mol	Chain	Residues	Atoms			AltConf
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



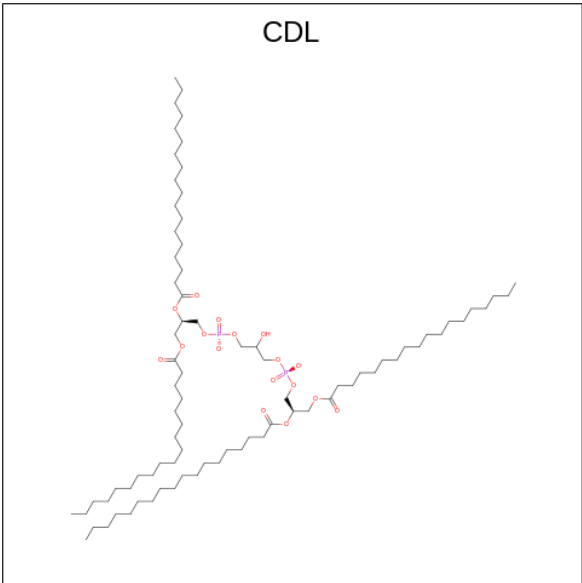
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 61 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



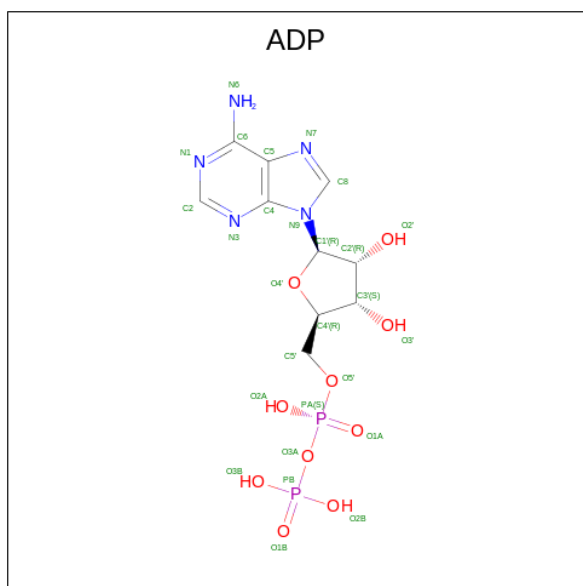
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			78	59	17	2	
62	X	1	Total	C	O	P	0
			67	48	17	2	

Continued on next page...

Continued from previous page...

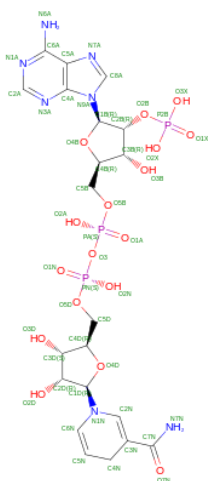
Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	Ag	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
63	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 64 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

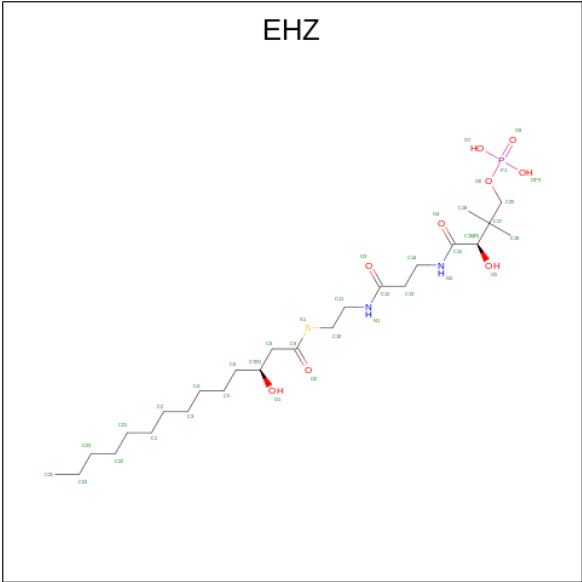


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

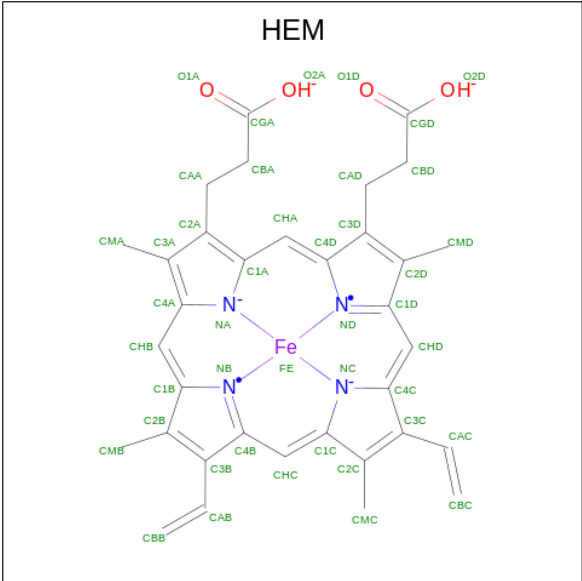
Mol	Chain	Residues	Atoms	AltConf
65	R	1	Total Zn 1 1	0

- Molecule 66 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



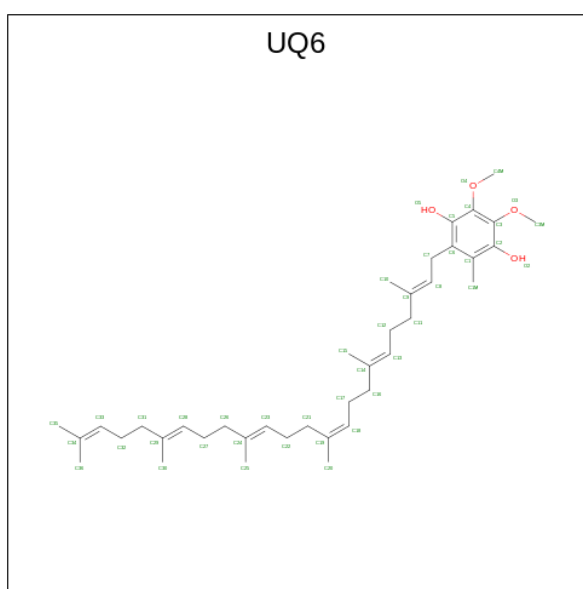
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

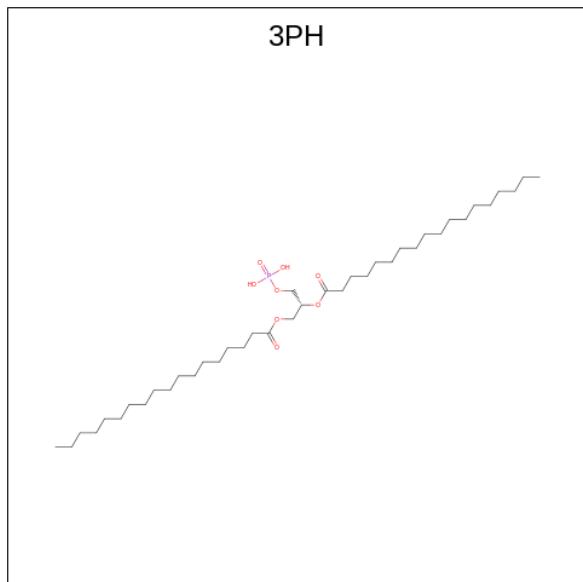
- Molecule 68 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			28	24	4	
68	Ac	1	Total	C	O	0
			28	24	4	

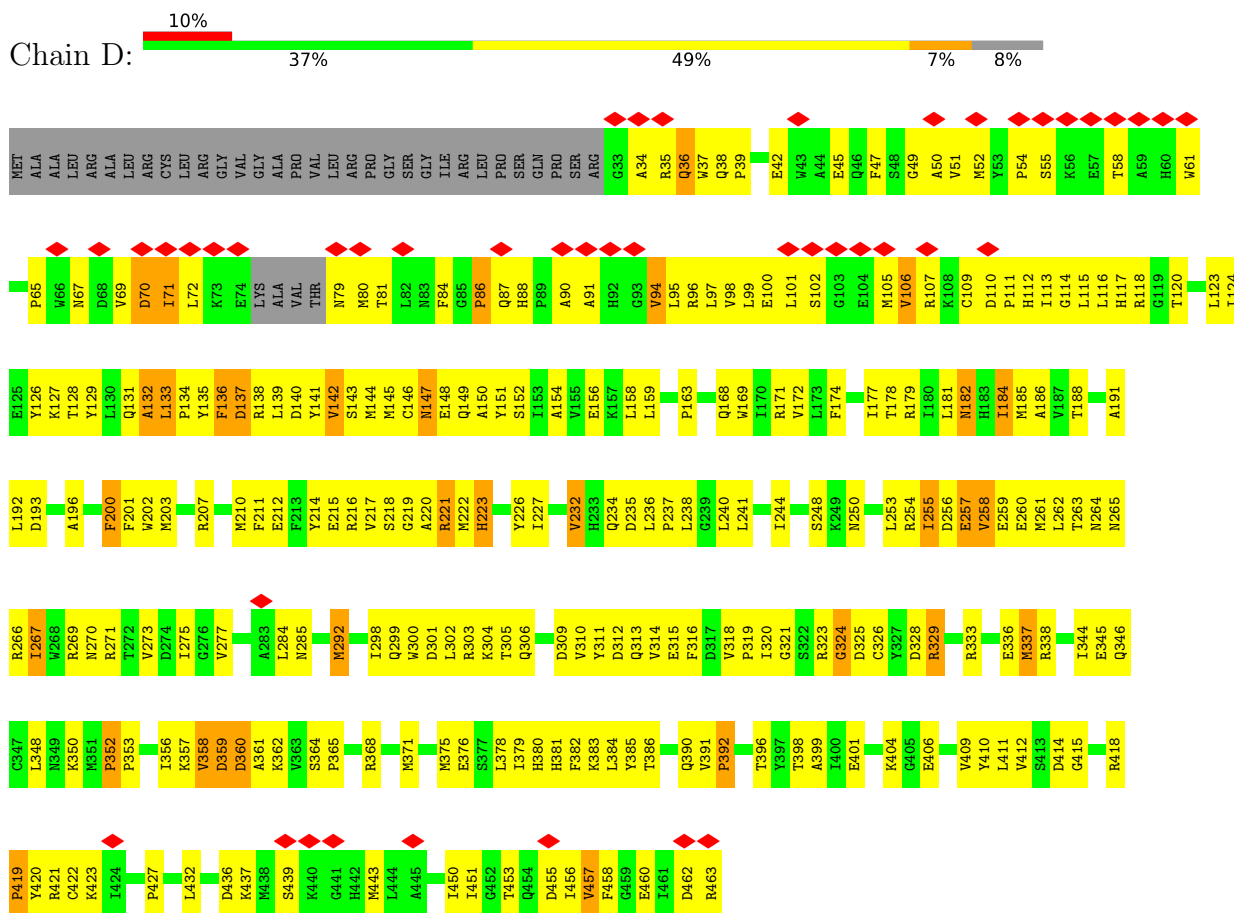
- Molecule 69 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).

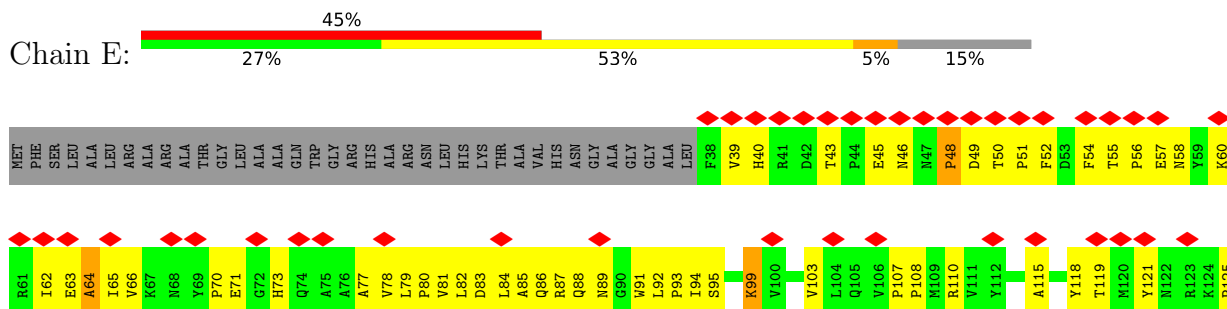


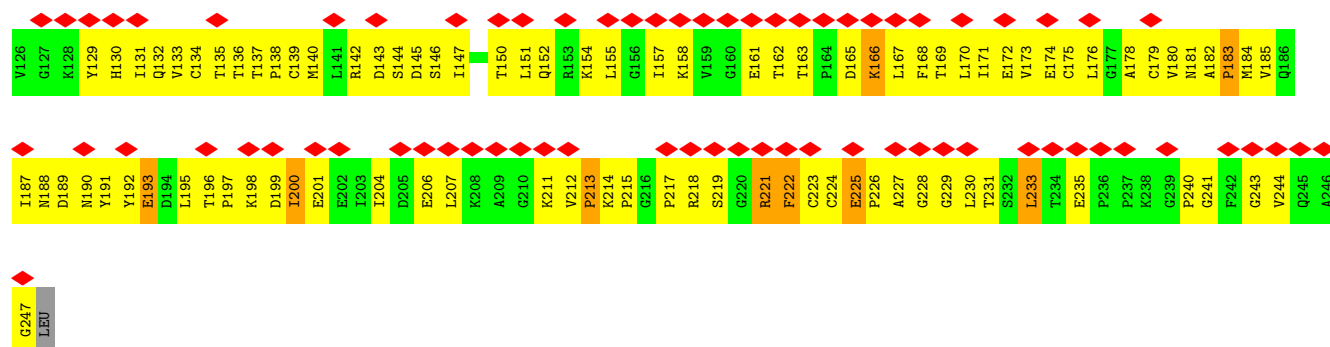
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
71	Ad	1	36	27	8	1	0

- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



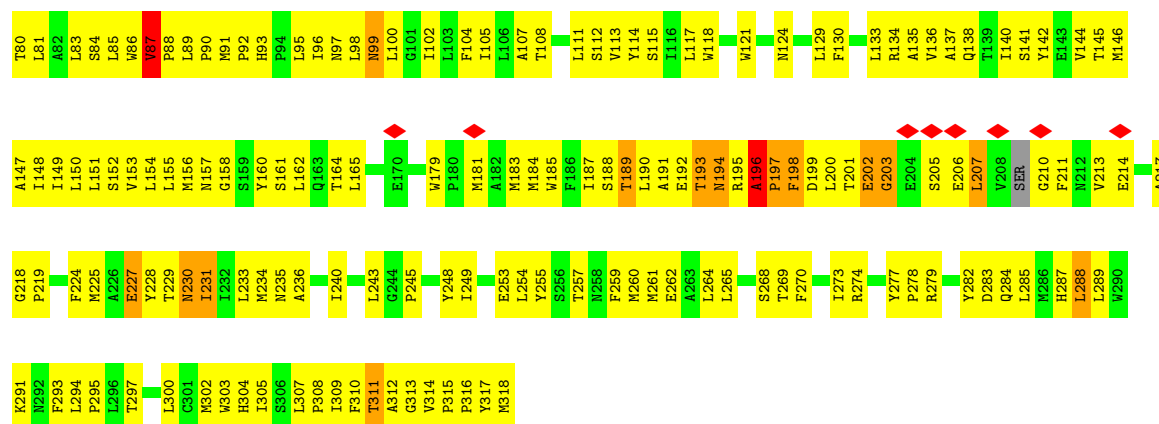


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

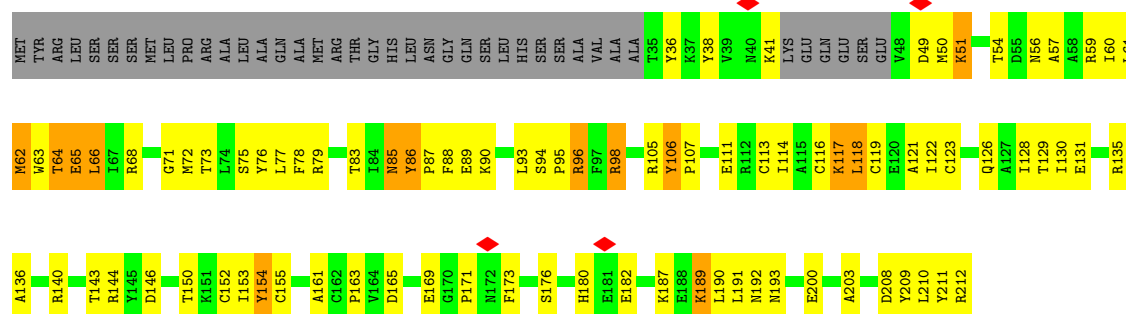


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

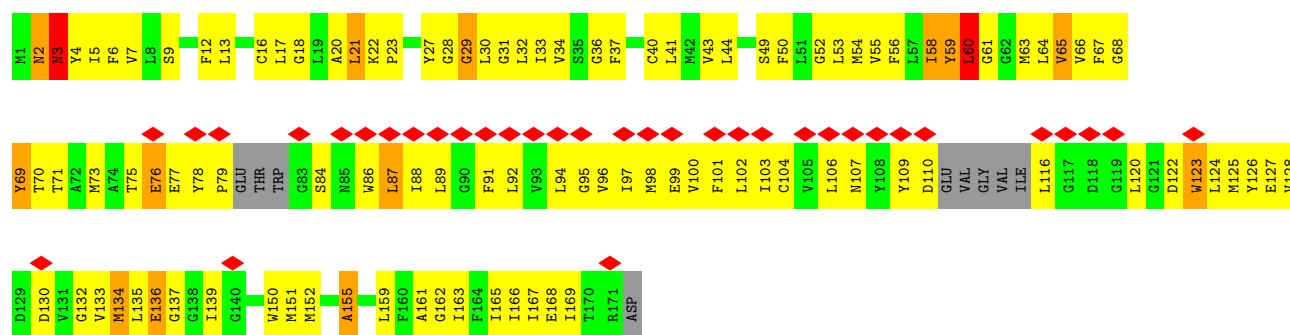




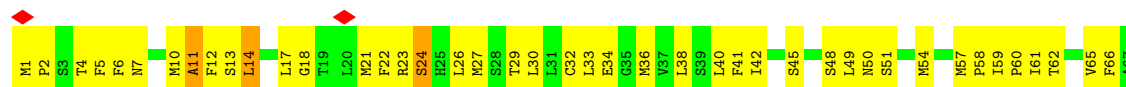
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

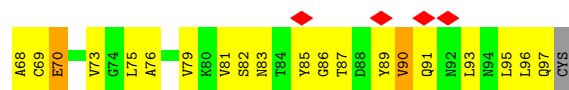


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

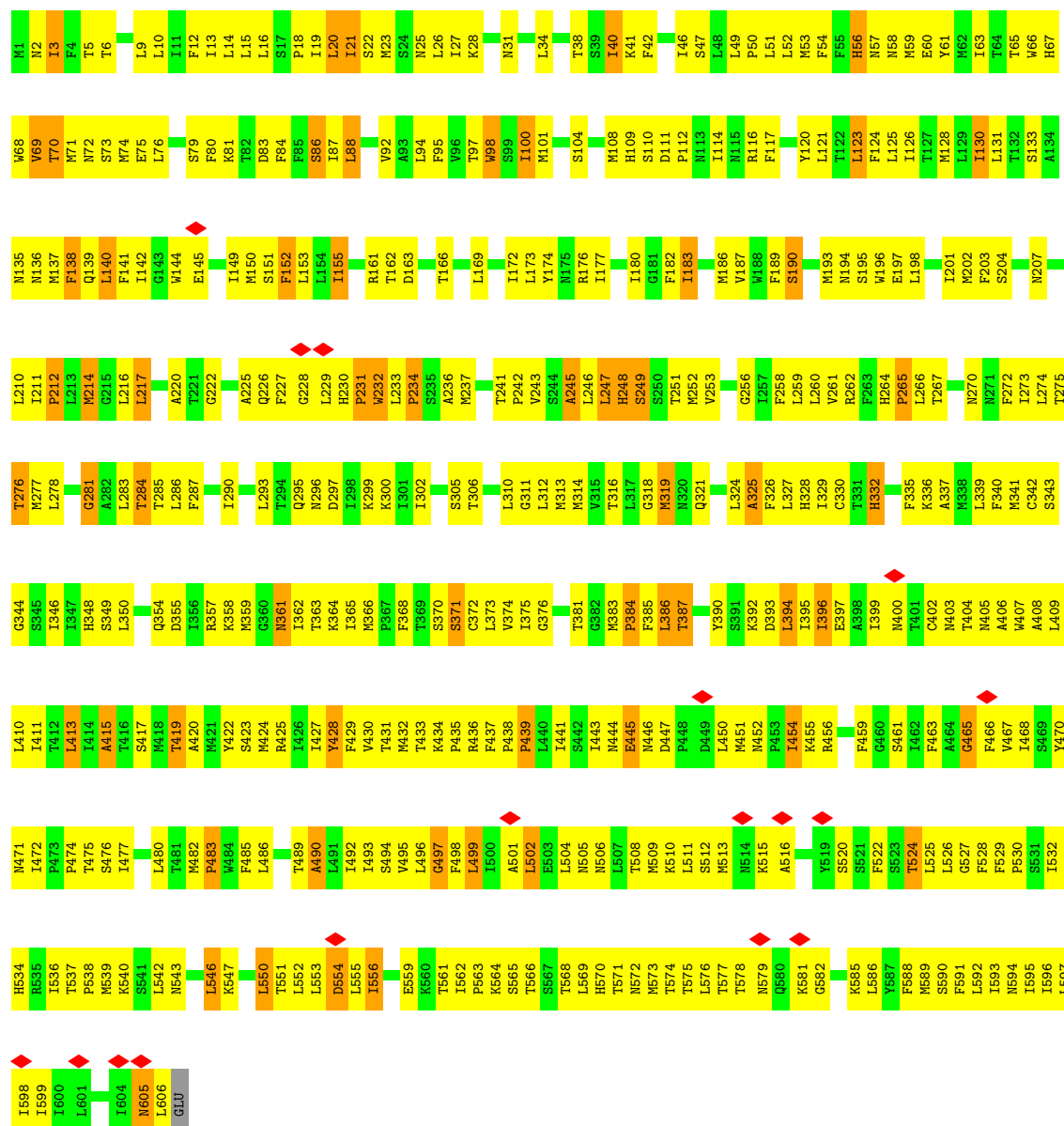
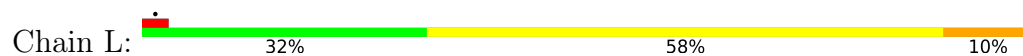


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

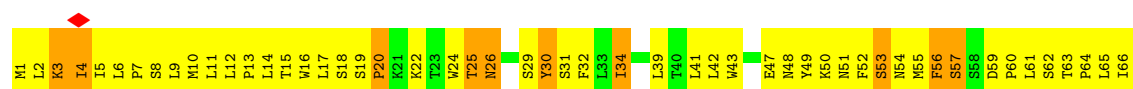


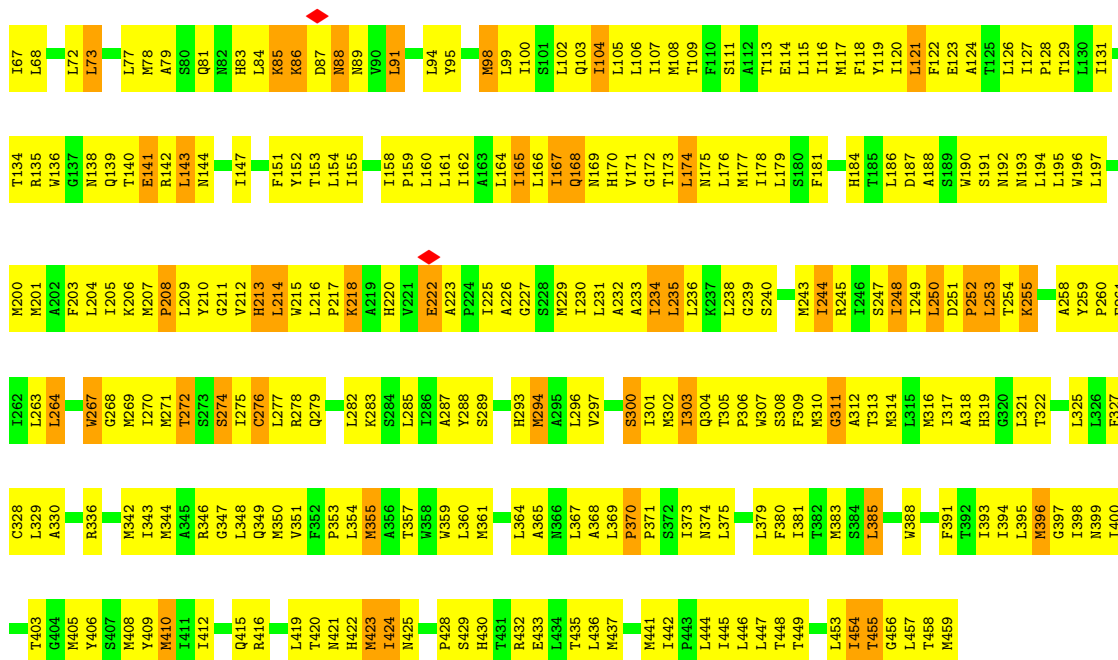


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

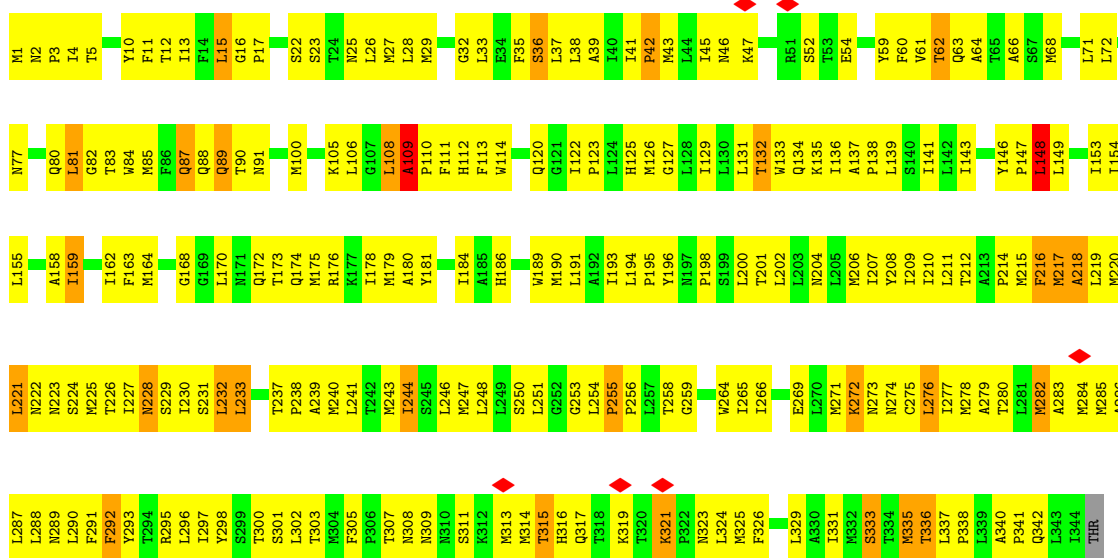


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

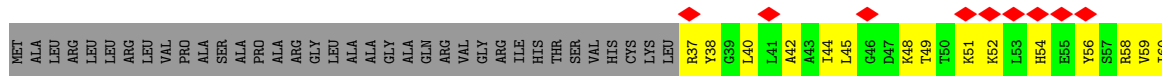


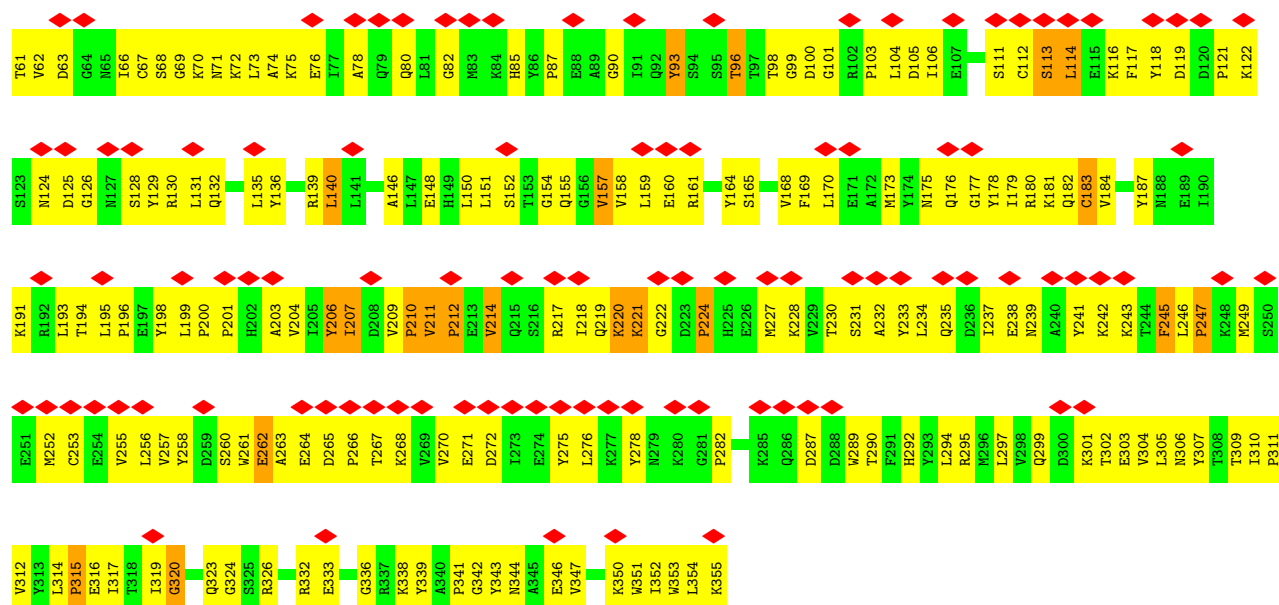


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

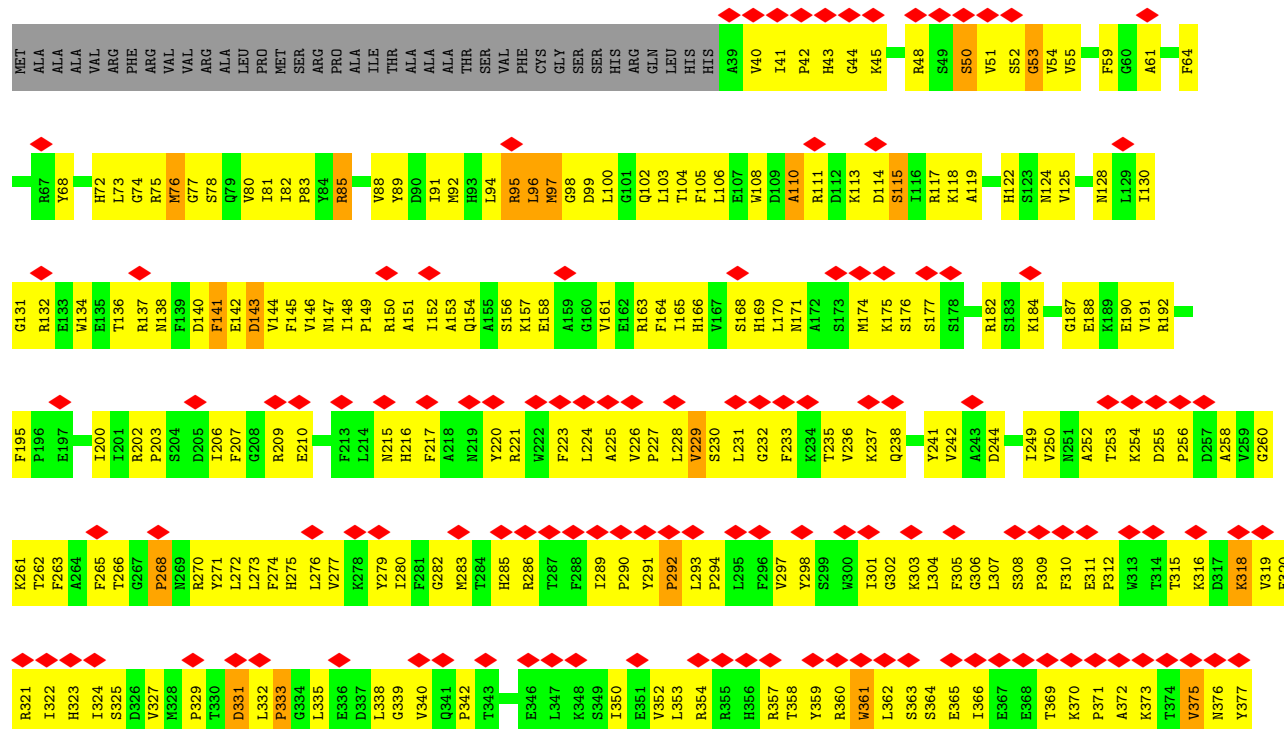


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

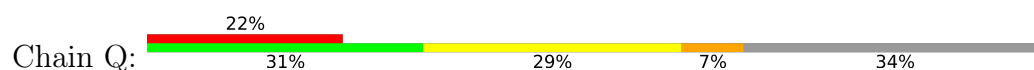


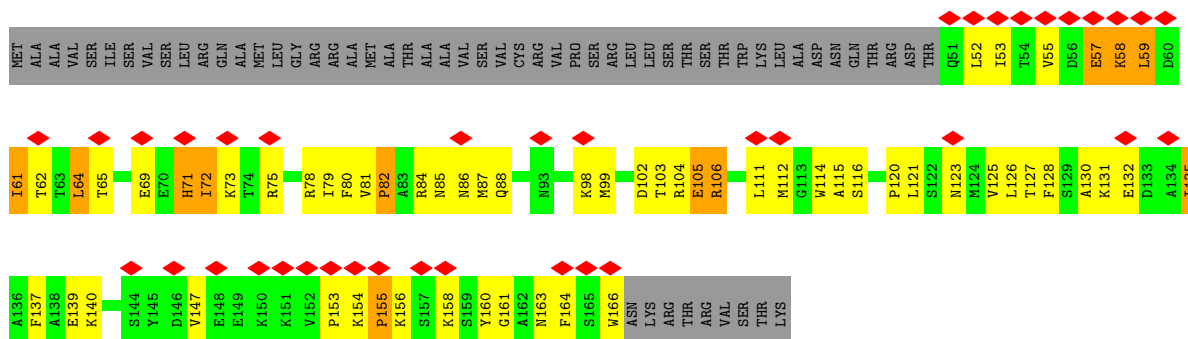


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

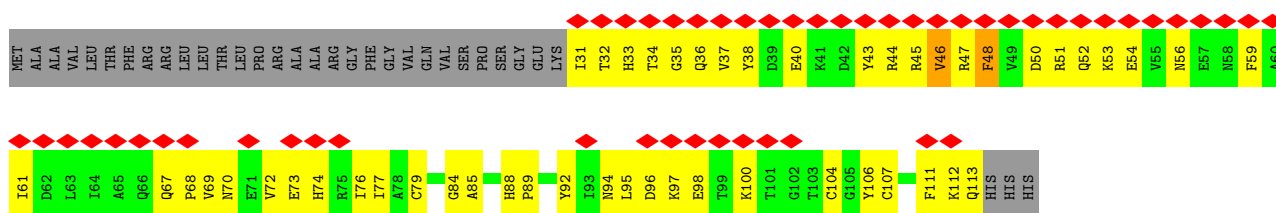


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

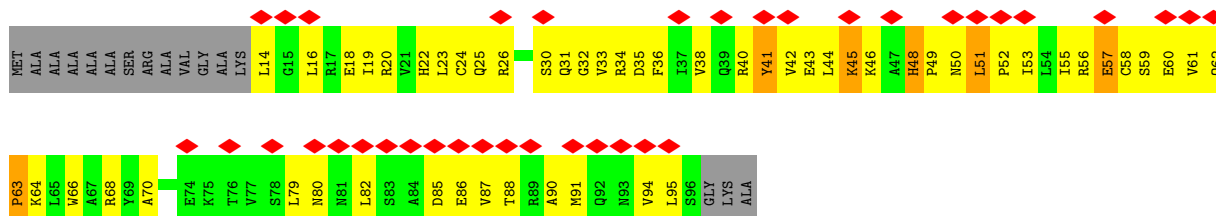




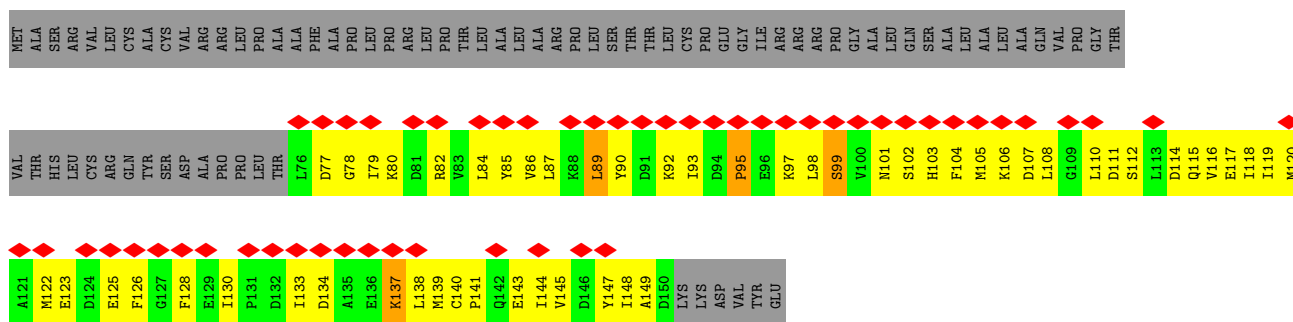
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

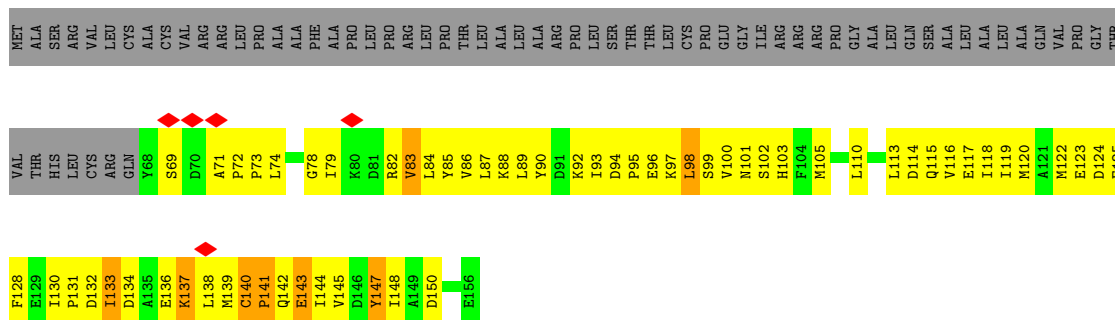


- Molecule 20: Acyl carrier protein, mitochondrial

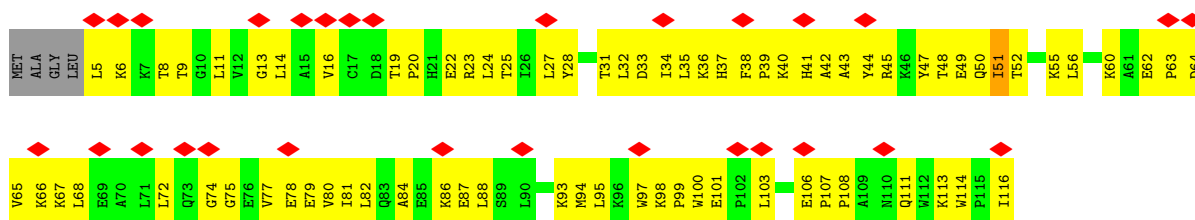


- Molecule 20: Acyl carrier protein, mitochondrial

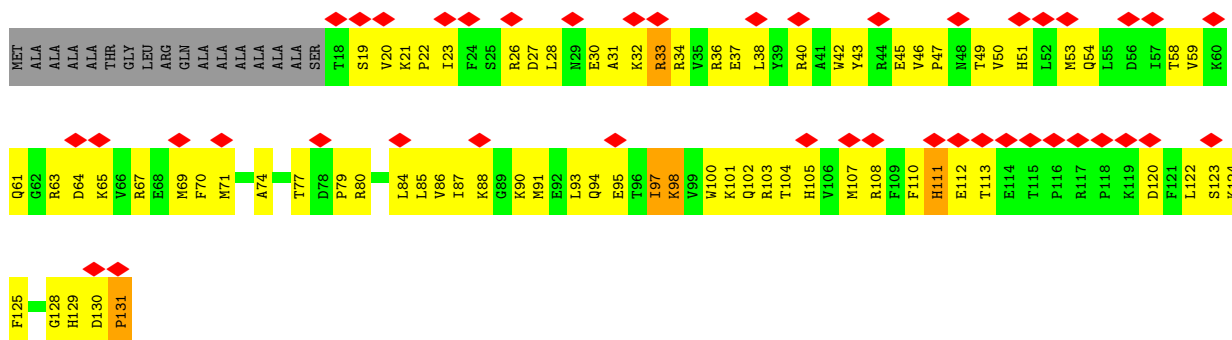




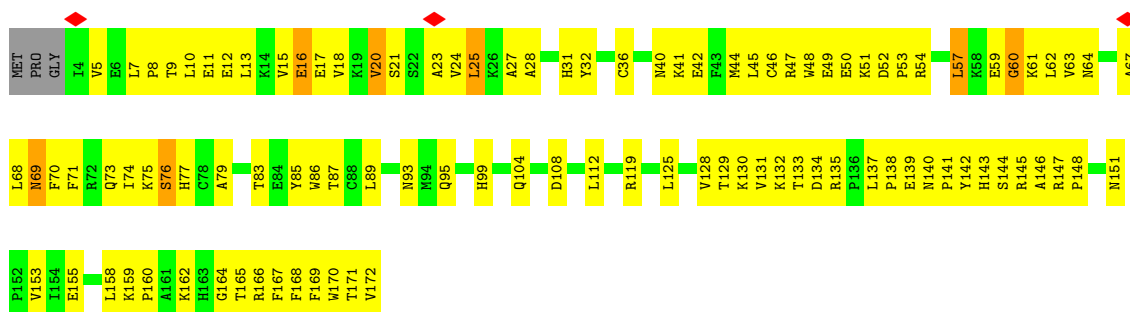
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



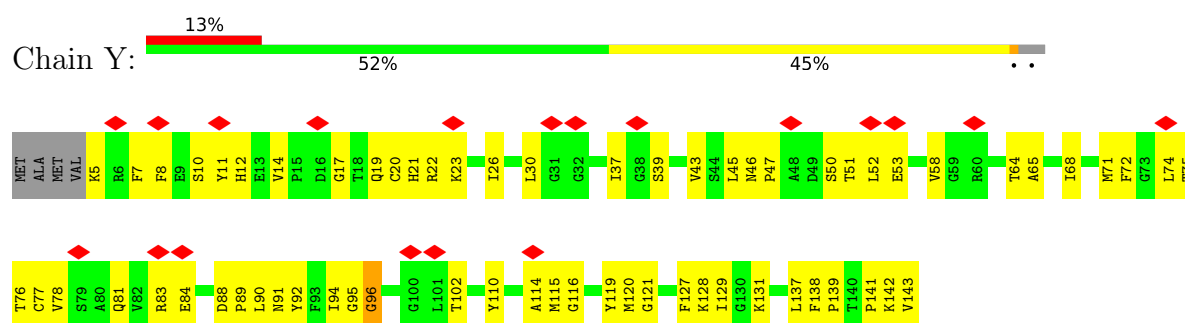
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



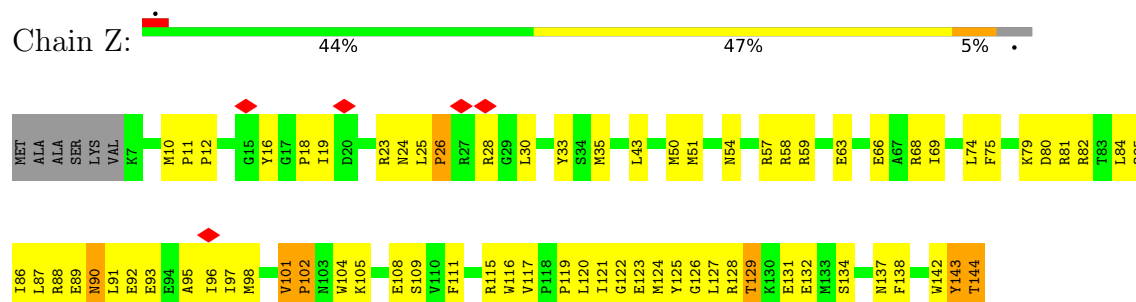
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



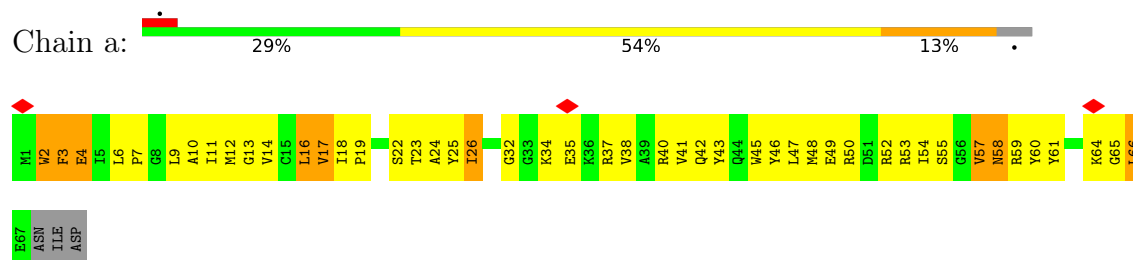
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



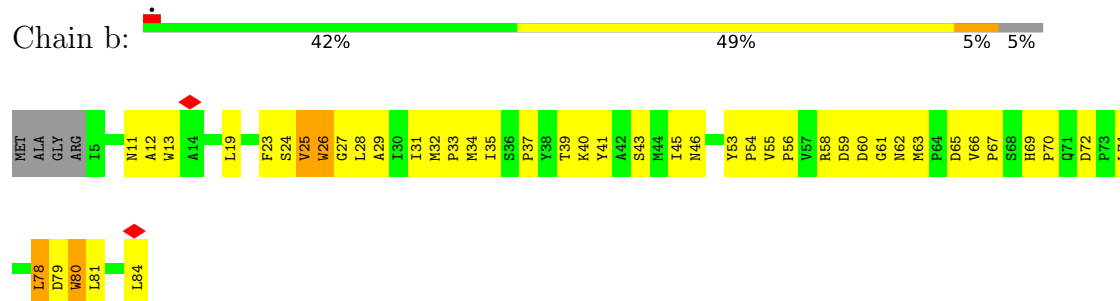
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



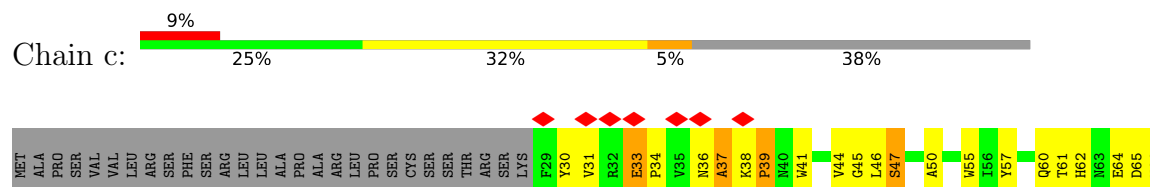
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



L67
E68
Y69
K70
R71
R72
N73
G74
L75
GLU

- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d: 5% 38% 59% .

M1 M2 N3 G4 R5 P6 G7 H8 E9 F10 L11 K12 F13 L14 P15 D16 E17 A18 R19 S20 L21 P22 P23 K24 K25 L26 N27 D28 P29 R30 Y33 L37 G38 Y39 C40 L43 M44 D45 N46 M47 L48 R49 M50 R51 P52 V53 M54 G57 L58 H59 R60 Q61 L62 I63 F64 Y65

T66 F70 A71 G72 Y73 K77 R78 Q79 N80 Y81 L82 D87 H88 D89 N90 F91 G92 R93 I94 E99 D100 F101 P102 E103 K106 K107 T108 Y109 A110 E111 I112 L113 E114 P115 F116 H117 P118 V119 R120

- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 5% 45% 48% 6% .

MET F2 F3 L4 D5 I6 L14 D15 R16 H17 F18 M19 F20 L21 R32 C33 H34 A35 F36 E37 K38 E39 W40 I41 E42 C43 A44 H45 G46 T47 G48 A49 T50 R51 A52 F60 E65 R69 Y70 K71 T72 M73 R74 R75 I79 Q82 R83 L86 M87 K88 E89 G90

K91 Y92 T93 P94 P95 P96 H97 H98 R101 E102 E103 P104 R105 P106

- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 5% 39% 42% 9% 11%

MET THR LEU PHE GLN LEU L7 R8 E9 H10 V11 V12 H13 V16 P17 F20 V21 F22 Y25 K29 D30 D31 A36 F37 R38 N39 K40 S41 M42 F43 F44 Q45 E47 L48 R49 P50 N51 E52 E53 V54 T55 W56 K57

- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

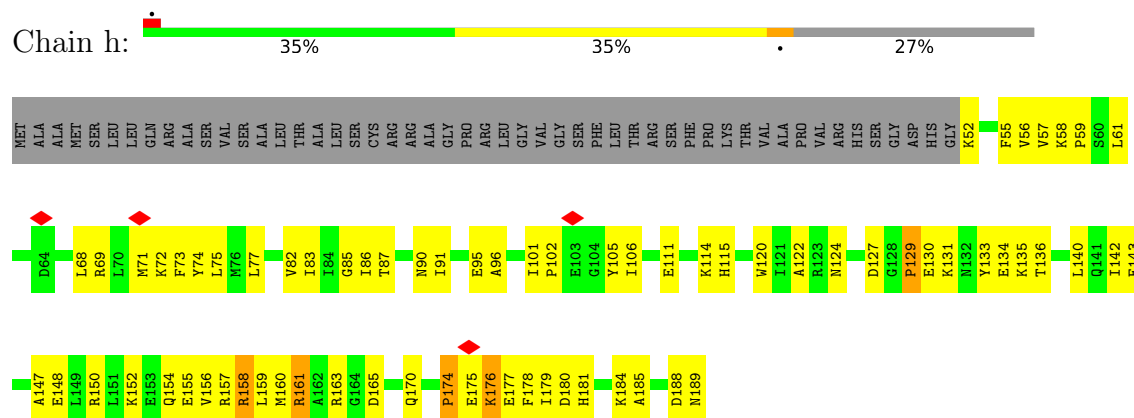
Chain g: 6% 35% 26% 7% 32%

MET ALA ALA ARG LEU LEU SER LEU TYR ARG ARG CYS LEU SER ALA ALA GLY MET ARG ARG LEU LEU PRO ALA ALA ARG VAL ARG TRP GLU SER SER ARG ARG VAL ILE ALA PRO SER GLY VAL LYS LYS ARG GLN ARG ARG PRO T50 M51 Q52 W53 Q54 E55 D56 F57 E58 P59 E60

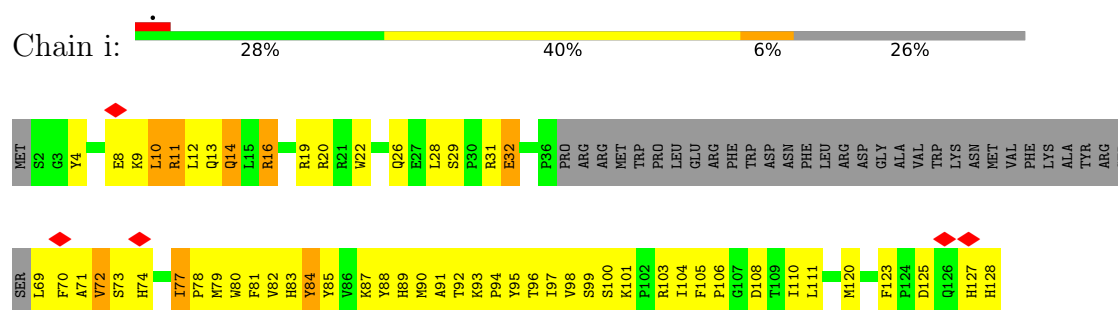
N63 V64 K67 N68 P69 D70 F71 H72 G73 Y74 Y75 S76 D77 P78 V79 V80 N84 M85 F89 F90 F91 G92 L97 T101 Y106 Y107 P108 D109 M112 Q113 E114 W115 A116 R117 R118 E119 A120 R121 R122 L123 V124 S137 N138 Y139 F140 I145 Q146 L147 P148

D151

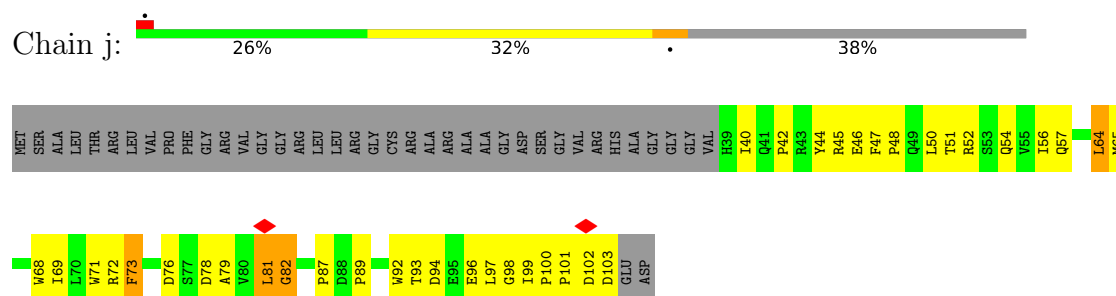
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



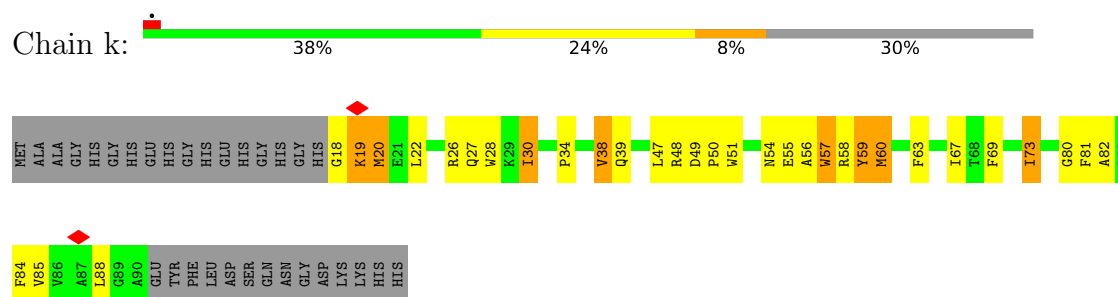
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



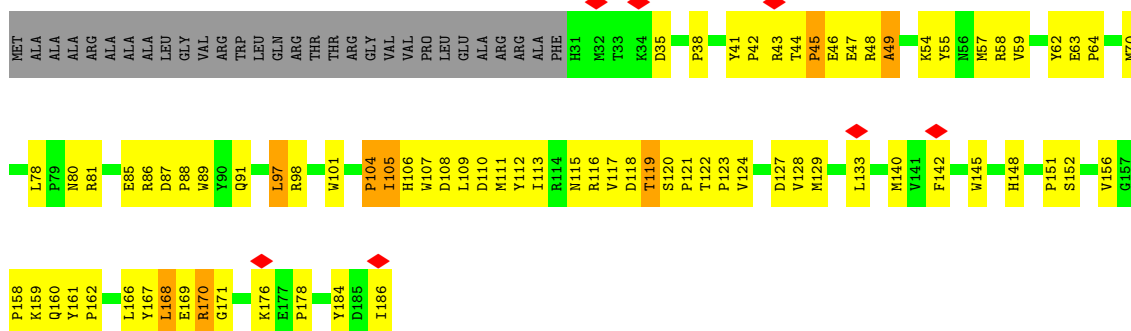
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



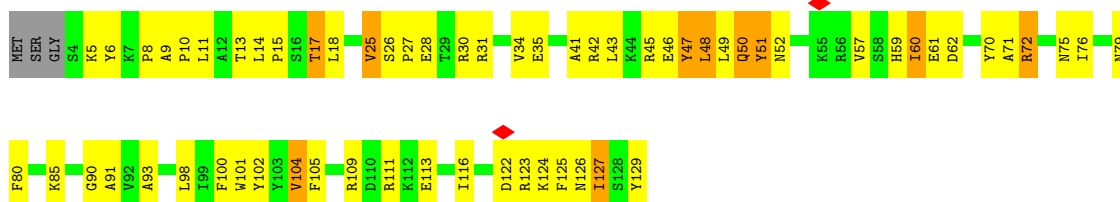
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



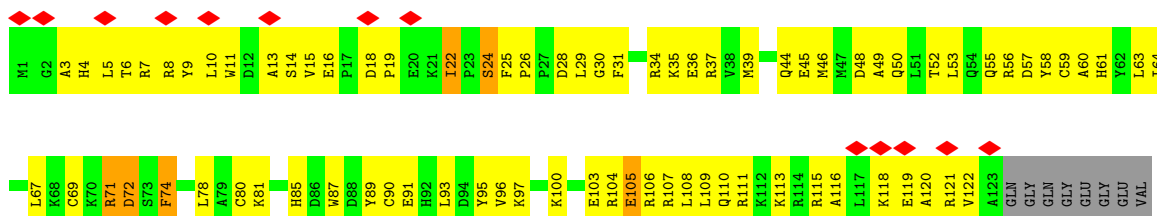
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



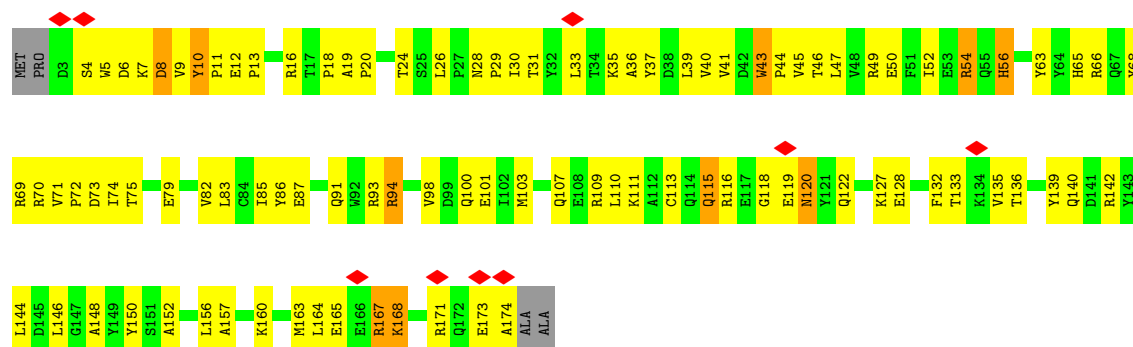
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



GLY
PRO
GLU
VAL
ALA
LEU

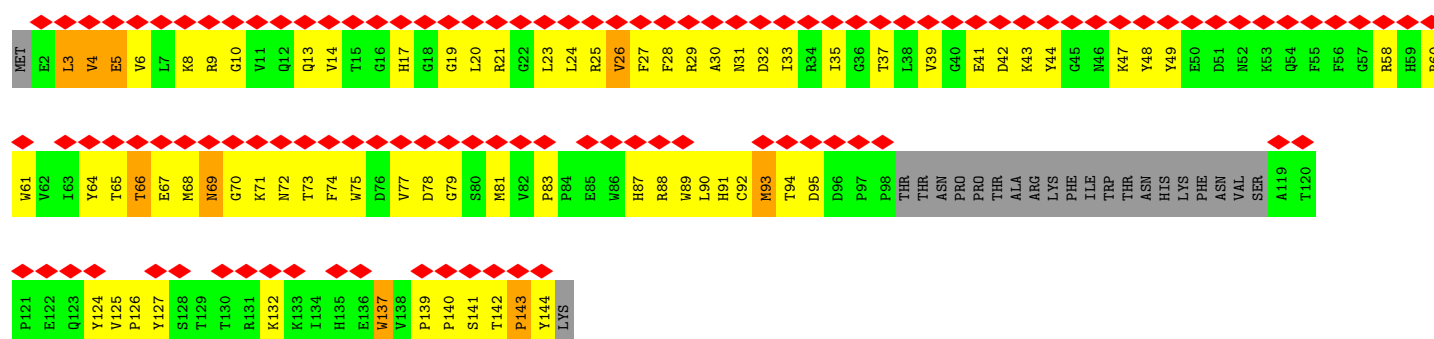
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p: 

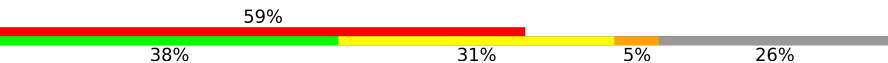


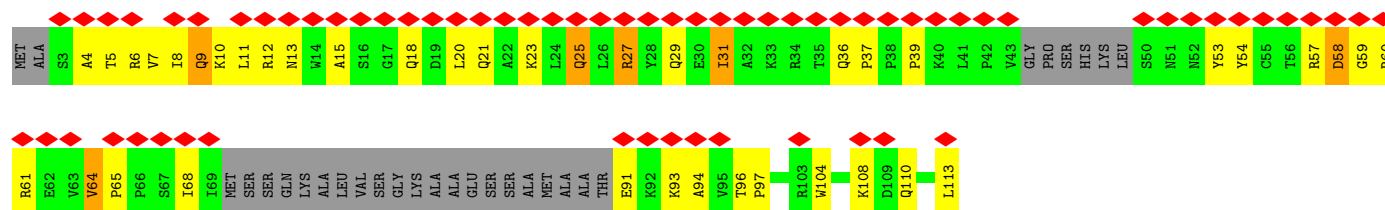
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 



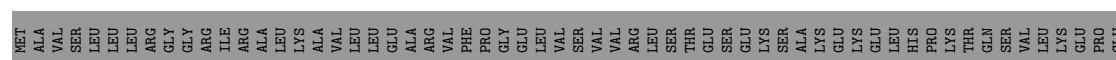
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

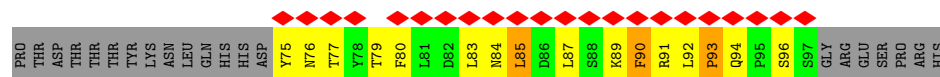
Chain r: 



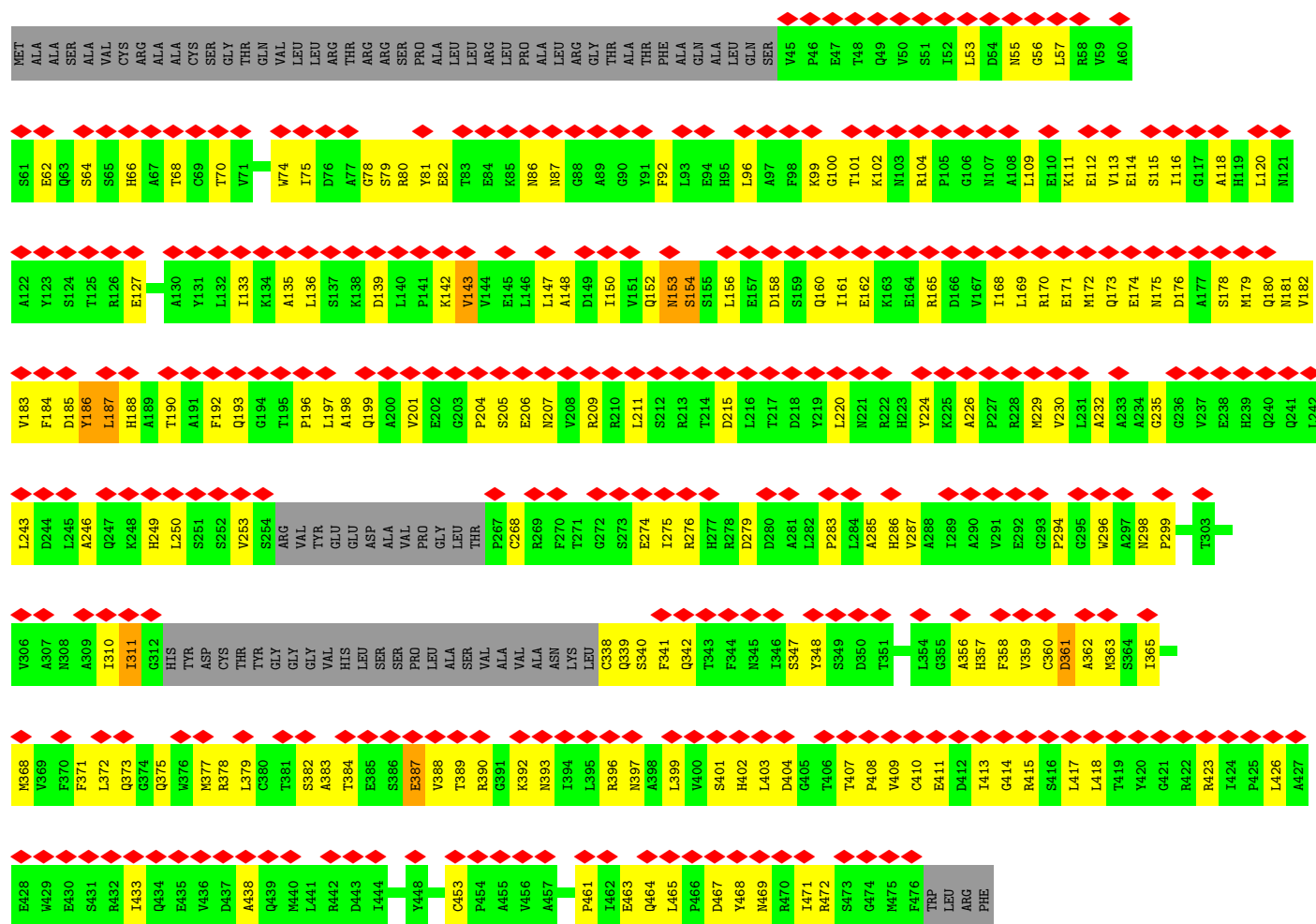
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s: 

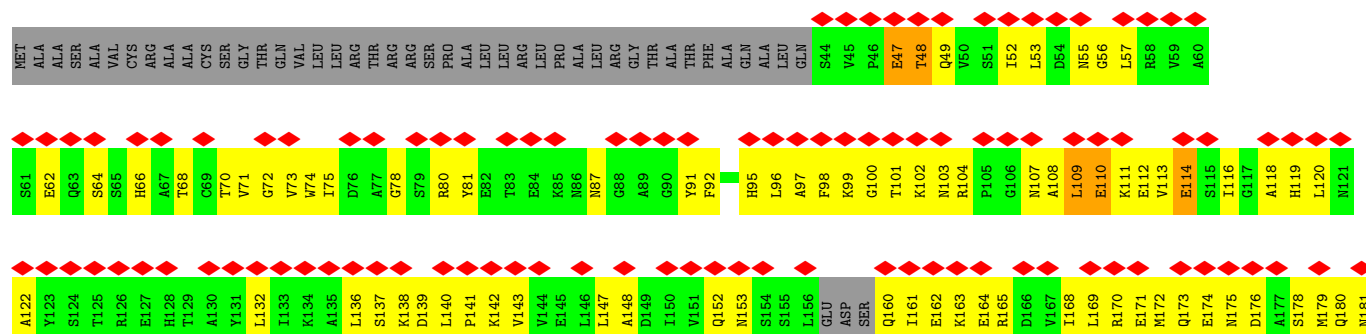


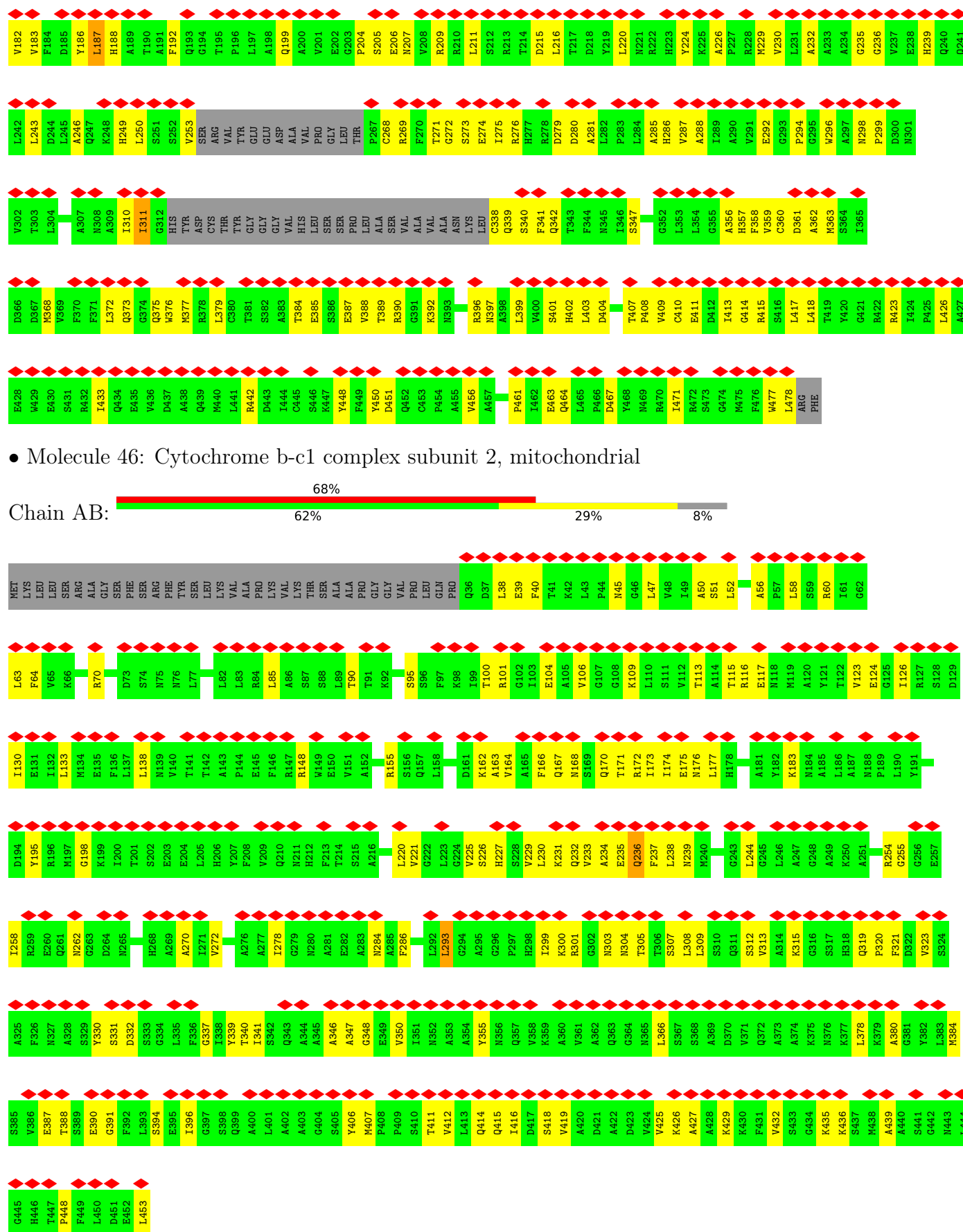


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

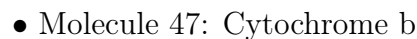


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

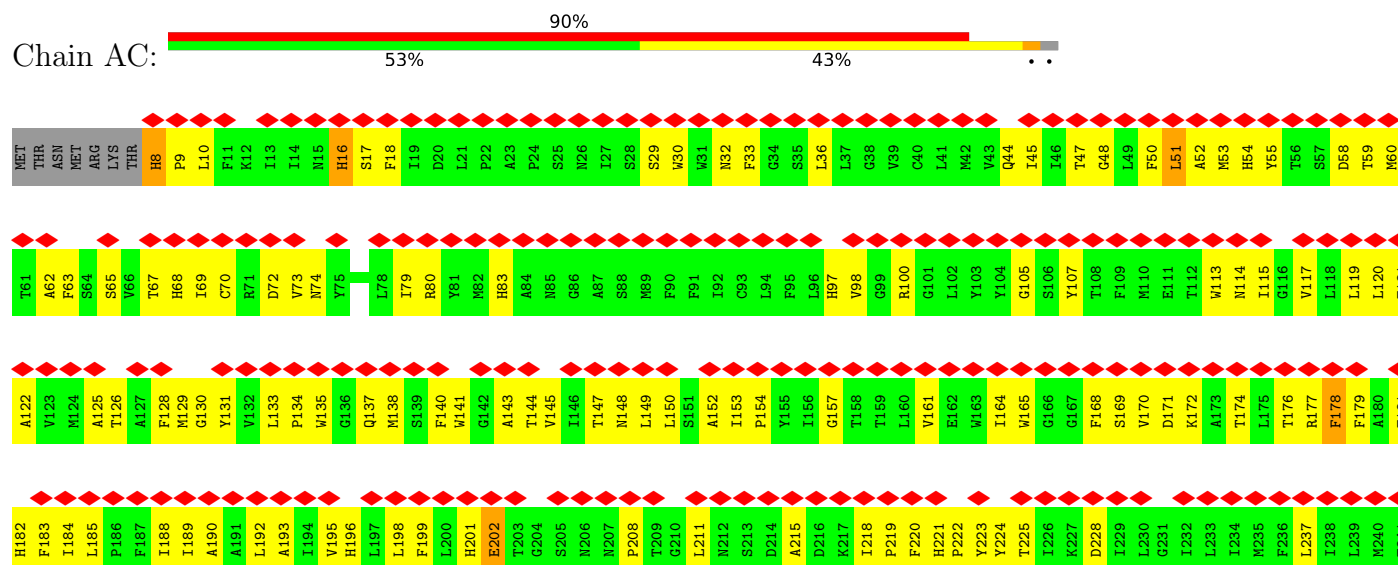


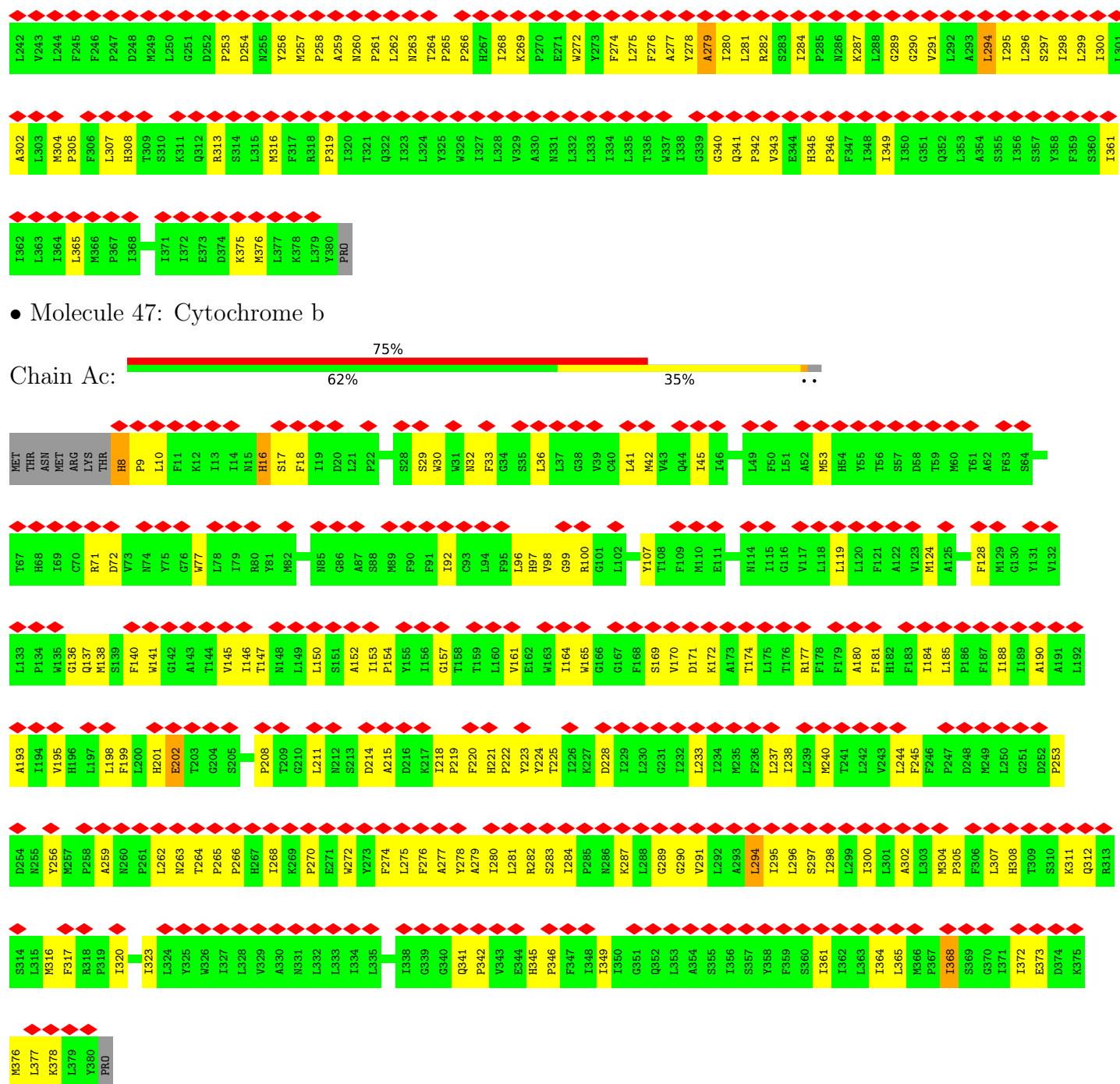


Chain Ab:

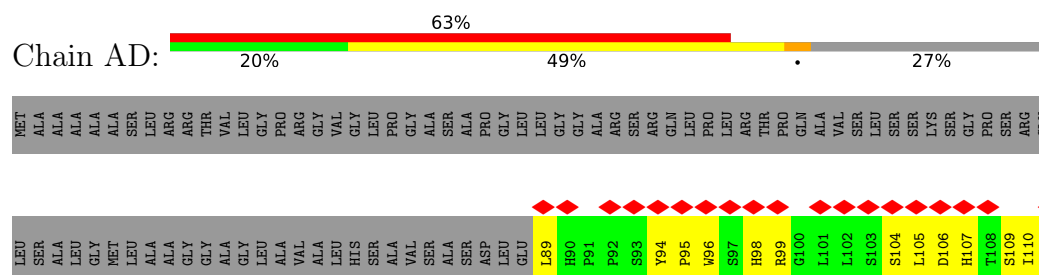


Chain AC:



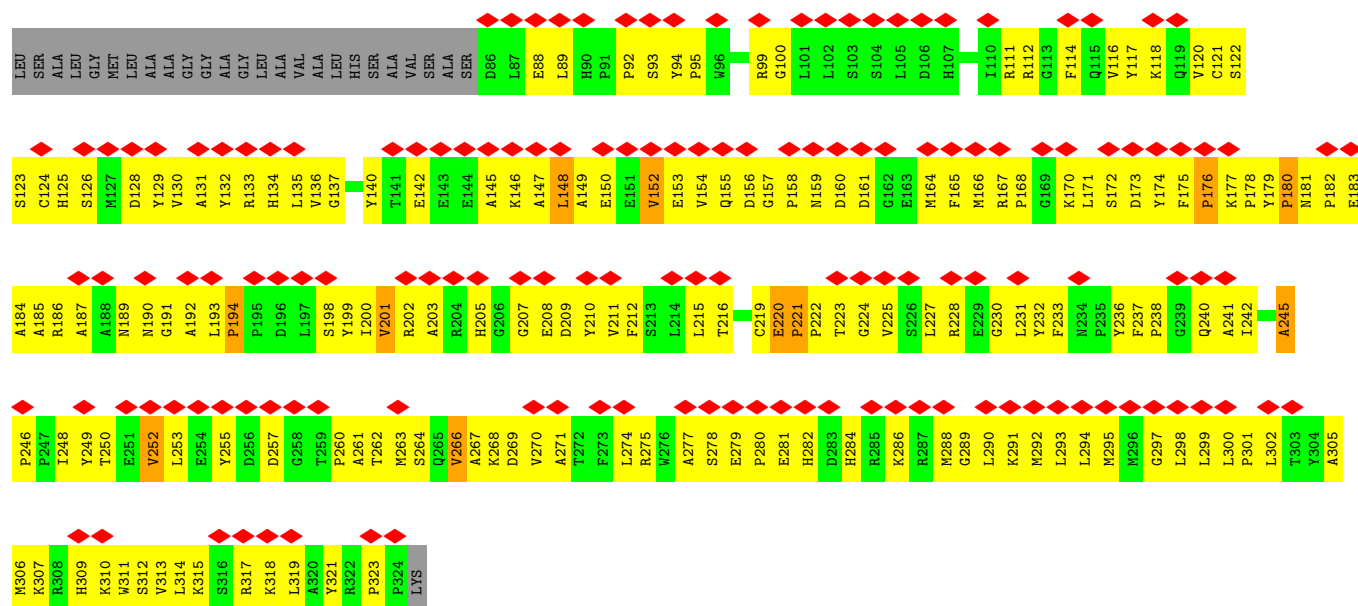
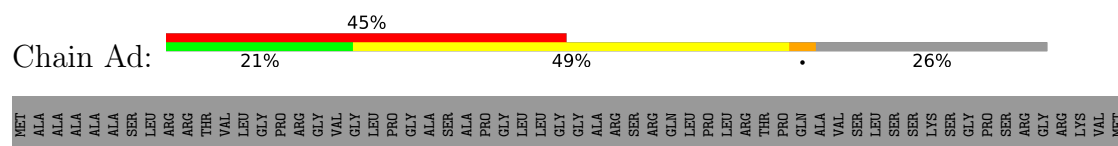


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

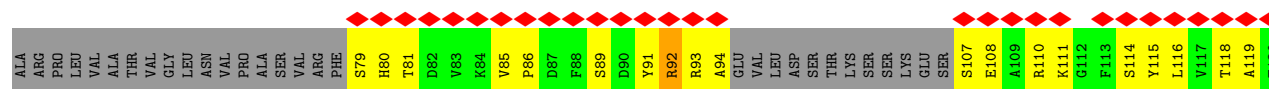
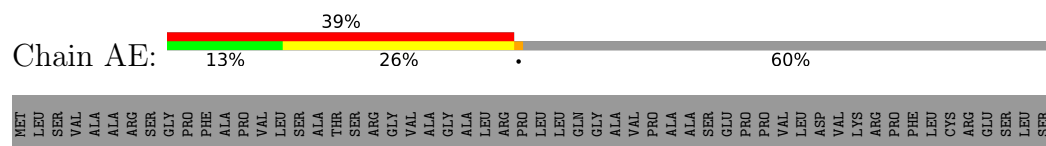


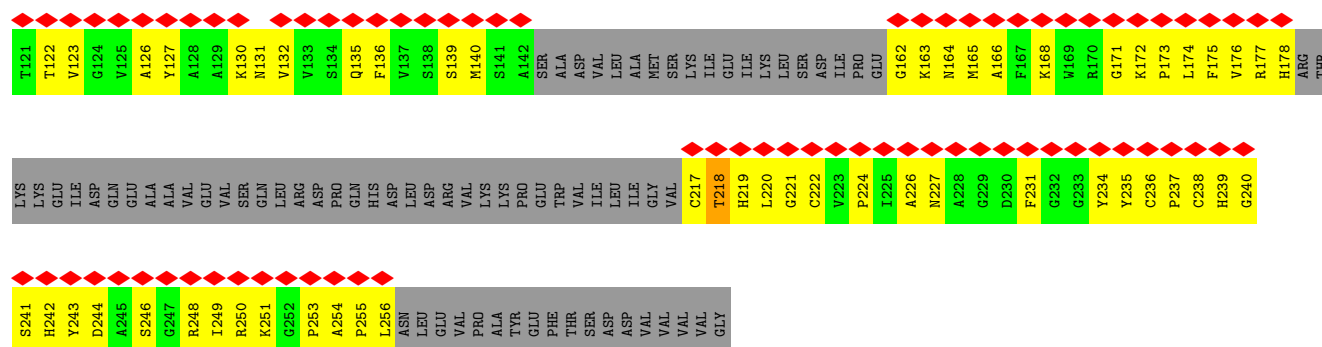


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

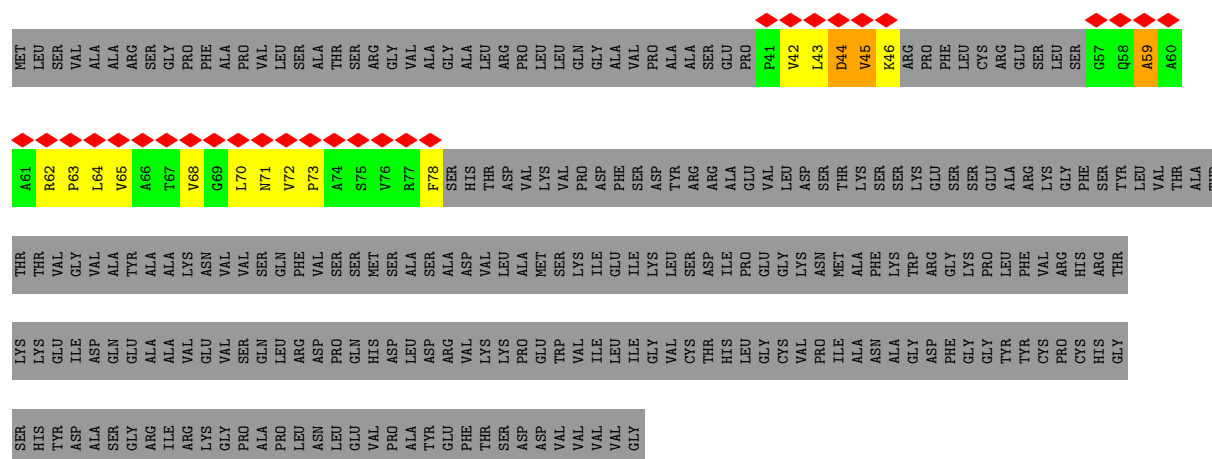


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

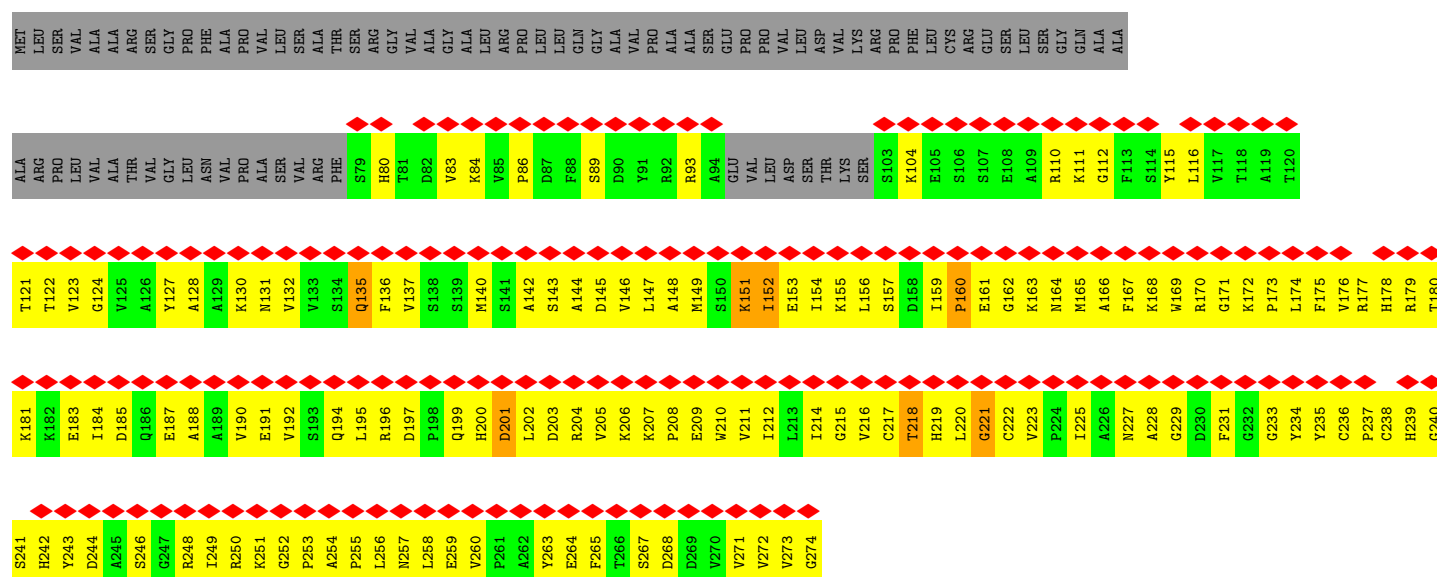
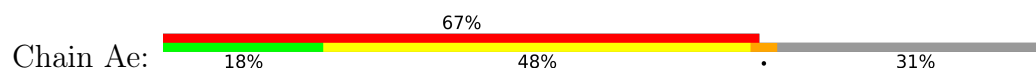


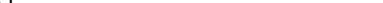


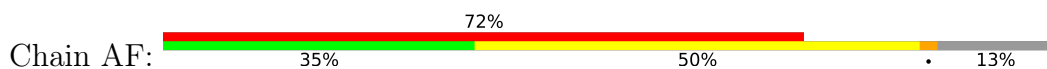
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

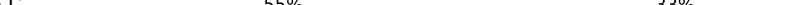


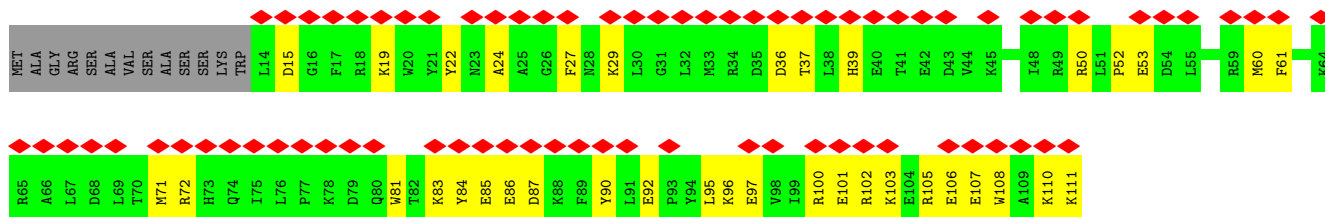
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

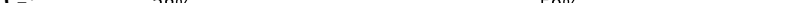


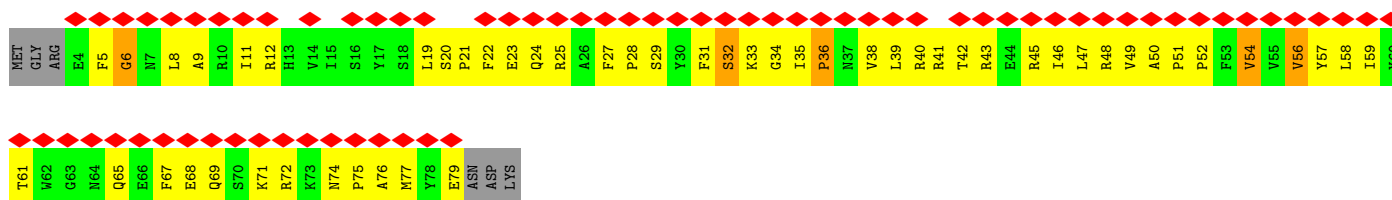
- Chain Ai:  10% 90%



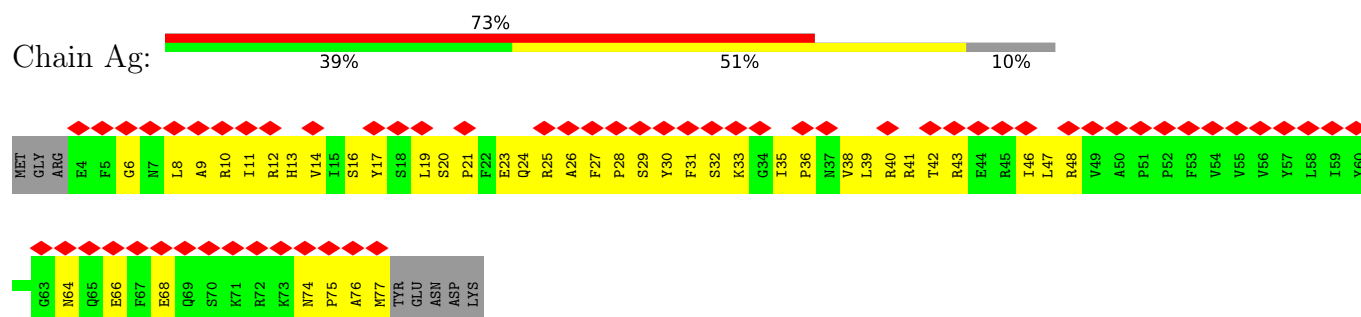
- Chain Af: 



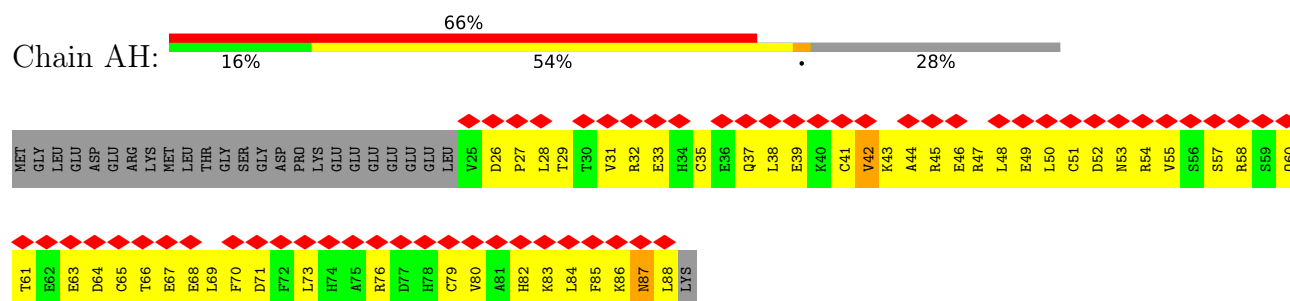
- Chain AG:  28% 87% 59% 6% 7%



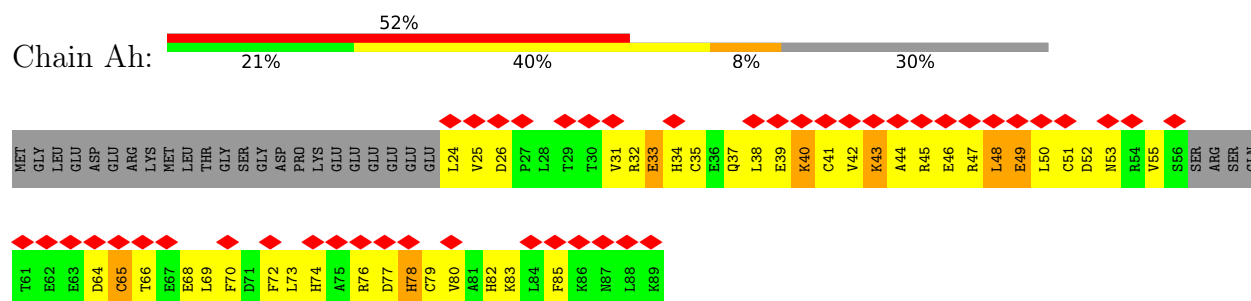
- Molecule 51: Cytochrome b-c1 complex subunit 8



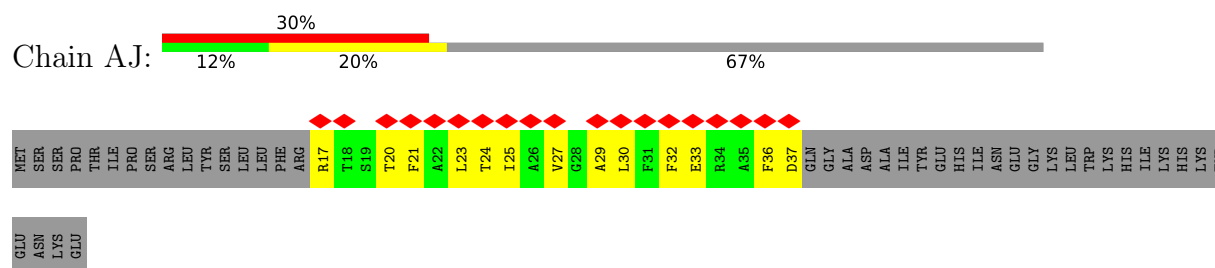
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



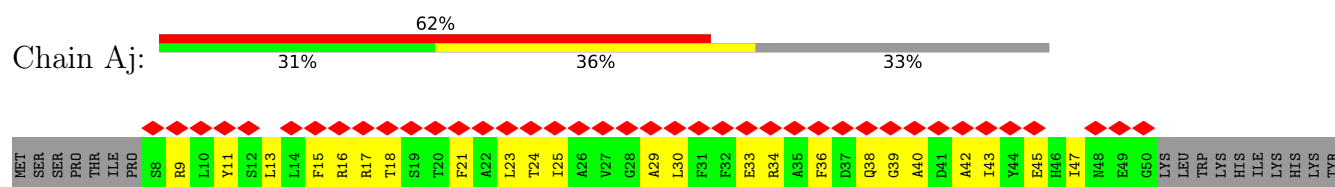
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 53: Cytochrome b-c1 complex subunit 9



- Molecule 53: Cytochrome b-c1 complex subunit 9



GLU
ASN
LYS
GLU

● Molecule 54: Cytochrome b-c1 complex subunit 10



MET	LEU	SER	ARG	PHE	LEU	GLY	PRO	ARG	TYR	ARG	GLU	LEU	ALA	ARG	ASN	TRP	ILE	PRO	THR	A21	G22	M23	M24	G25	T26	V27	G28	A29	V30	G31	L32	V33	W34	A35	T36	D37	TRP	ARG	LEU	ILE	LEU	ASP	TRP	VAL	PRO	TYR	ILE	ASN	GLY	LYS	PHE	LYS	LYS	ASP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 54: Cytochrome b-c1 complex subunit 10



MET	L2	S3	R4	F5	L6	G7	P8	R9	Y10	R11	E12	L13	A14	R15	N16	W17	I18	F19	T20	A21	G22	M23	W24	G25	T26	V27	G28	A29	V30	G31	L32	V33	W34	A35	T36	D37	W38	R39	LEU	ILE	LEU	ASP	TRP	VAL	PRO	TYR	ILE	ASN	GLY	LYS	PHE	LYS	LYS	ASP	ASP
-----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PC1, NDP, UQ9, U10, UQ6, CDL, EHZ, 3PE, HEM, ADP, FES, UQ1, FMN, 3PH, SF4, HEC

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	0.94	1/820 (0.1%)	1.18	8/1118 (0.7%)
2	B	1.16	6/1272 (0.5%)	1.73	26/1722 (1.5%)
3	C	1.04	1/1689 (0.1%)	1.42	24/2300 (1.0%)
4	D	0.96	3/3527 (0.1%)	1.46	52/4776 (1.1%)
5	E	0.82	2/1675 (0.1%)	1.30	26/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	66/4543 (1.5%)
7	G	0.97	13/5374 (0.2%)	1.59	112/7281 (1.5%)
8	H	0.87	2/2608 (0.1%)	1.23	30/3563 (0.8%)
9	I	0.80	3/1409 (0.2%)	1.27	21/1904 (1.1%)
10	J	0.84	1/1257 (0.1%)	1.26	20/1704 (1.2%)
11	K	0.90	0/740	1.54	13/1005 (1.3%)
12	L	0.99	7/4921 (0.1%)	1.57	107/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.57	86/5062 (1.7%)
14	N	1.01	3/2756 (0.1%)	1.44	51/3751 (1.4%)
15	O	1.00	8/2666 (0.3%)	1.40	41/3615 (1.1%)
16	P	0.77	2/2793 (0.1%)	1.19	23/3787 (0.6%)
17	Q	0.97	3/963 (0.3%)	1.40	11/1302 (0.8%)
18	R	0.63	0/671	1.06	4/903 (0.4%)
19	S	0.86	2/678 (0.3%)	1.37	13/915 (1.4%)
20	T	0.75	0/613	1.11	7/826 (0.8%)
20	U	0.98	1/731 (0.1%)	1.30	14/988 (1.4%)
21	V	0.82	0/937	1.24	4/1270 (0.3%)
22	W	0.89	2/993 (0.2%)	0.99	7/1335 (0.5%)
23	X	0.63	0/1422	1.01	8/1921 (0.4%)
24	Y	0.86	0/1054	0.98	2/1429 (0.1%)
25	Z	0.75	2/1176 (0.2%)	1.17	10/1587 (0.6%)
26	a	0.89	0/561	1.60	14/755 (1.9%)
27	b	0.69	0/651	1.11	7/895 (0.8%)
28	c	0.93	1/400 (0.2%)	1.49	12/544 (2.2%)
29	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
30	e	0.69	1/900 (0.1%)	1.01	5/1199 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.95	1/451 (0.2%)	1.38	12/607 (2.0%)
32	g	0.89	3/886 (0.3%)	1.35	19/1207 (1.6%)
33	h	0.77	1/1197 (0.1%)	1.26	8/1621 (0.5%)
34	i	0.84	0/829	1.35	14/1127 (1.2%)
35	j	0.80	0/588	1.32	8/805 (1.0%)
36	k	0.98	2/600 (0.3%)	1.44	14/810 (1.7%)
37	l	0.98	3/1367 (0.2%)	1.22	9/1866 (0.5%)
38	m	0.92	2/1079 (0.2%)	1.24	17/1463 (1.2%)
39	n	0.94	2/1596 (0.1%)	1.32	18/2162 (0.8%)
40	o	0.82	1/1075 (0.1%)	1.14	10/1442 (0.7%)
41	p	0.71	1/1485 (0.1%)	1.05	15/2007 (0.7%)
42	q	0.83	5/1059 (0.5%)	1.25	15/1439 (1.0%)
43	r	0.94	2/701 (0.3%)	1.56	12/948 (1.3%)
44	s	1.11	0/198	1.68	5/269 (1.9%)
45	AA	0.62	2/3134 (0.1%)	0.89	11/4248 (0.3%)
45	Aa	0.58	1/3134 (0.0%)	0.89	14/4248 (0.3%)
46	AB	0.44	0/3187	0.65	3/4308 (0.1%)
46	Ab	0.58	1/3187 (0.0%)	0.91	18/4308 (0.4%)
47	AC	0.51	0/3089	0.84	10/4221 (0.2%)
47	Ac	0.45	0/3089	0.73	7/4221 (0.2%)
48	AD	0.54	0/1937	0.97	11/2632 (0.4%)
48	Ad	0.85	3/1962 (0.2%)	1.07	17/2666 (0.6%)
49	AE	0.47	0/851	0.94	3/1146 (0.3%)
49	AI	1.86	2/202 (1.0%)	1.43	4/274 (1.5%)
49	Ae	0.63	0/1483	1.10	7/2007 (0.3%)
49	Ai	1.87	2/205 (1.0%)	1.49	5/277 (1.8%)
50	AF	0.64	0/875	0.90	6/1173 (0.5%)
50	Af	0.38	0/884	0.52	0/1184
51	AG	0.57	1/662 (0.2%)	1.10	5/895 (0.6%)
51	Ag	0.55	0/640	0.93	1/865 (0.1%)
52	AH	0.53	0/534	0.84	2/717 (0.3%)
52	Ah	0.76	0/518	1.14	7/694 (1.0%)
53	AJ	0.41	0/168	0.62	0/226
53	Aj	0.59	0/352	0.78	0/474
54	AK	0.47	0/121	0.84	1/166 (0.6%)
54	Ak	0.52	0/320	1.14	6/437 (1.4%)
All	All	0.83	114/97010 (0.1%)	1.24	1149/131525 (0.9%)

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	AI	44	ASP	C-N	20.17	1.52	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Ai	44	ASP	C-N	19.98	1.52	1.33
48	Ad	221	PRO	N-CD	18.51	1.73	1.47
15	O	247	PRO	N-CD	16.66	1.71	1.47
49	Ai	45	VAL	C-N	15.71	1.53	1.33
49	AI	45	VAL	C-N	14.48	1.53	1.33
29	d	115	PRO	N-CD	-14.15	1.27	1.47
12	L	265	PRO	N-CD	13.84	1.67	1.47
14	N	255	PRO	N-CD	-13.65	1.28	1.47
28	c	39	PRO	N-CD	-13.22	1.29	1.47
38	m	27	PRO	N-CD	-12.93	1.29	1.47
7	G	532	PRO	N-CD	-12.62	1.30	1.47
22	W	131	PRO	N-CD	-12.39	1.30	1.47
15	O	315	PRO	N-CD	-12.04	1.30	1.47
48	Ad	180	PRO	N-CD	11.27	1.63	1.47
12	L	234	PRO	N-CD	11.15	1.63	1.47
1	A	36	PRO	N-CD	-11.09	1.32	1.47
42	q	143	PRO	N-CD	-10.52	1.33	1.47
15	O	210	PRO	N-CD	-10.46	1.33	1.47
13	M	370	PRO	N-CD	-10.46	1.33	1.47
36	k	20	MET	C-N	10.35	1.47	1.33
6	F	234	GLY	CA-C	-10.22	1.41	1.52
15	O	224	PRO	N-CD	-10.21	1.33	1.47
12	L	57	ASN	C-O	-10.18	1.11	1.24
16	P	333	PRO	N-CD	-10.15	1.33	1.47
6	F	227	PRO	N-CD	10.13	1.61	1.47
2	B	121	PHE	C-O	-10.09	1.11	1.23
6	F	235	VAL	N-CA	-9.71	1.34	1.46
4	D	365	PRO	N-CD	-9.60	1.34	1.47
32	g	78	PRO	N-CD	-9.57	1.34	1.47
2	B	92	PRO	N-CD	9.41	1.60	1.47
7	G	275	PRO	N-CD	-9.40	1.34	1.47
29	d	15	PRO	N-CD	-9.37	1.34	1.47
6	F	319	PRO	N-CD	9.03	1.60	1.47
17	Q	106	ARG	C-O	8.93	1.34	1.24
9	I	154	TYR	C-O	8.83	1.35	1.23
15	O	212	PRO	N-CD	-8.82	1.35	1.47
25	Z	102	PRO	N-CD	-8.76	1.35	1.47
13	M	20	PRO	N-CD	8.61	1.59	1.47
9	I	107	PRO	N-CD	8.61	1.59	1.47
25	Z	143	TYR	CA-C	-8.47	1.42	1.52
12	L	212	PRO	N-CD	-8.26	1.36	1.47
9	I	118	LEU	CA-C	8.16	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	155	PRO	N-CD	8.08	1.59	1.47
42	q	139	PRO	N-CD	-7.95	1.36	1.47
5	E	218	ARG	CA-C	7.86	1.62	1.53
2	B	121	PHE	CA-C	-7.75	1.42	1.52
7	G	31	LEU	CA-C	-7.25	1.43	1.52
43	r	65	PRO	N-CD	7.17	1.57	1.47
37	l	104	PRO	N-CD	-7.17	1.37	1.47
13	M	208	PRO	N-CD	7.16	1.57	1.47
2	B	122	ARG	CA-CB	-7.08	1.41	1.53
14	N	238	PRO	N-CD	-7.02	1.38	1.47
15	O	211	VAL	CA-C	6.97	1.60	1.52
8	H	196	ALA	C-N	6.90	1.41	1.34
3	C	203	LEU	CA-C	-6.90	1.43	1.52
37	l	119	THR	CA-C	-6.86	1.45	1.53
7	G	449	PRO	N-CD	6.85	1.57	1.47
7	G	541	PRO	N-CD	-6.82	1.38	1.47
30	e	106	PRO	N-CD	6.71	1.57	1.47
7	G	203	ASP	CA-C	6.71	1.62	1.52
6	F	233	VAL	CA-C	-6.68	1.44	1.52
32	g	113	GLN	CA-C	6.68	1.61	1.52
48	Ad	176	PRO	N-CD	-6.62	1.38	1.47
42	q	69	ASN	CA-C	6.60	1.61	1.52
51	AG	36	PRO	N-CD	6.58	1.56	1.47
7	G	600	GLU	CA-C	6.47	1.61	1.52
46	Ab	117	GLU	CA-C	6.33	1.61	1.52
17	Q	155	PRO	N-CD	-6.32	1.38	1.47
12	L	384	PRO	N-CD	6.24	1.56	1.47
41	p	10	TYR	CA-C	-6.19	1.46	1.52
42	q	69	ASN	C-O	6.19	1.31	1.24
7	G	127	ASP	CA-C	6.17	1.62	1.52
32	g	137	SER	C-O	-6.15	1.16	1.24
6	F	384	PRO	N-CD	-6.14	1.39	1.47
7	G	76	ARG	CA-C	6.14	1.61	1.53
16	P	292	PRO	N-CD	-6.13	1.39	1.47
4	D	359	ASP	CA-C	6.11	1.60	1.52
2	B	170	TYR	CA-CB	-6.04	1.43	1.53
7	G	192	VAL	CA-C	-6.04	1.47	1.53
45	AA	153	ASN	CA-C	5.98	1.61	1.53
5	E	93	PRO	N-CD	-5.96	1.39	1.47
12	L	112	PRO	N-CD	5.95	1.56	1.47
10	J	69	TYR	CA-C	-5.91	1.45	1.52
4	D	392	PRO	C-O	-5.88	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	m	72	ARG	CA-C	5.83	1.60	1.52
7	G	361	VAL	CA-C	5.80	1.60	1.52
36	k	19	LYS	C-N	5.76	1.41	1.33
15	O	87	PRO	N-CD	-5.74	1.39	1.47
37	l	45	PRO	N-CD	-5.73	1.39	1.47
19	S	50	ASN	CA-C	5.70	1.60	1.53
13	M	454	ILE	CA-C	5.69	1.60	1.52
19	S	63	PRO	N-CD	-5.64	1.39	1.47
14	N	333	SER	C-O	-5.58	1.17	1.23
17	Q	82	PRO	N-CD	-5.58	1.40	1.47
13	M	252	PRO	N-CD	-5.54	1.40	1.47
43	r	37	PRO	N-CD	5.41	1.55	1.47
20	U	140	CYS	C-O	-5.40	1.17	1.24
7	G	683	PRO	N-CD	-5.38	1.40	1.47
15	O	103	PRO	N-CD	-5.31	1.40	1.47
22	W	111	HIS	C-O	5.30	1.30	1.23
8	H	51	ASP	CA-C	5.25	1.59	1.52
45	Aa	311	ILE	C-N	5.19	1.40	1.33
31	f	38	ARG	CA-C	-5.14	1.46	1.52
33	h	174	PRO	N-CD	-5.14	1.40	1.47
40	o	24	SER	C-N	-5.12	1.23	1.33
13	M	424	ILE	CA-C	-5.11	1.45	1.52
39	n	80	TYR	CA-C	-5.10	1.46	1.52
2	B	195	PRO	CA-C	-5.09	1.47	1.52
13	M	159	PRO	N-CD	5.09	1.54	1.47
7	G	83	GLU	CA-C	5.08	1.59	1.52
42	q	4	VAL	CA-C	5.07	1.58	1.52
12	L	56	HIS	CA-C	-5.03	1.46	1.52
45	AA	311	ILE	C-N	5.02	1.40	1.33

All (1149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	231	ILE	N-CA-C	-19.19	90.97	113.42
2	B	99	CYS	N-CA-C	-18.00	91.45	113.41
2	B	170	TYR	N-CA-C	-17.69	89.93	111.33
7	G	174	THR	N-CA-C	-16.82	89.07	114.64
2	B	122	ARG	N-CA-CB	-16.68	85.52	110.04
2	B	121	PHE	N-CA-C	-16.25	86.23	110.28
6	F	125	CYS	N-CA-C	-15.66	93.43	113.17
6	F	332	CYS	N-CA-C	15.64	130.11	111.02
7	G	380	ASP	N-CA-C	15.31	129.32	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	370	PRO	N-CA-C	14.57	128.48	110.70
14	N	255	PRO	N-CA-C	14.50	128.39	110.70
8	H	196	ALA	CA-C-N	-14.42	105.69	119.82
8	H	196	ALA	C-N-CA	-14.42	105.69	119.82
15	O	118	TYR	N-CA-C	13.84	125.88	111.07
25	Z	102	PRO	N-CA-C	13.52	130.15	111.22
39	n	165	PRO	N-CA-C	13.34	130.41	111.33
7	G	251	ILE	N-CA-C	13.30	126.79	108.17
15	O	222	GLY	N-CA-C	13.25	129.73	112.77
7	G	77	MET	N-CA-C	-13.08	97.29	113.38
4	D	360	ASP	N-CA-C	-12.88	87.74	108.73
9	I	64	THR	N-CA-C	-12.74	98.38	114.56
25	Z	143	TYR	N-CA-C	12.73	129.48	108.73
41	p	128	GLU	N-CA-C	12.67	125.17	111.36
16	P	115	SER	N-CA-C	-12.59	97.38	113.12
44	s	85	LEU	N-CA-C	-12.55	97.65	111.07
7	G	500	ILE	N-CA-C	-12.47	98.81	110.53
26	a	3	PHE	CB-CA-C	-12.34	89.71	110.68
6	F	171	VAL	N-CA-C	-11.85	99.39	110.53
13	M	424	ILE	N-CA-C	-11.68	93.99	109.30
15	O	157	VAL	N-CA-C	11.67	124.45	108.11
7	G	204	MET	N-CA-C	-11.66	91.41	109.25
34	i	14	GLN	N-CA-C	11.60	123.92	111.28
6	F	449	ARG	N-CA-C	-11.59	98.73	111.36
15	O	114	LEU	N-CA-C	-11.53	98.79	111.36
6	F	334	THR	N-CA-CB	11.51	127.31	109.82
13	M	104	ILE	N-CA-C	-11.48	99.17	110.30
9	I	118	LEU	N-CA-C	11.47	126.77	113.01
12	L	194	ASN	N-CA-C	11.43	125.34	109.11
14	N	244	ILE	N-CA-C	-11.37	99.24	110.72
13	M	311	GLY	N-CA-C	-11.35	99.33	112.50
7	G	599	THR	N-CA-C	11.28	126.14	112.38
12	L	278	LEU	N-CA-C	-11.25	98.99	111.14
47	AC	115	ILE	N-CA-C	-11.23	99.16	110.62
11	K	83	ASN	N-CA-C	-11.16	100.21	114.04
7	G	83	GLU	N-CA-C	11.12	127.43	109.76
8	H	197	PRO	N-CA-C	-10.97	99.82	113.98
10	J	4	TYR	N-CA-C	-10.94	99.44	113.12
4	D	358	VAL	N-CA-C	-10.93	95.26	109.80
2	B	121	PHE	CA-C-O	-10.82	109.04	121.16
10	J	76	GLU	N-CA-C	-10.81	97.09	110.61
4	D	257	GLU	N-CA-C	-10.81	99.47	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	582	GLY	N-CA-C	-10.80	99.52	114.64
54	Ak	38	TRP	N-CA-C	10.76	126.05	110.24
2	B	122	ARG	N-CA-C	10.74	124.96	110.35
8	H	197	PRO	N-CA-CB	10.74	113.73	103.52
35	j	82	GLY	N-CA-C	-10.74	91.04	111.02
12	L	556	ILE	N-CA-C	10.69	121.34	110.23
12	L	231	PRO	N-CA-C	10.67	127.72	113.84
33	h	101	ILE	N-CA-C	-10.57	98.59	108.95
8	H	231	ILE	N-CA-CB	10.56	126.93	112.35
8	H	196	ALA	N-CA-C	10.48	132.97	109.81
43	r	64	VAL	N-CA-CB	-10.41	96.63	111.21
15	O	96	THR	N-CA-C	-10.40	100.03	111.36
15	O	247	PRO	N-CA-CB	10.35	114.30	103.23
13	M	276	CYS	N-CA-C	-10.34	100.01	111.28
4	D	365	PRO	N-CA-CB	-10.31	97.42	103.19
7	G	280	ASP	N-CA-C	10.28	122.48	111.28
42	q	5	GLU	N-CA-C	10.13	123.59	111.33
9	I	119	CYS	N-CA-C	10.11	126.86	113.72
37	l	170	ARG	N-CA-C	-10.10	101.60	113.21
7	G	414	PHE	N-CA-C	-10.08	101.49	113.88
15	O	220	LYS	N-CA-C	10.07	124.92	112.23
2	B	80	ASP	N-CA-C	-10.06	100.31	111.28
26	a	4	GLU	N-CA-C	10.04	124.79	112.54
19	S	57	GLU	N-CA-C	9.97	126.02	109.46
13	M	117	MET	N-CA-C	-9.96	100.42	111.28
7	G	325	ARG	N-CA-C	-9.88	100.20	110.97
46	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
46	Ab	306	THR	N-CA-C	9.83	123.22	111.33
6	F	178	GLU	N-CA-C	-9.81	99.34	111.11
45	Aa	187	LEU	N-CA-C	-9.79	100.43	112.38
11	K	90	VAL	N-CA-C	-9.79	100.32	112.76
45	Aa	47	GLU	N-CA-C	9.78	125.53	113.50
6	F	144	VAL	N-CA-C	-9.76	101.36	110.53
13	M	423	MET	N-CA-C	-9.76	96.89	110.35
45	AA	154	SER	N-CA-C	-9.75	94.79	110.20
6	F	103	ASN	N-CA-C	-9.75	101.08	113.16
6	F	141	GLY	N-CA-C	-9.73	101.21	112.50
14	N	255	PRO	CA-N-CD	9.72	125.61	112.00
14	N	286	ALA	N-CA-C	-9.70	100.71	111.28
7	G	35	PHE	N-CA-C	9.69	124.37	108.96
7	G	694	PHE	N-CA-C	9.68	121.42	111.07
25	Z	144	THR	N-CA-CB	-9.68	95.05	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Ad	142	GLU	N-CA-C	9.66	121.40	111.07
5	E	64	ALA	N-CA-C	-9.65	99.53	111.11
13	M	83	HIS	N-CA-C	-9.63	97.25	110.35
29	d	115	PRO	N-CA-CB	-9.61	94.99	103.35
34	i	12	LEU	N-CA-C	-9.60	101.11	113.12
6	F	418	GLN	N-CA-C	-9.60	100.77	111.14
7	G	337	ALA	N-CA-C	-9.59	100.79	114.12
39	n	29	SER	N-CA-C	-9.56	101.50	113.55
8	H	207	LEU	N-CA-C	-9.56	94.75	109.95
4	D	427	PRO	N-CA-C	-9.54	95.52	110.50
12	L	375	ILE	N-CA-C	-9.53	101.27	110.42
26	a	2	TRP	N-CA-C	-9.53	101.66	113.28
43	r	31	ILE	N-CA-C	9.51	121.76	109.30
27	b	78	LEU	CB-CA-C	-9.48	98.04	112.07
10	J	36	GLY	N-CA-C	-9.46	101.04	112.49
14	N	228	ASN	N-CA-C	-9.46	100.95	111.07
41	p	56	HIS	N-CA-C	9.45	121.58	111.28
2	B	155	PRO	N-CA-C	-9.43	95.68	110.95
42	q	3	LEU	N-CA-C	-9.43	100.55	112.90
29	d	115	PRO	CA-N-CD	9.41	125.18	112.00
31	f	51	ASN	CB-CA-C	-9.38	97.33	112.06
12	L	40	ILE	N-CA-C	-9.33	101.30	110.72
7	G	692	LYS	N-CA-C	-9.32	100.48	112.23
36	k	60	MET	N-CA-C	9.32	121.12	110.97
36	k	56	ALA	N-CA-C	9.30	121.50	111.36
13	M	104	ILE	N-CA-CB	9.27	120.73	110.62
7	G	640	ASP	N-CA-C	-9.27	101.26	111.36
12	L	394	LEU	N-CA-C	-9.24	101.19	111.07
9	I	95	PRO	N-CA-C	-9.23	102.32	113.86
38	m	48	LEU	N-CA-C	9.22	124.07	113.01
5	E	85	ALA	N-CA-C	-9.18	101.36	111.36
4	D	223	HIS	N-CA-C	-9.16	98.69	111.52
12	L	483	PRO	N-CA-C	-9.16	96.81	111.38
12	L	524	THR	N-CA-C	9.13	122.20	111.71
15	O	247	PRO	CA-N-CD	-9.12	99.23	112.00
14	N	87	GLN	N-CA-C	9.11	123.25	109.41
28	c	64	GLU	N-CA-C	-9.08	101.35	111.07
13	M	442	ILE	N-CA-CB	9.08	117.53	110.45
12	L	467	VAL	N-CA-C	9.06	119.12	110.42
28	c	39	PRO	N-CA-CB	-9.00	95.33	103.25
27	b	26	TRP	N-CA-C	-8.96	101.48	111.07
41	p	115	GLN	N-CA-C	-8.94	102.88	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	65	PRO	N-CA-CB	8.93	107.86	103.22
11	K	70	GLU	N-CA-C	-8.93	100.39	111.11
19	S	61	VAL	N-CA-C	-8.92	96.04	108.27
3	C	149	LEU	N-CA-C	8.90	124.20	113.16
3	C	180	HIS	N-CA-C	-8.90	95.76	109.64
2	B	122	ARG	CB-CA-C	8.89	125.53	109.62
6	F	411	SER	N-CA-C	-8.87	101.58	111.07
12	L	344	GLY	N-CA-C	-8.87	102.22	112.50
12	L	406	ALA	N-CA-C	-8.87	101.70	111.36
15	O	206	TYR	N-CA-CB	-8.85	92.77	110.64
14	N	233	LEU	N-CA-C	-8.84	101.64	111.28
50	AF	108	TRP	N-CA-C	-8.84	101.75	112.54
15	O	183	CYS	N-CA-C	-8.82	100.53	111.11
7	G	212	LYS	N-CA-C	-8.80	94.56	108.90
7	G	365	ASN	N-CA-C	-8.79	102.11	112.92
26	a	66	LEU	N-CA-C	-8.78	102.35	113.23
13	M	255	LYS	N-CA-C	-8.77	101.69	111.07
7	G	133	GLN	N-CA-CB	8.76	121.48	110.45
38	m	27	PRO	CA-N-CD	8.74	124.24	112.00
14	N	255	PRO	N-CA-CB	-8.74	94.61	103.08
14	N	81	LEU	N-CA-C	-8.72	94.42	108.55
42	q	66	THR	N-CA-C	-8.70	101.88	111.36
39	n	70	GLU	N-CA-C	-8.69	101.77	111.07
49	Ai	46	LYS	N-CA-C	8.69	121.54	110.33
40	o	72	ASP	N-CA-C	-8.69	99.06	110.53
9	I	62	MET	N-CA-C	-8.67	92.12	107.73
19	S	51	LEU	N-CA-C	-8.67	91.07	109.01
46	Ab	118	ASN	N-CA-CB	-8.67	97.45	110.97
7	G	310	GLU	CB-CA-C	-8.63	106.62	116.54
13	M	248	ILE	N-CA-C	-8.60	102.17	110.42
12	L	212	PRO	N-CA-C	8.59	125.76	113.47
10	J	29	GLY	N-CA-C	-8.59	102.25	112.64
26	a	3	PHE	CA-CB-CG	8.57	122.37	113.80
45	AA	143	VAL	N-CA-C	8.54	119.33	110.36
15	O	315	PRO	CA-N-CD	8.52	123.93	112.00
12	L	265	PRO	N-CA-C	-8.51	101.31	113.47
17	Q	59	LEU	N-CA-CB	-8.49	99.13	111.70
15	O	245	PHE	N-CA-C	8.48	120.15	111.07
14	N	221	LEU	N-CA-C	-8.45	101.11	111.33
14	N	272	LYS	N-CA-C	-8.42	102.10	111.28
12	L	281	GLY	N-CA-C	-8.41	102.75	112.50
49	Ae	148	ALA	N-CA-C	-8.40	102.58	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	287	PHE	N-CA-C	-8.40	102.08	111.07
43	r	25	GLN	N-CA-C	-8.40	103.04	113.28
15	O	212	PRO	N-CA-C	8.39	126.26	113.75
4	D	258	VAL	N-CA-C	-8.35	102.28	110.72
14	N	109	ALA	CA-C-N	-8.35	110.85	120.12
14	N	109	ALA	C-N-CA	-8.35	110.85	120.12
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
43	r	58	ASP	N-CA-C	8.35	123.62	108.17
39	n	19	LEU	N-CA-C	-8.35	103.23	113.41
42	q	64	TYR	N-CA-C	8.35	121.10	110.33
7	G	452	LEU	N-CA-C	-8.33	102.20	111.28
43	r	29	GLN	N-CA-C	-8.33	102.31	114.39
22	W	131	PRO	CA-N-CD	8.32	123.65	112.00
25	Z	90	ASN	N-CA-C	-8.32	103.26	113.41
14	N	218	ALA	N-CA-C	-8.26	98.92	111.56
51	AG	6	GLY	N-CA-C	-8.26	102.27	112.68
7	G	691	ILE	N-CA-C	8.22	123.72	111.89
13	M	274	SER	N-CA-C	8.22	120.24	111.28
12	L	88	LEU	N-CA-C	-8.21	102.28	111.14
7	G	387	LEU	N-CA-C	-8.20	98.00	110.30
6	F	298	GLU	N-CA-C	8.17	120.19	111.28
3	C	196	PRO	N-CA-C	8.17	124.89	113.53
12	L	151	SER	N-CA-C	-8.17	102.46	111.36
5	E	218	ARG	CB-CA-C	-8.16	99.87	112.12
14	N	32	GLY	N-CA-C	-8.16	103.03	112.50
4	D	36	GLN	N-CA-C	-8.16	98.50	110.42
21	V	87	GLU	N-CA-C	-8.16	102.38	111.28
7	G	484	ASP	N-CA-C	8.15	121.08	111.71
12	L	169	LEU	N-CA-C	-8.15	102.48	111.36
45	AA	360	CYS	N-CA-C	8.14	121.53	109.24
6	F	411	SER	N-CA-CB	8.12	121.79	110.01
13	M	26	ASN	N-CA-C	-8.12	102.37	111.14
36	k	38	VAL	N-CA-C	-8.11	102.53	110.72
7	G	500	ILE	N-CA-CB	8.11	120.95	110.57
6	F	191	TYR	N-CA-C	8.10	121.67	110.24
16	P	143	ASP	N-CA-C	8.10	119.74	111.07
45	Aa	360	CYS	N-CA-C	8.09	121.45	109.24
8	H	99	ASN	N-CA-C	-8.09	99.35	110.35
17	Q	155	PRO	N-CA-CB	-8.08	96.83	103.30
8	H	52	ALA	N-CA-C	-8.08	100.82	111.24
13	M	385	LEU	N-CA-C	-8.06	102.50	111.28
5	E	219	SER	N-CA-CB	8.05	124.04	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	217	ARG	N-CA-C	-8.05	102.46	111.07
39	n	170	ILE	N-CA-C	-8.03	103.06	111.58
8	H	193	THR	N-CA-C	-8.02	102.53	112.88
4	D	457	VAL	N-CA-C	-8.01	96.90	108.11
12	L	276	THR	N-CA-CB	8.00	121.61	110.01
7	G	534	VAL	N-CA-C	-7.99	104.80	111.91
1	A	61	THR	N-CA-C	-7.99	102.52	111.07
29	d	15	PRO	N-CA-CB	-7.99	96.40	103.35
43	r	10	LYS	N-CA-C	-7.98	103.00	112.89
7	G	664	TYR	N-CA-C	-7.97	97.67	109.62
10	J	60	LEU	N-CA-C	7.96	120.72	111.02
6	F	364	VAL	N-CA-C	7.94	118.72	110.62
1	A	36	PRO	N-CA-CB	-7.93	94.28	103.00
13	M	205	ILE	N-CA-C	7.92	118.02	110.42
28	c	39	PRO	CA-N-CD	7.92	123.08	112.00
13	M	141	GLU	N-CA-C	7.90	122.76	113.20
4	D	359	ASP	CB-CA-C	-7.90	94.71	110.42
7	G	270	VAL	N-CA-CB	-7.89	100.61	110.31
30	e	105	ARG	N-CA-C	7.86	122.45	110.50
41	p	128	GLU	N-CA-CB	-7.85	98.54	110.16
28	c	45	GLY	N-CA-C	7.85	123.53	113.24
2	B	165	ALA	N-CA-C	-7.85	104.19	114.31
12	L	111	ASP	N-CA-C	-7.84	100.20	109.93
12	L	265	PRO	N-CA-CB	7.84	111.62	103.23
13	M	85	LYS	N-CA-C	-7.82	101.37	113.02
38	m	50	GLN	N-CA-C	-7.81	102.77	114.64
9	I	118	LEU	CA-C-O	7.79	129.18	119.05
17	Q	72	ILE	N-CA-C	-7.79	105.90	113.53
5	E	193	GLU	N-CA-C	7.78	120.55	108.96
13	M	330	ALA	N-CA-C	-7.77	102.75	111.14
11	K	51	SER	N-CA-C	-7.75	102.91	113.30
7	G	377	ALA	N-CA-C	-7.75	102.92	112.38
12	L	265	PRO	CA-N-CD	-7.75	101.14	112.00
16	P	95	ARG	N-CA-C	7.75	120.62	111.71
8	H	230	ASN	N-CA-C	-7.74	101.89	112.03
25	Z	102	PRO	N-CA-CB	-7.74	93.20	103.42
14	N	336	THR	N-CA-C	-7.74	103.36	114.12
2	B	195	PRO	N-CA-C	-7.73	101.27	110.70
12	L	415	ALA	N-CA-C	-7.72	102.86	111.28
17	Q	139	GLU	N-CA-C	-7.70	102.83	111.07
6	F	334	THR	N-CA-C	-7.67	101.66	111.02
6	F	58	ARG	N-CA-C	-7.66	103.01	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	51	ASN	N-CA-C	7.66	121.97	111.17
46	Ab	118	ASN	N-CA-C	7.64	118.33	108.24
7	G	56	VAL	N-CA-C	-7.63	103.01	110.72
16	P	50	SER	N-CA-C	-7.63	98.25	109.63
4	D	184	ILE	N-CA-C	-7.62	102.84	110.62
50	AF	106	GLU	N-CA-C	7.62	119.23	111.07
31	f	48	LEU	N-CA-C	7.60	121.69	110.30
5	E	235	GLU	N-CA-C	-7.59	98.34	109.50
32	g	124	VAL	N-CA-C	-7.59	103.06	110.72
7	G	569	GLN	N-CA-C	7.58	121.97	108.24
6	F	171	VAL	N-CA-CB	7.57	120.26	110.57
5	E	166	LYS	N-CA-C	-7.57	102.22	113.72
20	U	147	TYR	N-CA-C	-7.55	102.98	111.14
40	o	81	LYS	N-CA-C	-7.55	104.59	113.88
48	AD	226	SER	N-CA-C	7.54	126.87	110.80
25	Z	142	TRP	N-CA-C	-7.54	99.12	110.28
21	V	41	HIS	N-CA-CB	-7.54	101.91	110.35
9	I	190	LEU	N-CA-C	-7.53	104.70	114.04
18	R	74	HIS	N-CA-C	7.53	121.11	110.50
38	m	27	PRO	N-CA-CB	-7.52	95.36	103.25
1	A	36	PRO	CA-N-CD	7.51	122.52	112.00
7	G	467	LYS	N-CA-C	-7.51	102.24	111.33
7	G	277	MET	N-CA-C	7.50	120.62	109.59
12	L	392	LYS	N-CA-C	7.50	119.09	111.07
48	AD	154	VAL	N-CA-C	7.49	119.30	107.98
12	L	245	ALA	N-CA-C	7.47	119.07	111.07
6	F	430	GLY	N-CA-C	7.46	121.69	112.73
11	K	14	LEU	N-CA-C	-7.46	103.23	111.36
30	e	46	GLY	N-CA-C	-7.46	104.97	114.37
2	B	169	GLY	N-CA-C	7.46	120.80	111.85
12	L	605	ASN	N-CA-CB	7.45	121.27	110.47
7	G	510	TRP	N-CA-CB	7.42	120.90	109.85
12	L	123	LEU	N-CA-C	-7.41	103.28	111.36
12	L	138	PHE	N-CA-C	-7.40	103.21	111.28
13	M	250	LEU	N-CA-C	-7.40	103.56	112.58
7	G	303	THR	N-CA-C	7.39	123.01	113.18
12	L	21	ILE	N-CA-CB	7.39	121.66	110.58
47	Ac	202	GLU	N-CA-C	-7.39	103.25	111.82
29	d	113	LEU	N-CA-CB	-7.38	99.93	111.23
47	AC	202	GLU	N-CA-C	-7.36	103.29	111.82
12	L	28	LYS	N-CA-C	-7.35	103.27	111.28
54	AK	39	ARG	N-CA-CB	7.33	122.97	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Ab	212	HIS	N-CA-C	7.33	121.98	112.89
6	F	259	GLY	N-CA-C	-7.31	103.91	112.83
38	m	72	ARG	N-CA-C	7.31	122.49	113.50
37	l	97	LEU	N-CA-C	-7.31	103.96	113.17
49	Ae	221	GLY	N-CA-C	7.30	126.90	113.76
49	AE	221	GLY	N-CA-C	7.30	126.90	113.76
47	Ac	8	HIS	CA-C-N	7.29	127.00	119.56
47	Ac	8	HIS	C-N-CA	7.29	127.00	119.56
13	M	455	THR	N-CA-C	-7.28	100.44	110.35
49	AI	45	VAL	CA-C-N	-7.27	108.61	121.70
49	AI	45	VAL	C-N-CA	-7.27	108.61	121.70
11	K	81	VAL	N-CA-C	7.27	118.04	110.62
28	c	37	ALA	N-CA-C	7.27	119.83	111.11
23	X	69	ASN	N-CA-C	-7.26	102.97	111.03
4	D	365	PRO	N-CA-C	7.26	117.44	110.47
12	L	19	ILE	N-CA-C	7.26	117.39	110.42
13	M	289	SER	N-CA-C	-7.25	103.31	111.07
10	J	21	LEU	N-CA-C	-7.24	104.53	113.15
33	h	174	PRO	N-CA-C	7.24	122.62	111.11
39	n	165	PRO	CB-CA-C	-7.24	100.25	111.40
47	AC	8	HIS	CA-C-N	7.24	126.94	119.56
47	AC	8	HIS	C-N-CA	7.24	126.94	119.56
46	Ab	125	GLY	N-CA-C	7.23	121.20	110.42
20	T	99	SER	N-CA-C	-7.23	99.18	109.96
19	S	33	VAL	N-CA-C	-7.22	103.25	110.62
15	O	224	PRO	N-CA-CB	-7.20	96.76	103.46
11	K	24	SER	CB-CA-C	-7.20	107.44	117.23
15	O	210	PRO	CA-N-CD	7.19	122.06	112.00
7	G	497	VAL	N-CA-C	-7.18	103.29	110.62
20	U	136	GLU	N-CA-C	-7.18	104.51	113.20
38	m	25	VAL	CB-CA-C	-7.18	102.89	111.65
4	D	257	GLU	N-CA-CB	7.18	120.48	110.07
6	F	73	PRO	N-CA-C	-7.17	103.79	113.40
4	D	303	ARG	N-CA-C	-7.17	104.16	114.12
8	H	198	PHE	CB-CA-C	-7.16	101.19	111.14
3	C	195	HIS	CB-CA-C	7.15	117.25	110.17
36	k	73	ILE	N-CA-C	-7.15	103.33	110.62
12	L	554	ASP	N-CA-CB	7.14	121.28	110.42
6	F	81	LYS	N-CA-C	-7.13	103.58	111.36
13	M	244	ILE	N-CA-C	7.13	117.89	110.62
45	Aa	47	GLU	CA-C-O	7.12	126.98	119.14
13	M	325	LEU	N-CA-C	-7.12	103.45	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	198	PHE	N-CA-C	7.11	121.92	112.25
35	j	78	ASP	N-CA-C	-7.11	103.17	112.41
41	p	168	LYS	N-CA-C	-7.11	104.24	113.12
16	P	97	MET	N-CA-CB	7.10	121.32	110.60
35	j	65	MET	N-CA-C	-7.10	103.48	111.07
7	G	465	VAL	N-CA-CB	7.09	118.38	110.51
7	G	461	SER	N-CA-C	7.09	119.91	111.33
15	O	210	PRO	N-CA-C	7.08	122.32	111.34
47	Ac	17	SER	N-CA-C	7.08	122.09	113.38
6	F	78	GLY	N-CA-C	-7.08	104.24	112.73
7	G	217	GLU	N-CA-C	-7.07	101.71	110.41
11	K	48	SER	N-CA-C	-7.07	103.58	111.28
1	A	67	LEU	N-CA-C	-7.05	103.64	111.82
2	B	194	CYS	N-CA-C	-7.05	102.58	112.17
7	G	148	SER	N-CA-C	7.05	120.89	109.40
13	M	34	ILE	N-CA-C	-7.05	103.43	110.62
48	Ad	221	PRO	N-CA-C	-7.05	102.10	110.70
13	M	365	ALA	N-CA-C	-7.04	103.69	111.36
39	n	102	TRP	N-CA-C	-7.03	105.06	112.93
8	H	52	ALA	N-CA-CB	7.03	120.40	110.07
40	o	11	TRP	CB-CA-C	-7.02	108.48	116.63
35	j	81	LEU	CA-C-O	7.02	126.02	119.00
12	L	319	MET	N-CA-C	-7.01	104.72	112.72
51	AG	54	VAL	N-CA-C	-7.01	103.69	110.42
46	Ab	74	SER	N-CA-C	7.00	119.77	111.71
13	M	264	LEU	N-CA-C	-7.00	103.58	111.07
47	AC	17	SER	N-CA-C	7.00	122.00	113.38
6	F	246	GLU	N-CA-C	-7.00	103.65	111.28
12	L	100	ILE	N-CA-C	6.99	119.79	111.05
6	F	169	LEU	N-CA-C	6.99	118.90	111.28
13	M	213	HIS	CB-CA-C	-6.99	96.83	110.11
52	Ah	33	GLU	N-CA-C	-6.98	103.75	111.36
14	N	132	THR	N-CA-C	6.97	122.90	113.97
3	C	80	LEU	N-CA-C	-6.97	104.65	113.02
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
6	F	428	GLY	N-CA-C	-6.97	103.85	112.77
21	V	74	GLY	N-CA-C	-6.96	104.43	112.79
49	Ai	45	VAL	CA-C-N	-6.96	108.56	120.95
49	Ai	45	VAL	C-N-CA	-6.96	108.56	120.95
4	D	193	ASP	N-CA-C	-6.95	103.63	111.07
49	Ae	218	THR	N-CA-C	-6.95	102.86	111.75
6	F	418	GLN	N-CA-CB	6.94	120.14	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	86	SER	N-CA-C	6.94	118.50	111.07
12	L	546	LEU	N-CA-C	6.94	119.49	111.02
15	O	220	LYS	CB-CA-C	-6.94	96.22	110.38
49	AE	218	THR	N-CA-C	-6.94	102.86	111.75
42	q	137	TRP	N-CA-C	-6.94	99.55	109.96
26	a	57	VAL	N-CA-C	-6.93	105.97	112.83
34	i	9	LYS	N-CA-C	-6.93	104.82	112.72
8	H	156	MET	N-CA-C	6.93	118.91	111.36
4	D	255	ILE	N-CA-C	6.93	117.07	110.42
7	G	294	TYR	N-CA-C	-6.92	104.64	113.23
6	F	103	ASN	N-CA-CB	6.92	121.03	110.44
8	H	194	ASN	N-CA-C	-6.92	101.84	111.39
15	O	231	SER	N-CA-C	-6.92	103.81	111.36
13	M	91	LEU	N-CA-C	-6.92	103.84	112.90
34	i	11	ARG	N-CA-C	-6.92	104.84	113.28
7	G	582	VAL	N-CA-C	6.92	118.44	108.48
48	AD	244	MET	N-CA-C	-6.91	97.28	108.41
45	Aa	110	GLU	N-CA-CB	6.91	120.28	110.12
22	W	131	PRO	N-CA-CB	-6.91	95.40	103.00
6	F	148	ALA	N-CA-C	-6.90	103.84	111.36
3	C	233	ASP	CB-CA-C	-6.89	102.16	111.88
13	M	235	LEU	N-CA-C	6.89	119.38	111.11
13	M	442	ILE	N-CA-C	-6.89	104.08	112.35
5	E	152	GLN	N-CA-C	-6.89	103.70	111.07
12	L	471	ASN	N-CA-C	6.88	118.86	111.36
8	H	77	LEU	N-CA-C	-6.88	103.47	110.97
7	G	133	GLN	N-CA-C	-6.88	101.11	110.68
7	G	300	GLN	N-CA-CB	6.88	122.46	112.08
12	L	26	LEU	N-CA-C	6.87	119.61	111.71
17	Q	61	ILE	N-CA-C	-6.87	105.79	111.91
39	n	117	ASP	N-CA-C	-6.87	103.85	111.82
36	k	59	TYR	N-CA-CB	-6.87	98.87	110.41
13	M	276	CYS	N-CA-CB	6.87	120.21	110.12
5	E	235	GLU	N-CA-CB	6.86	122.23	109.68
7	G	362	ASP	N-CA-C	6.86	125.41	110.80
12	L	547	LYS	N-CA-C	6.86	118.75	111.28
32	g	78	PRO	CA-N-CD	6.86	121.60	112.00
7	G	385	TYR	N-CA-C	6.85	120.94	111.55
15	O	93	TYR	N-CA-C	-6.85	103.89	111.36
6	F	233	VAL	O-C-N	6.85	131.11	123.10
10	J	58	ILE	N-CA-C	6.84	117.44	111.56
13	M	165	ILE	N-CA-C	-6.84	102.54	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	65	PRO	N-CA-C	-6.84	103.26	110.58
46	AB	293	LEU	N-CA-C	-6.83	100.92	110.35
11	K	83	ASN	N-CA-CB	6.83	120.92	110.81
6	F	329	LYS	N-CA-C	6.83	119.59	111.33
52	Ah	43	LYS	N-CA-C	-6.83	103.84	111.28
7	G	268	GLY	N-CA-C	6.81	124.76	115.30
46	Ab	234	ALA	N-CA-C	-6.81	105.51	113.88
18	R	46	VAL	N-CA-C	-6.80	103.68	110.62
35	j	79	ALA	N-CA-C	-6.80	103.95	111.36
6	F	244	ASN	N-CA-C	-6.79	100.93	110.50
19	S	49	PRO	N-CA-C	6.78	120.71	111.22
16	P	333	PRO	CA-N-CD	6.78	121.49	112.00
11	K	70	GLU	N-CA-CB	6.77	120.03	109.94
23	X	104	GLN	N-CA-C	6.77	118.45	111.14
9	I	119	CYS	N-CA-CB	-6.77	100.70	110.65
3	C	204	THR	N-CA-C	6.77	120.51	112.93
7	G	434	SER	N-CA-C	-6.74	100.99	110.29
8	H	203	GLY	N-CA-C	-6.73	97.22	113.18
6	F	233	VAL	CA-C-O	-6.73	113.33	120.53
17	Q	58	LYS	CA-C-O	6.72	128.81	119.80
29	d	88	HIS	N-CA-C	-6.72	103.04	111.11
4	D	329	ARG	CB-CA-C	6.72	121.95	110.79
38	m	127	ILE	N-CA-C	-6.72	106.25	112.43
50	AF	108	TRP	N-CA-CB	6.72	121.54	110.39
15	O	207	ILE	N-CA-C	-6.71	97.27	107.73
13	M	248	ILE	N-CA-CB	6.71	118.39	110.55
9	I	86	TYR	CB-CA-C	-6.70	101.29	113.49
13	M	374	ASN	N-CA-C	-6.70	103.90	111.07
23	X	57	LEU	N-CA-C	-6.70	104.20	112.38
45	AA	361	ASP	N-CA-C	-6.70	101.24	110.35
20	U	140	CYS	CA-C-N	-6.70	114.00	120.83
20	U	140	CYS	C-N-CA	-6.70	114.00	120.83
9	I	49	ASP	N-CA-C	-6.69	99.77	110.14
14	N	228	ASN	N-CA-CB	6.69	119.71	110.01
32	g	76	SER	N-CA-C	6.69	118.22	111.07
12	L	95	PHE	N-CA-C	-6.68	103.93	111.07
15	O	315	PRO	N-CA-CB	-6.67	95.99	103.33
7	G	640	ASP	N-CA-CB	6.67	120.03	110.16
20	U	150	ASP	CB-CA-C	6.67	121.86	110.79
37	l	86	ARG	N-CA-C	-6.67	99.66	110.20
45	Aa	361	ASP	N-CA-C	-6.67	101.28	110.35
3	C	49	ARG	N-CA-C	6.67	120.38	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	121	PHE	CA-C-N	6.66	130.81	120.75
2	B	121	PHE	C-N-CA	6.66	130.81	120.75
15	O	224	PRO	CA-N-CD	6.66	121.32	112.00
6	F	344	GLN	N-CA-C	-6.66	104.03	111.28
26	a	65	GLY	N-CA-C	-6.65	105.57	114.95
45	AA	187	LEU	N-CA-C	-6.65	103.72	110.97
7	G	287	SER	N-CA-C	6.64	119.30	110.53
2	B	88	SER	N-CA-C	-6.64	103.97	111.14
8	H	311	THR	N-CA-C	-6.64	104.81	113.17
11	K	76	ALA	N-CA-C	-6.63	104.13	111.36
9	I	51	LYS	N-CA-C	-6.63	103.97	111.07
13	M	410	MET	N-CA-C	-6.63	103.98	111.07
7	G	601	GLY	N-CA-C	6.62	124.84	115.30
13	M	143	LEU	N-CA-C	-6.62	103.98	111.07
13	M	303	ILE	N-CA-C	-6.62	104.03	110.72
2	B	124	SER	N-CA-C	6.62	119.54	109.41
4	D	70	ASP	N-CA-C	6.62	120.68	110.42
6	F	228	PRO	N-CA-C	-6.61	98.85	112.47
15	O	140	LEU	N-CA-C	-6.61	104.00	111.07
6	F	206	CYS	N-CA-C	-6.60	105.08	113.01
5	E	166	LYS	CB-CA-C	6.60	123.52	110.65
22	W	98	LYS	N-CA-C	-6.59	102.01	110.19
34	i	8	GLU	N-CA-C	-6.58	104.84	114.39
6	F	336	LEU	N-CA-CB	-6.58	100.97	111.43
12	L	499	LEU	N-CA-C	-6.57	103.81	110.97
46	Ab	305	THR	N-CA-CB	-6.57	100.32	109.91
12	L	130	ILE	N-CA-C	-6.57	103.92	110.62
17	Q	58	LYS	CB-CA-C	-6.57	101.12	111.17
7	G	435	PRO	N-CA-C	-6.56	100.20	110.50
19	S	50	ASN	CA-C-O	6.56	129.28	121.08
9	I	98	ARG	N-CA-C	6.55	118.96	108.41
1	A	59	ALA	N-CA-C	6.55	118.42	111.28
36	k	57	TRP	N-CA-C	-6.55	104.55	112.54
6	F	234	GLY	CA-C-N	-6.54	111.73	120.50
6	F	234	GLY	C-N-CA	-6.54	111.73	120.50
45	AA	153	ASN	CA-C-O	6.54	129.26	121.08
7	G	275	PRO	CB-CA-C	-6.54	102.41	110.98
12	L	232	TRP	N-CA-C	6.54	120.52	112.54
39	n	115	TYR	N-CA-CB	6.54	122.00	110.37
13	M	161	LEU	N-CA-C	-6.53	104.08	111.07
49	Ai	44	ASP	O-C-N	6.53	131.27	122.59
2	B	163	SER	N-CA-C	-6.53	105.28	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	16	LEU	CA-C-N	-6.53	112.96	122.69
26	a	16	LEU	C-N-CA	-6.53	112.96	122.69
12	L	423	SER	N-CA-C	-6.53	104.09	111.07
41	p	54	ARG	N-CA-C	-6.52	103.67	111.69
7	G	605	GLN	N-CA-C	6.52	119.14	108.52
15	O	118	TYR	N-CA-CB	-6.52	100.56	110.01
45	AA	215	ASP	N-CA-C	-6.50	103.89	110.97
4	D	365	PRO	CA-N-CD	6.50	121.09	112.00
26	a	58	ASN	N-CA-C	6.49	119.31	108.73
12	L	329	ILE	N-CA-C	-6.49	104.19	110.42
45	Aa	215	ASP	N-CA-C	-6.49	103.89	110.97
19	S	61	VAL	N-CA-CB	6.49	123.05	111.63
7	G	189	ILE	N-CA-C	-6.49	105.38	111.48
38	m	51	TYR	N-CA-C	-6.49	105.67	113.97
7	G	653	LEU	N-CA-CB	6.48	121.45	110.49
24	Y	96	GLY	N-CA-C	-6.47	104.48	112.77
14	N	315	THR	N-CA-C	-6.47	104.15	111.07
37	l	119	THR	N-CA-C	-6.46	95.78	107.60
20	T	95	PRO	N-CA-C	-6.46	106.41	114.68
7	G	190	ALA	N-CA-C	-6.45	99.13	109.96
7	G	275	PRO	CA-N-CD	6.45	121.02	112.00
19	S	41	TYR	N-CA-C	-6.44	103.95	110.97
40	o	22	ILE	CA-C-N	-6.44	113.22	121.91
40	o	22	ILE	C-N-CA	-6.44	113.22	121.91
6	F	178	GLU	N-CA-CB	6.44	119.53	109.94
7	G	250	SER	N-CA-C	6.43	116.77	108.34
7	G	273	ILE	N-CA-C	-6.43	98.36	107.75
15	O	221	LYS	N-CA-C	-6.43	101.44	110.50
16	P	224	LEU	CB-CA-C	-6.43	109.15	116.54
48	AD	196	ASP	N-CA-C	-6.43	101.61	110.35
7	G	662	THR	N-CA-C	-6.41	96.45	107.61
15	O	320	GLY	N-CA-C	-6.41	96.69	111.04
48	Ad	245	ALA	CA-C-N	-6.41	113.78	120.38
48	Ad	245	ALA	C-N-CA	-6.41	113.78	120.38
46	Ab	117	GLU	CA-C-O	6.41	127.24	119.49
11	K	11	ALA	N-CA-C	-6.40	104.22	111.07
16	P	119	ALA	N-CA-C	-6.40	104.22	111.14
52	Ah	78	HIS	N-CA-C	-6.40	103.59	111.33
45	AA	186	TYR	N-CA-C	-6.39	106.02	113.88
12	L	325	ALA	N-CA-C	-6.38	104.32	111.28
45	Aa	48	THR	N-CA-CB	6.38	121.61	111.91
13	M	32	PHE	N-CA-C	-6.38	104.25	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	112	MET	N-CA-C	6.37	120.84	113.38
42	q	143	PRO	CA-N-CD	6.37	120.91	112.00
12	L	439	PRO	N-CA-C	6.36	122.37	113.53
43	r	27	ARG	N-CA-C	6.36	118.66	108.41
6	F	416	SER	N-CA-C	6.36	117.87	111.07
12	L	234	PRO	CA-N-CD	-6.36	103.10	112.00
12	L	387	THR	N-CA-C	6.36	119.02	111.71
8	H	288	LEU	N-CA-C	-6.35	103.65	111.40
29	d	15	PRO	CA-N-CD	6.35	120.89	112.00
12	L	490	ALA	N-CA-C	-6.34	104.28	111.07
6	F	144	VAL	N-CA-CB	6.34	118.68	110.57
6	F	370	LEU	N-CA-C	-6.34	104.45	111.36
4	D	337	MET	N-CA-C	-6.33	104.38	111.28
13	M	317	ILE	N-CA-C	-6.33	104.58	110.53
15	O	98	THR	N-CA-C	6.33	120.60	109.96
34	i	32	GLU	CA-C-N	-6.33	111.92	119.84
34	i	32	GLU	C-N-CA	-6.33	111.92	119.84
12	L	70	THR	N-CA-C	-6.32	103.91	111.69
10	J	136	GLU	CA-C-N	-6.32	113.56	120.44
10	J	136	GLU	C-N-CA	-6.32	113.56	120.44
17	Q	105	GLU	N-CA-C	6.30	119.35	109.96
44	s	93	PRO	N-CA-C	6.30	120.97	111.14
7	G	176	CYS	N-CA-C	6.30	119.61	110.42
31	f	52	GLU	N-CA-CB	6.29	121.16	110.71
5	E	64	ALA	N-CA-CB	6.28	119.30	109.94
14	N	89	GLN	N-CA-C	6.28	120.50	112.34
26	a	26	ILE	N-CA-C	-6.28	104.53	113.07
12	L	337	ALA	N-CA-C	-6.27	104.44	111.28
13	M	26	ASN	N-CA-CB	6.27	119.17	110.07
3	C	47	ARG	N-CA-C	6.27	116.81	109.60
37	l	105	ILE	CA-C-O	-6.26	115.14	121.59
48	Ad	152	VAL	N-CA-C	6.26	117.83	109.37
3	C	149	LEU	N-CA-CB	-6.26	100.86	110.44
28	c	47	SER	N-CA-CB	6.26	120.84	110.33
49	AI	44	ASP	O-C-N	6.25	131.04	121.23
8	H	217	ALA	CB-CA-C	-6.24	109.36	116.54
9	I	66	LEU	N-CA-C	-6.24	105.67	113.28
12	L	502	LEU	N-CA-C	-6.24	104.48	111.28
14	N	46	ASN	N-CA-C	-6.24	105.69	113.55
5	E	50	THR	N-CA-CB	6.23	121.47	110.37
6	F	409	ILE	N-CA-C	6.23	116.40	110.42
6	F	415	ILE	N-CA-C	-6.22	104.43	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	192	ASP	N-CA-C	6.22	119.08	109.07
7	G	356	ASP	N-CA-CB	6.22	119.26	110.12
15	O	210	PRO	N-CA-CB	-6.22	97.55	103.39
14	N	276	LEU	N-CA-C	-6.21	105.34	113.17
3	C	223	VAL	N-CA-C	6.21	117.03	108.84
6	F	101	PHE	N-CA-C	6.21	118.84	111.33
14	N	91	ASN	N-CA-CB	6.21	119.09	109.97
14	N	216	PHE	N-CA-C	6.21	118.12	111.36
15	O	113	SER	N-CA-C	6.20	118.52	108.41
38	m	72	ARG	CA-C-O	6.20	125.96	119.14
2	B	135	GLY	CA-C-O	-6.20	117.99	122.45
32	g	123	LEU	N-CA-CB	6.19	119.05	110.07
46	Ab	116	ARG	N-CA-C	-6.19	104.08	111.69
13	M	121	LEU	N-CA-C	-6.18	104.62	111.36
36	k	59	TYR	N-CA-C	6.18	120.66	113.18
4	D	262	LEU	N-CA-CB	-6.18	102.37	110.59
7	G	389	THR	N-CA-C	-6.18	101.27	110.23
7	G	451	ILE	N-CA-C	-6.17	104.97	113.00
7	G	418	ILE	N-CA-C	-6.17	103.40	112.04
9	I	86	TYR	N-CA-C	6.17	120.88	112.55
12	L	361	ASN	CB-CA-C	-6.17	102.79	111.80
14	N	337	LEU	CA-C-N	-6.16	113.78	119.82
14	N	337	LEU	C-N-CA	-6.16	113.78	119.82
7	G	325	ARG	N-CA-CB	6.16	118.90	109.91
2	B	80	ASP	N-CA-CB	6.15	119.16	110.12
31	f	49	ARG	N-CA-CB	6.14	119.08	110.11
52	Ah	49	GLU	N-CA-C	-6.14	104.50	111.07
4	D	145	MET	N-CA-C	6.14	123.88	110.80
54	AK	25	GLY	N-CA-C	-6.13	105.39	112.50
36	k	30	ILE	N-CA-C	6.13	118.75	111.09
51	AG	56	VAL	N-CA-C	6.13	116.61	110.23
39	n	63	LEU	N-CA-C	-6.13	104.15	111.69
48	Ad	180	PRO	N-CA-CB	6.13	109.56	102.33
44	s	83	LEU	N-CA-C	6.13	117.63	111.07
52	Ah	48	LEU	N-CA-C	-6.13	104.51	111.07
14	N	47	LYS	N-CA-C	-6.13	104.71	111.82
7	G	420	LYS	N-CA-C	6.12	118.74	111.33
10	J	123	TRP	N-CA-C	-6.12	102.55	111.30
40	o	105	GLU	N-CA-C	-6.12	104.69	111.36
48	AD	153	GLU	N-CA-CB	-6.12	102.14	110.95
17	Q	71	HIS	N-CA-C	-6.12	105.10	113.30
13	M	4	ILE	N-CA-C	-6.11	104.00	112.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	98	TRP	N-CA-C	-6.11	104.70	111.36
2	B	194	CYS	N-CA-CB	6.11	116.19	110.39
12	L	454	ILE	N-CA-C	-6.11	104.39	110.62
28	c	33	GLU	CA-C-N	-6.10	113.99	120.03
28	c	33	GLU	C-N-CA	-6.10	113.99	120.03
13	M	57	SER	N-CA-C	6.10	119.14	109.50
4	D	147	ASN	N-CA-C	-6.10	104.55	111.07
51	AG	32	SER	N-CA-C	6.10	117.59	111.07
31	f	39	ASN	N-CA-C	-6.09	104.02	112.30
32	g	109	ASP	CA-CB-CG	6.09	118.69	112.60
33	h	101	ILE	N-CA-CB	6.07	115.72	110.08
33	h	142	ILE	N-CA-C	-6.07	104.60	110.42
16	P	361	TRP	N-CA-C	-6.06	106.86	114.56
13	M	213	HIS	N-CA-C	6.06	120.53	113.20
16	P	268	PRO	N-CA-C	6.06	121.95	113.53
27	b	80	TRP	N-CA-CB	6.06	119.72	110.39
12	L	287	PHE	N-CA-CB	6.05	118.79	110.01
14	N	91	ASN	N-CA-C	-6.05	101.33	110.28
51	Ag	31	PHE	N-CA-C	-6.05	105.94	113.38
46	Ab	213	PHE	N-CA-CB	-6.04	102.07	110.65
42	q	141	SER	N-CA-C	6.04	117.86	111.28
12	L	140	LEU	N-CA-C	-6.04	104.70	111.28
7	G	508	ALA	N-CA-C	6.03	117.85	111.28
32	g	123	LEU	N-CA-C	-6.03	104.63	111.14
13	M	3	LYS	N-CA-C	-6.03	106.06	113.41
45	Aa	110	GLU	N-CA-C	-6.03	104.71	111.28
16	P	85	ARG	N-CA-C	-6.01	105.53	112.92
50	AF	37	THR	N-CA-C	6.01	120.61	113.28
7	G	353	ALA	N-CA-C	-6.00	104.67	112.23
13	M	396	MET	N-CA-C	-6.00	105.94	113.20
13	M	370	PRO	CA-N-CD	6.00	120.39	112.00
15	O	183	CYS	N-CA-CB	5.99	118.86	109.94
7	G	532	PRO	N-CA-CB	-5.98	97.10	103.38
42	q	132	LYS	N-CA-CB	-5.98	107.35	114.17
41	p	8	ASP	N-CA-C	5.97	120.64	113.23
48	Ad	148	LEU	N-CA-C	-5.97	104.77	111.28
7	G	638	THR	N-CA-C	-5.97	100.23	109.24
48	AD	227	LEU	N-CA-CB	5.97	118.38	109.19
13	M	168	GLN	N-CA-C	-5.97	104.86	111.36
12	L	234	PRO	N-CA-CB	5.97	109.61	103.23
14	N	295	ARG	N-CA-C	-5.96	104.78	111.28
28	c	47	SER	N-CA-C	-5.96	104.75	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	AB	244	LEU	N-CA-C	-5.96	106.01	113.28
6	F	291	GLU	N-CA-C	5.96	118.23	110.43
13	M	253	LEU	N-CA-C	5.95	117.77	111.28
16	P	76	MET	N-CA-C	-5.95	106.07	113.15
48	AD	242	ILE	N-CA-C	5.95	116.61	110.36
32	g	78	PRO	N-CA-C	5.95	121.80	113.53
13	M	300	SER	N-CA-C	-5.95	107.01	114.56
12	L	112	PRO	CB-CA-C	-5.95	103.00	111.68
13	M	222	GLU	N-CA-C	5.95	120.37	113.18
15	O	234	LEU	N-CA-C	-5.95	104.88	111.36
23	X	60	GLY	N-CA-C	-5.95	105.60	112.50
10	J	155	ALA	N-CA-C	-5.94	104.89	111.36
46	Ab	213	PHE	N-CA-C	5.93	119.26	112.97
22	W	33	ARG	N-CA-C	-5.93	104.81	111.28
25	Z	101	VAL	CA-C-N	-5.93	114.52	120.21
25	Z	101	VAL	C-N-CA	-5.93	114.52	120.21
4	D	350	LYS	CB-CA-C	-5.92	103.14	111.85
12	L	278	LEU	N-CA-CB	5.92	118.66	110.07
31	f	53	GLU	N-CA-CB	-5.92	101.37	110.20
41	p	127	LYS	N-CA-C	-5.92	104.17	111.40
23	X	16	GLU	N-CA-C	-5.92	102.30	110.35
7	G	651	PRO	N-CA-C	5.92	121.31	114.03
12	L	88	LEU	N-CA-CB	5.92	118.65	110.07
6	F	127	ASP	N-CA-C	5.91	118.51	111.71
13	M	88	ASN	N-CA-C	5.91	120.12	113.02
15	O	181	LYS	N-CA-C	5.90	117.39	111.07
48	AD	191	GLY	N-CA-C	-5.90	108.05	115.08
5	E	233	LEU	CB-CA-C	-5.90	101.61	111.23
12	L	247	LEU	N-CA-CB	5.90	120.61	110.34
12	L	248	HIS	CB-CA-C	5.90	120.88	110.85
23	X	76	SER	N-CA-C	-5.90	101.89	111.04
15	O	130	ARG	N-CA-C	-5.90	104.85	111.28
16	P	331	ASP	CB-CA-C	-5.89	103.41	111.95
52	Ah	65	CYS	N-CA-C	-5.89	106.07	113.20
54	Ak	16	ASN	N-CA-C	-5.88	105.00	111.82
30	e	101	ARG	CB-CA-C	-5.87	109.82	116.63
12	L	387	THR	CB-CA-C	-5.87	99.77	110.63
4	D	455	ASP	CB-CA-C	-5.86	103.56	111.89
36	k	80	GLY	N-CA-C	-5.86	105.70	112.50
13	M	272	THR	N-CA-C	-5.86	104.98	111.36
14	N	16	GLY	CA-C-N	-5.86	112.47	118.85
14	N	16	GLY	C-N-CA	-5.86	112.47	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	333	PRO	N-CA-CB	-5.86	97.10	103.25
9	I	85	ASN	N-CA-C	-5.85	100.72	109.15
15	O	217	ARG	N-CA-CB	5.85	118.50	110.01
20	U	143	GLU	N-CA-C	-5.85	104.26	111.75
8	H	2	PHE	N-CA-C	-5.84	104.87	112.23
36	k	82	ALA	N-CA-C	-5.84	104.92	111.28
19	S	51	LEU	N-CA-CB	5.84	119.52	110.12
39	n	27	LEU	N-CA-C	-5.84	106.13	113.72
38	m	116	ILE	N-CA-C	-5.84	104.82	110.42
36	k	50	PRO	N-CA-C	5.83	121.64	113.53
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
14	N	66	ALA	N-CA-C	-5.82	105.02	111.36
44	s	90	PHE	N-CA-CB	5.82	118.50	110.07
52	AH	53	ASN	N-CA-C	-5.81	104.95	111.28
15	O	262	GLU	N-CA-C	-5.81	104.95	111.28
14	N	15	LEU	N-CA-C	-5.80	105.69	112.89
22	W	97	ILE	N-CA-C	-5.80	104.85	110.42
48	AD	243	GLY	N-CA-C	-5.80	107.87	115.47
29	d	62	LEU	N-CA-C	5.80	117.60	111.28
31	f	52	GLU	N-CA-C	-5.79	98.05	108.48
7	G	672	ALA	N-CA-C	-5.79	104.97	111.28
12	L	428	TYR	N-CA-C	-5.79	104.89	111.14
4	D	232	VAL	N-CA-C	-5.79	101.47	109.46
25	Z	26	PRO	N-CA-C	5.79	120.34	110.74
34	i	10	LEU	N-CA-C	-5.79	107.21	114.56
37	l	186	ILE	N-CA-CB	-5.78	101.67	111.50
35	j	73	PHE	N-CA-C	-5.78	104.88	111.07
4	D	414	ASP	N-CA-C	-5.78	101.40	110.36
17	Q	57	GLU	N-CA-C	-5.78	100.63	109.41
34	i	105	PHE	CA-C-N	-5.77	113.75	119.99
34	i	105	PHE	C-N-CA	-5.77	113.75	119.99
7	G	275	PRO	N-CA-CB	-5.77	97.97	103.33
32	g	78	PRO	N-CA-CB	-5.77	96.98	103.33
7	G	289	LYS	N-CA-C	5.76	117.56	111.28
39	n	52	LYS	N-CA-C	-5.76	105.92	113.12
4	D	114	GLY	N-CA-C	-5.76	99.53	113.18
12	L	177	ILE	N-CA-C	-5.76	104.75	110.62
7	G	181	ARG	N-CA-C	-5.76	104.61	111.69
6	F	102	MET	CB-CA-C	-5.75	101.45	110.94
6	F	299	LEU	N-CA-C	5.75	118.49	111.82
31	f	36	ALA	N-CA-C	-5.75	103.34	110.41
6	F	393	ASN	N-CA-C	-5.74	104.92	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	77	ASP	N-CA-C	-5.74	107.27	114.56
16	P	375	VAL	N-CA-C	5.74	117.94	108.99
9	I	64	THR	N-CA-CB	-5.74	103.37	111.00
13	M	279	GLN	N-CA-C	-5.74	98.54	108.69
13	M	424	ILE	O-C-N	5.73	128.35	122.79
14	N	321	LYS	N-CA-C	5.73	118.45	110.20
31	f	10	HIS	N-CA-C	-5.73	104.51	112.30
27	b	61	GLY	N-CA-C	-5.73	107.76	115.21
10	J	134	MET	CA-C-N	-5.73	114.89	122.85
10	J	134	MET	C-N-CA	-5.73	114.89	122.85
12	L	467	VAL	N-CA-CB	-5.73	103.85	110.55
16	P	44	GLY	N-CA-C	5.72	119.49	110.96
20	U	83	VAL	N-CA-C	-5.72	104.94	110.72
46	Ab	242	GLY	N-CA-C	5.72	120.74	113.24
13	M	124	ALA	N-CA-C	-5.72	105.12	111.36
47	Ac	17	SER	N-CA-CB	-5.72	102.01	110.53
1	A	61	THR	N-CA-CB	5.71	118.29	110.01
13	M	19	SER	N-CA-C	5.71	117.78	109.84
26	a	3	PHE	N-CA-CB	5.71	118.62	110.06
29	d	53	VAL	N-CA-C	5.71	116.36	110.36
12	L	605	ASN	N-CA-C	-5.71	106.17	113.02
5	E	183	PRO	N-CA-C	-5.70	102.19	110.80
5	E	119	THR	N-CA-C	-5.70	105.82	112.89
12	L	495	VAL	N-CA-C	5.70	115.89	110.42
12	L	419	THR	N-CA-C	-5.69	105.07	111.28
32	g	67	LYS	N-CA-C	-5.69	102.04	110.46
48	Ad	180	PRO	CA-N-CD	-5.69	104.03	112.00
40	o	71	ARG	N-CA-C	-5.69	104.46	111.40
52	Ah	40	LYS	N-CA-C	5.69	117.93	111.11
1	A	65	PHE	N-CA-C	-5.68	106.27	113.43
47	AC	17	SER	N-CA-CB	-5.68	102.06	110.53
20	U	137	LYS	CA-C-N	-5.67	113.66	122.05
20	U	137	LYS	C-N-CA	-5.67	113.66	122.05
34	i	84	TYR	N-CA-C	-5.67	105.10	111.28
38	m	104	VAL	N-CA-C	-5.67	105.57	111.58
45	AA	185	ASP	N-CA-C	5.67	120.19	113.16
17	Q	64	LEU	N-CA-C	-5.67	106.50	113.41
7	G	59	GLN	N-CA-C	5.66	118.02	107.99
9	I	65	GLU	N-CA-C	5.66	120.19	113.28
15	O	214	VAL	N-CA-CB	5.66	119.07	110.58
12	L	371	SER	N-CA-C	-5.66	105.03	111.14
3	C	117	ASP	CA-C-N	-5.65	116.41	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	117	ASP	C-N-CA	-5.65	116.41	122.85
12	L	214	MET	N-CA-C	-5.65	105.20	111.36
34	i	14	GLN	N-CA-CB	-5.65	101.81	110.12
50	AF	25	ALA	N-CA-C	-5.65	105.12	111.28
9	I	106	TYR	N-CA-C	-5.65	101.99	109.84
14	N	232	LEU	N-CA-C	-5.64	106.61	112.93
50	AF	27	PHE	N-CA-C	-5.64	105.50	112.38
12	L	151	SER	N-CA-CB	5.63	118.50	110.16
6	F	176	ALA	N-CA-C	5.63	118.14	111.33
12	L	342	CYS	N-CA-CB	5.62	118.16	110.01
13	M	214	LEU	N-CA-C	-5.62	105.68	112.54
6	F	457	HIS	N-CA-CB	-5.62	100.95	110.50
37	l	49	ALA	N-CA-C	-5.61	106.59	113.50
7	G	475	VAL	N-CA-C	5.61	115.94	107.75
12	L	20	LEU	N-CA-C	5.61	119.85	112.89
6	F	304	ALA	CB-CA-C	-5.61	110.09	116.54
7	G	599	THR	CA-C-N	-5.61	114.20	122.83
7	G	599	THR	C-N-CA	-5.61	114.20	122.83
4	D	136	PHE	N-CA-C	5.60	119.29	112.23
27	b	24	SER	N-CA-C	-5.60	107.08	114.31
4	D	186	ALA	N-CA-C	5.60	117.06	111.07
5	E	222	PHE	CB-CA-C	-5.60	100.62	109.80
32	g	107	VAL	N-CA-C	-5.60	102.86	108.96
9	I	189	LYS	N-CA-C	-5.59	106.12	113.17
47	Ac	368	ILE	N-CA-C	-5.59	105.07	110.72
48	Ad	180	PRO	N-CA-C	-5.59	106.86	114.80
29	d	5	ARG	CA-C-N	-5.59	114.19	119.90
29	d	5	ARG	C-N-CA	-5.59	114.19	119.90
4	D	143	SER	CB-CA-C	5.59	120.80	111.30
14	N	251	LEU	N-CA-C	-5.59	105.19	111.28
38	m	60	ILE	N-CA-C	-5.59	101.98	109.30
7	G	615	LEU	N-CA-C	-5.59	106.23	113.16
4	D	221	ARG	N-CA-C	-5.59	106.23	113.16
7	G	530	TYR	N-CA-C	-5.59	102.01	110.28
12	L	445	GLU	CB-CA-C	-5.59	101.97	111.02
41	p	115	GLN	N-CA-CB	5.58	118.02	110.59
45	AA	153	ASN	CB-CA-C	-5.58	102.89	111.66
46	Ab	233	VAL	CB-CA-C	-5.58	105.17	110.70
16	P	177	SER	CB-CA-C	-5.58	103.66	111.80
48	Ad	297	GLY	N-CA-C	-5.58	107.75	114.66
4	D	309	ASP	CB-CA-C	-5.57	109.65	117.23
51	AG	34	GLY	N-CA-C	5.57	118.97	112.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	370	PRO	N-CA-CB	-5.57	97.68	103.08
8	H	50	ALA	N-CA-C	5.57	117.81	111.02
4	D	267	ILE	N-CA-C	5.57	120.92	109.34
1	A	80	GLN	CB-CA-C	-5.56	102.66	111.17
2	B	88	SER	N-CA-CB	5.56	118.14	110.07
32	g	140	PHE	N-CA-CB	5.56	118.27	109.71
32	g	122	ARG	N-CA-C	5.56	118.27	111.82
12	L	234	PRO	N-CA-C	-5.56	105.53	113.47
43	r	108	LYS	N-CA-C	5.55	117.33	111.28
12	L	370	SER	N-CA-C	-5.55	105.31	111.36
3	C	153	ASP	N-CA-C	5.55	117.23	110.41
12	L	155	ILE	N-CA-C	-5.54	105.32	110.53
20	T	78	GLY	N-CA-C	-5.54	106.08	112.73
5	E	233	LEU	N-CA-C	5.54	119.86	113.38
12	L	394	LEU	N-CA-CB	5.53	118.03	110.01
16	P	110	ALA	N-CA-CB	-5.53	101.70	110.28
16	P	141	PHE	N-CA-C	-5.53	104.67	111.75
52	AH	87	ASN	N-CA-C	-5.53	105.16	111.14
4	D	137	ASP	N-CA-C	-5.53	106.49	113.18
41	p	120	ASN	N-CA-C	-5.53	105.15	113.89
10	J	2	ASN	N-CA-C	-5.53	104.76	112.45
10	J	134	MET	N-CA-C	-5.53	105.31	113.72
7	G	127	ASP	CA-C-O	5.53	129.02	121.89
32	g	113	GLN	CA-C-O	5.53	126.18	119.11
14	N	148	LEU	N-CA-C	5.52	120.02	113.28
13	M	355	MET	N-CA-C	-5.52	104.65	111.33
38	m	46	GLU	N-CA-C	-5.52	106.55	113.72
40	o	74	PHE	CA-C-N	-5.52	113.93	119.56
40	o	74	PHE	C-N-CA	-5.52	113.93	119.56
8	H	192	GLU	N-CA-C	-5.52	105.76	112.88
27	b	25	VAL	N-CA-C	-5.52	106.96	113.42
4	D	91	ALA	CB-CA-C	-5.51	110.23	116.63
49	AI	59	ALA	N-CA-CB	-5.51	101.41	109.95
4	D	182	ASN	N-CA-CB	5.51	118.06	110.07
6	F	118	ASP	N-CA-C	-5.51	102.13	110.28
12	L	465	GLY	N-CA-C	-5.50	105.73	112.77
13	M	73	LEU	N-CA-C	-5.50	105.27	112.75
6	F	294	VAL	CA-C-N	-5.50	114.09	119.76
6	F	294	VAL	C-N-CA	-5.50	114.09	119.76
49	Ae	151	LYS	CA-C-O	-5.50	115.72	121.99
26	a	25	TYR	N-CA-C	-5.50	107.83	114.75
12	L	194	ASN	CB-CA-C	-5.48	103.33	111.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	64	GLU	N-CA-CB	5.48	117.96	110.01
49	Ae	148	ALA	N-CA-CB	5.48	118.56	110.56
4	D	292	MET	N-CA-C	-5.47	105.39	111.36
39	n	136	GLU	CB-CA-C	5.47	121.31	110.42
49	Ai	59	ALA	N-CA-CB	-5.47	101.47	109.95
13	M	223	ALA	N-CA-CB	5.46	118.09	110.11
7	G	363	SER	N-CA-C	-5.46	100.28	109.07
27	b	79	ASP	CA-C-O	5.46	127.64	119.23
42	q	33	ILE	N-CA-C	-5.46	107.96	113.20
12	L	152	PHE	N-CA-C	-5.46	105.23	111.07
41	p	94	ARG	N-CA-C	5.45	116.91	111.07
35	j	64	LEU	N-CA-C	-5.45	105.50	111.82
36	k	20	MET	CA-C-N	-5.45	111.20	121.66
36	k	20	MET	C-N-CA	-5.45	111.20	121.66
32	g	137	SER	N-CA-CB	-5.44	101.27	110.41
19	S	50	ASN	CB-CA-C	-5.44	103.12	111.66
46	Ab	124	GLU	N-CA-C	5.44	118.27	109.40
14	N	62	THR	N-CA-C	-5.44	105.25	111.07
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80
20	U	98	LEU	N-CA-C	-5.43	102.16	110.30
7	G	82	ILE	N-CA-C	-5.43	104.08	110.21
46	AB	236	GLN	N-CA-C	-5.42	105.92	112.54
14	N	89	GLN	N-CA-CB	-5.42	100.43	110.18
13	M	409	TYR	N-CA-C	-5.40	105.55	111.82
3	C	228	GLU	N-CA-C	-5.40	103.35	110.43
38	m	52	ASN	N-CA-C	-5.40	105.13	112.26
13	M	234	ILE	N-CA-C	5.40	116.27	111.90
14	N	108	LEU	N-CA-C	5.39	118.03	109.24
43	r	9	GLN	N-CA-C	5.39	118.08	111.82
34	i	77	ILE	CB-CA-C	-5.39	108.63	114.35
13	M	174	LEU	N-CA-C	-5.39	106.48	112.57
22	W	21	LYS	CA-C-N	-5.39	114.17	119.99
22	W	21	LYS	C-N-CA	-5.39	114.17	119.99
12	L	543	ASN	N-CA-C	-5.39	105.41	111.28
12	L	550	LEU	CA-C-O	-5.38	115.24	120.89
7	G	420	LYS	N-CA-CB	-5.38	101.99	110.06
8	H	227	GLU	N-CA-C	-5.38	107.09	113.97
12	L	21	ILE	N-CA-C	-5.38	105.29	110.72
15	O	175	ASN	N-CA-C	-5.37	105.42	111.28
4	D	223	HIS	N-CA-CB	-5.37	103.75	111.91
12	L	311	GLY	N-CA-C	-5.37	106.28	112.73
16	P	53	GLY	N-CA-C	5.37	121.32	113.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	682	ASP	CA-C-N	-5.37	114.23	119.76
7	G	682	ASP	C-N-CA	-5.37	114.23	119.76
12	L	183	ILE	N-CA-C	-5.37	105.14	110.62
4	D	142	VAL	N-CA-C	-5.36	105.62	110.82
12	L	413	LEU	N-CA-C	5.36	117.13	111.28
7	G	510	TRP	N-CA-C	-5.36	101.92	109.96
18	R	48	PHE	N-CA-C	5.36	119.57	113.19
47	AC	178	PHE	N-CA-C	-5.36	105.55	111.71
45	Aa	48	THR	N-CA-C	-5.36	104.01	111.52
7	G	652	ASN	CB-CA-C	-5.36	102.12	111.23
4	D	86	PRO	N-CA-C	-5.35	106.56	113.57
13	M	343	ILE	N-CA-C	5.35	116.08	110.62
12	L	415	ALA	N-CA-CB	5.35	117.98	110.12
13	M	169	ASN	N-CA-C	-5.35	105.53	111.36
13	M	53	SER	N-CA-C	5.35	115.60	108.38
47	AC	279	ALA	N-CA-C	-5.35	105.45	111.28
54	Ak	18	ILE	N-CA-C	5.34	120.42	108.88
42	q	143	PRO	N-CA-CB	-5.34	96.26	103.15
49	Ae	89	SER	N-CA-C	5.34	118.58	111.75
12	L	386	LEU	N-CA-C	-5.33	101.01	108.96
40	o	24	SER	O-C-N	-5.33	115.98	122.22
6	F	199	ARG	N-CA-C	5.33	117.43	109.59
7	G	654	VAL	N-CA-C	-5.33	105.82	113.07
25	Z	102	PRO	CA-N-CD	5.33	119.46	112.00
13	M	117	MET	N-CA-CB	5.32	117.95	110.12
32	g	80	VAL	N-CA-C	-5.32	105.31	110.42
5	E	219	SER	N-CA-C	-5.32	100.65	108.79
2	B	141	MET	N-CA-C	-5.32	106.79	113.28
13	M	25	THR	CB-CA-C	-5.32	100.46	110.67
4	D	344	ILE	N-CA-C	-5.32	105.20	110.62
15	O	219	GLN	N-CA-C	5.32	117.49	111.11
5	E	48	PRO	N-CA-C	5.31	120.75	113.84
12	L	494	SER	N-CA-C	-5.31	105.40	111.14
48	Ad	210	TYR	N-CA-C	-5.31	105.39	111.07
20	U	141	PRO	N-CA-C	-5.31	109.16	114.68
16	P	229	VAL	N-CA-C	-5.30	104.22	110.21
39	n	26	HIS	N-CA-C	-5.30	106.40	112.92
14	N	218	ALA	N-CA-CB	5.30	118.41	110.14
7	G	356	ASP	N-CA-C	-5.30	105.51	111.28
8	H	87	VAL	CA-C-N	-5.29	114.90	120.94
8	H	87	VAL	C-N-CA	-5.29	114.90	120.94
13	M	167	ILE	N-CA-C	5.29	117.67	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S	51	LEU	CA-C-N	-5.29	113.23	119.84
19	S	51	LEU	C-N-CA	-5.29	113.23	119.84
48	Ad	230	GLY	N-CA-C	-5.29	108.34	115.21
47	Ac	16	HIS	N-CA-C	5.28	117.78	111.71
7	G	362	ASP	CA-CB-CG	5.28	117.88	112.60
45	Aa	56	GLY	N-CA-C	-5.27	107.26	114.64
5	E	66	VAL	N-CA-C	5.27	116.63	110.62
15	O	206	TYR	N-CA-C	5.27	118.88	107.49
15	O	264	GLU	N-CA-C	-5.26	107.22	113.38
48	AD	156	ASP	N-CA-C	-5.26	105.62	111.36
12	L	137	MET	N-CA-C	5.26	119.33	113.01
12	L	231	PRO	CB-CA-C	-5.26	104.38	111.85
48	AD	164	MET	CB-CA-C	-5.26	110.49	116.54
9	I	96	ARG	N-CA-C	5.26	119.55	113.18
39	n	104	LEU	N-CA-C	-5.26	106.89	113.15
4	D	248	SER	N-CA-C	-5.25	105.63	111.36
33	h	129	PRO	N-CA-C	-5.25	106.69	113.57
47	AC	183	PHE	N-CA-C	-5.25	107.04	113.50
7	G	449	PRO	N-CA-CB	5.25	109.06	103.39
12	L	375	ILE	N-CA-CB	5.25	116.69	110.55
42	q	93	MET	N-CA-C	-5.25	105.73	111.82
5	E	48	PRO	CB-CA-C	-5.25	104.40	111.85
12	L	190	SER	N-CA-C	-5.25	106.72	113.23
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
32	g	68	ASN	N-CA-CB	5.25	119.01	111.51
13	M	294	MET	N-CA-C	-5.25	106.90	113.72
39	n	12	HIS	N-CA-C	-5.25	105.00	111.40
49	AE	92	ARG	N-CA-C	5.25	117.92	110.10
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
41	p	13	PRO	O-C-N	5.24	123.61	121.15
13	M	212	VAL	CB-CA-C	-5.23	105.19	112.36
6	F	300	ILE	N-CA-CB	5.23	119.30	110.56
20	U	133	ILE	CB-CA-C	-5.23	104.05	112.16
48	Ad	266	VAL	N-CA-C	-5.23	104.87	110.36
12	L	497	GLY	N-CA-C	-5.23	106.44	112.50
10	J	3	ASN	N-CA-C	-5.22	99.43	108.52
7	G	435	PRO	CB-CA-C	-5.22	105.87	111.56
35	j	76	ASP	CB-CA-C	-5.22	104.63	112.09
47	AC	16	HIS	N-CA-C	5.22	117.71	111.71
54	Ak	38	TRP	CB-CA-C	-5.22	102.01	109.84
16	P	96	LEU	CB-CA-C	-5.22	99.70	109.72
33	h	176	LYS	N-CA-C	-5.22	105.77	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	235	ASN	N-CA-C	-5.21	99.70	110.80
41	p	167	ARG	CB-CA-C	5.21	117.26	109.13
2	B	76	THR	N-CA-C	-5.21	105.04	111.40
30	e	104	PRO	CB-CA-C	5.21	118.49	111.71
54	Ak	37	ASP	CB-CA-C	5.21	119.72	112.11
5	E	221	ARG	N-CA-C	5.21	117.78	110.23
45	AA	56	GLY	N-CA-C	-5.21	107.35	114.64
49	Ae	201	ASP	N-CA-C	-5.21	104.86	111.11
20	U	133	ILE	N-CA-C	5.21	117.56	111.05
23	X	20	VAL	N-CA-C	-5.21	100.70	108.46
3	C	237	PRO	CB-CA-C	-5.20	104.19	109.92
26	a	17	VAL	CB-CA-C	-5.20	104.75	111.20
13	M	317	ILE	N-CA-CB	5.20	117.23	110.57
20	T	137	LYS	N-CA-C	5.20	117.85	111.82
48	Ad	220	GLU	CA-C-N	-5.20	115.03	120.38
48	Ad	220	GLU	C-N-CA	-5.20	115.03	120.38
14	N	90	THR	N-CA-C	5.20	117.63	110.35
3	C	235	ASN	N-CA-CB	5.20	119.27	110.49
4	D	133	LEU	CA-C-N	-5.19	113.45	119.47
4	D	133	LEU	C-N-CA	-5.19	113.45	119.47
13	M	20	PRO	N-CA-C	-5.19	106.31	113.53
7	G	63	PHE	CA-C-O	-5.19	115.04	121.06
12	L	284	THR	N-CA-C	-5.19	105.70	111.36
38	m	17	THR	N-CA-C	-5.19	103.68	110.53
19	S	45	LYS	N-CA-C	-5.19	105.52	111.07
3	C	109	SER	N-CA-C	5.18	118.26	109.76
12	L	332	HIS	N-CA-C	-5.18	105.63	111.28
12	L	217	LEU	N-CA-C	-5.18	105.64	111.28
7	G	83	GLU	N-CA-CB	-5.18	101.93	109.95
4	D	132	ALA	N-CA-C	-5.17	107.99	114.56
7	G	600	GLU	CB-CA-C	-5.17	103.04	111.06
12	L	396	ILE	O-C-N	5.17	126.98	121.91
13	M	98	MET	N-CA-C	-5.17	105.53	111.07
10	J	69	TYR	N-CA-C	-5.17	104.71	111.02
42	q	26	VAL	N-CA-CB	5.17	119.76	111.23
42	q	87	HIS	N-CA-C	-5.17	105.73	111.36
12	L	386	LEU	CA-C-O	-5.17	115.92	121.45
14	N	335	MET	CB-CA-C	-5.17	104.46	111.95
45	Aa	47	GLU	N-CA-CB	-5.16	102.94	110.53
42	q	139	PRO	CA-N-CD	5.16	119.23	112.00
14	N	222	ASN	N-CA-C	-5.16	106.22	112.88
37	l	168	LEU	N-CA-C	-5.16	105.57	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	25	LEU	N-CA-C	-5.16	105.66	111.28
4	D	439	SER	CB-CA-C	-5.15	104.39	112.12
38	m	47	TYR	N-CA-C	-5.15	105.83	112.68
6	F	337	MET	CB-CA-C	-5.15	103.03	111.68
7	G	172	ILE	N-CA-C	-5.15	98.63	109.34
41	p	43	TRP	CA-C-N	-5.15	113.61	118.97
41	p	43	TRP	C-N-CA	-5.15	113.61	118.97
10	J	87	LEU	N-CA-C	-5.15	105.75	111.36
7	G	713	ALA	N-CA-C	-5.15	105.56	111.07
6	F	131	MET	N-CA-C	-5.14	105.84	112.68
7	G	192	VAL	CB-CA-C	-5.14	105.25	111.88
7	G	569	GLN	CB-CA-C	-5.14	104.23	112.05
3	C	240	ALA	N-CA-CB	-5.14	102.30	110.06
8	H	189	THR	N-CA-C	-5.14	107.04	113.72
13	M	86	LYS	N-CA-C	-5.14	106.25	112.88
7	G	458	GLY	N-CA-C	-5.14	108.23	115.32
7	G	150	ARG	N-CA-CB	-5.13	101.81	110.49
33	h	158	ARG	N-CA-C	-5.13	105.60	111.14
29	d	37	LEU	N-CA-C	-5.12	105.70	111.28
14	N	225	MET	N-CA-C	-5.12	106.62	112.92
31	f	12	VAL	N-CA-C	-5.12	107.99	112.90
38	m	61	GLU	N-CA-C	5.12	119.60	112.90
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
7	G	203	ASP	CA-C-O	5.11	127.25	121.32
44	s	85	LEU	N-CA-CB	5.11	117.41	110.01
8	H	202	GLU	N-CA-C	-5.10	105.17	111.90
13	M	234	ILE	CB-CA-C	5.10	116.20	111.30
21	V	87	GLU	N-CA-CB	5.09	117.61	110.12
13	M	330	ALA	N-CA-CB	5.09	117.45	110.07
4	D	71	ILE	N-CA-C	5.09	118.26	111.44
4	D	352	PRO	N-CA-C	5.09	116.91	110.70
11	K	48	SER	N-CA-CB	5.09	117.60	110.12
24	Y	72	PHE	N-CA-C	-5.09	105.63	111.07
7	G	660	GLU	N-CA-C	5.08	118.10	109.76
46	Ab	212	HIS	CA-C-O	5.08	125.62	119.31
28	c	60	GLN	N-CA-C	-5.08	105.63	111.07
43	r	59	GLY	N-CA-C	-5.08	106.61	112.50
20	T	89	LEU	N-CA-C	-5.08	105.75	111.28
4	D	106	VAL	N-CA-CB	-5.08	105.27	111.21
12	L	249	SER	N-CA-C	5.07	116.62	111.14
42	q	8	LYS	N-CA-C	-5.07	105.66	111.14
5	E	222	PHE	N-CA-C	5.07	117.88	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Ad	221	PRO	CA-N-CD	-5.07	104.90	112.00
7	G	280	ASP	N-CA-CB	-5.07	102.67	110.12
14	N	292	PHE	CA-CB-CG	5.07	118.87	113.80
3	C	241	PHE	CB-CA-C	5.06	117.99	109.69
13	M	229	MET	N-CA-C	-5.06	105.66	111.07
20	T	149	ALA	N-CA-C	5.06	116.48	110.97
13	M	32	PHE	N-CA-CB	5.06	117.34	110.01
46	Ab	38	LEU	N-CA-C	-5.06	103.47	110.35
31	f	55	THR	N-CA-C	5.06	116.48	110.97
3	C	237	PRO	N-CD-CG	-5.05	95.62	103.20
45	Aa	109	LEU	CB-CA-C	-5.05	102.92	110.90
5	E	225	GLU	CA-C-N	-5.05	114.37	119.83
5	E	225	GLU	C-N-CA	-5.05	114.37	119.83
13	M	56	PHE	N-CA-C	5.05	116.75	108.52
36	k	19	LYS	N-CA-C	-5.05	104.27	111.24
3	C	108	LYS	N-CA-C	5.05	116.78	111.28
10	J	161	ALA	N-CA-C	-5.05	107.07	113.18
14	N	64	ALA	N-CA-C	5.05	116.47	111.07
5	E	213	PRO	CB-CA-C	-5.05	106.28	112.89
6	F	366	ALA	N-CA-C	-5.05	105.47	110.97
13	M	30	TYR	N-CA-C	5.05	116.78	111.28
14	N	42	PRO	CB-CA-C	-5.05	105.04	113.06
20	U	132	ASP	N-CA-C	5.05	117.18	111.02
37	l	45	PRO	N-CA-C	5.05	120.46	113.65
3	C	139	ARG	N-CA-CB	-5.04	102.19	111.37
9	I	117	LYS	N-CA-C	-5.04	103.03	113.31
14	N	217	MET	N-CA-C	-5.04	106.96	113.01
13	M	267	TRP	N-CA-C	-5.04	105.87	111.36
2	B	194	CYS	CA-C-N	-5.03	115.19	120.38
2	B	194	CYS	C-N-CA	-5.03	115.19	120.38
28	c	39	PRO	N-CA-C	5.03	119.10	111.15
7	G	388	ASN	N-CA-C	-5.03	103.86	111.56
32	g	137	SER	N-CA-C	5.03	119.27	113.18
14	N	36	SER	N-CA-C	-5.03	105.25	111.33
30	e	102	GLU	N-CA-C	-5.03	106.73	112.86
39	n	169	HIS	CB-CA-C	5.02	118.66	110.17
4	D	419	PRO	N-CA-C	5.02	118.51	111.33
12	L	384	PRO	N-CA-CB	5.02	107.71	103.35
14	N	282	MET	N-CA-C	-5.01	105.71	111.07
34	i	16	ARG	N-CA-C	-5.01	105.82	111.28
39	n	42	CYS	N-CA-C	-5.01	107.00	113.01
32	g	109	ASP	CB-CA-C	5.00	119.00	111.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	h	161	ARG	N-CA-C	-5.00	105.51	110.97
48	Ad	137	GLY	N-CA-C	-5.00	102.97	110.38
18	R	53	LYS	N-CA-C	5.00	116.56	108.41
45	Aa	114	GLU	N-CA-C	-5.00	105.91	111.36
10	J	59	TYR	N-CA-C	-5.00	105.30	111.40
16	P	52	SER	N-CA-C	-5.00	106.43	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	799	0	851	162	0
2	B	1241	0	1252	179	0
3	C	1643	0	1598	133	0
4	D	3438	0	3379	391	0
5	E	1635	0	1625	183	0
6	F	3288	0	3243	373	0
7	G	5287	0	5322	583	0
8	H	2532	0	2621	350	0
9	I	1380	0	1339	169	0
10	J	1229	0	1250	230	0
11	K	729	0	764	101	0
12	L	4798	0	4986	608	0
13	M	3630	0	3854	544	0
14	N	2694	0	2896	336	0
15	O	2599	0	2552	306	0
16	P	2720	0	2740	257	0
17	Q	940	0	930	96	0
18	R	660	0	639	69	0
19	S	667	0	685	75	0
20	T	604	0	596	70	0
20	U	718	0	705	89	0
21	V	915	0	954	78	0
22	W	970	0	991	92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	X	1385	0	1366	150	0
24	Y	1030	0	1015	75	0
25	Z	1145	0	1139	171	0
26	a	548	0	562	83	0
27	b	628	0	628	72	0
28	c	389	0	385	48	0
29	d	996	0	1001	93	0
30	e	877	0	869	130	0
31	f	439	0	433	37	0
32	g	858	0	787	75	0
33	h	1162	0	1163	139	0
34	i	802	0	802	84	0
35	j	563	0	510	72	0
36	k	582	0	584	46	0
37	l	1312	0	1204	103	0
38	m	1050	0	1061	109	0
39	n	1541	0	1470	151	0
40	o	1050	0	1045	103	0
41	p	1452	0	1413	140	0
42	q	1025	0	980	80	0
43	r	686	0	710	70	0
44	s	193	0	187	36	0
45	AA	3077	0	2996	199	0
45	Aa	3076	0	3001	230	0
46	AB	3137	0	3143	153	0
46	Ab	3137	0	3143	252	0
47	AC	2988	0	3045	294	0
47	Ac	2988	0	3045	216	0
48	AD	1878	0	1827	294	0
48	Ad	1903	0	1848	279	0
49	AE	830	0	802	136	0
49	AI	200	0	216	32	0
49	Ae	1451	0	1433	264	0
49	Ai	204	0	221	34	0
50	AF	855	0	841	64	0
50	Af	864	0	854	38	0
51	AG	643	0	643	88	0
51	Ag	622	0	628	54	0
52	AH	527	0	507	76	0
52	Ah	512	0	497	85	0
53	AJ	165	0	162	81	0
53	Aj	345	0	333	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AK	118	0	111	39	0
54	AK	309	0	304	27	0
55	A	42	0	58	8	0
55	Aa	23	0	20	3	0
55	Ac	35	0	44	7	0
55	Ag	38	0	53	9	0
55	H	48	0	73	12	0
55	I	51	0	82	8	0
55	K	46	0	66	9	0
55	L	167	0	233	28	0
55	M	88	0	130	8	0
55	N	51	0	82	11	0
55	Y	41	0	56	8	0
55	d	31	0	36	8	0
55	i	40	0	54	19	0
55	m	139	0	209	23	0
56	B	8	0	0	6	0
56	F	8	0	0	10	0
56	G	16	0	0	8	0
56	I	16	0	0	9	0
57	B	18	0	18	11	0
58	B	78	0	107	23	0
59	E	4	0	0	3	0
59	G	4	0	0	4	0
60	F	31	0	19	3	0
61	H	35	0	43	4	0
62	Ag	98	0	84	9	0
62	L	78	0	100	16	0
62	X	67	0	81	9	0
62	a	57	0	58	12	0
62	h	70	0	87	17	0
63	O	27	0	12	11	0
64	P	48	0	26	7	0
65	R	1	0	0	0	0
66	W	32	0	0	3	0
66	n	32	0	0	0	0
67	AC	86	0	60	27	0
67	Ac	86	0	60	11	0
68	AC	28	0	31	11	0
68	Ac	28	0	31	15	0
69	AD	43	0	32	18	0
69	Ad	43	0	32	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Ac	23	0	23	20	0
71	Ad	36	0	45	39	0
All	All	96599	0	96831	8621	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 45.

All (8621) 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:A:52:SER:HB2	1:A:55:PHE:CD2	1.31	1.61
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.38
49:Ae:239:HIS:ND1	49:Ae:253:PRO:HG3	1.39	1.37
1:A:52:SER:CB	1:A:55:PHE:CD2	2.10	1.33
1:A:52:SER:CB	1:A:55:PHE:HD2	1.41	1.32
46:Ab:212:HIS:CE1	46:Ab:246:LEU:HD23	1.63	1.32
48:Ad:221:PRO:CD	48:Ad:221:PRO:N	1.73	1.32
47:AC:268:ILE:HD12	49:Ae:238:CYS:SG	1.67	1.31
46:Ab:297:PRO:CG	46:Ab:304:ASN:HD21	1.43	1.31
15:O:168:VAL:HG21	15:O:241:TYR:CZ	1.66	1.29
47:AC:199:PHE:CZ	47:Ac:8:HIS:CE1	2.23	1.25
4:D:181:LEU:CD1	4:D:210:MET:SD	2.27	1.23
4:D:181:LEU:HD11	4:D:210:MET:SD	1.79	1.23
47:AC:145:VAL:HA	49:Ae:220:LEU:O	1.35	1.23
45:Aa:109:LEU:HD12	45:Aa:110:GLU:N	1.52	1.22
3:C:234:LEU:HD12	3:C:234:LEU:O	1.36	1.22
7:G:130:ILE:HA	9:I:140:ARG:NH1	1.56	1.21
46:Ab:59:SER:CB	46:Ab:224:GLY:HA3	1.69	1.21
53:AJ:23:LEU:HD22	54:AK:23:MET:SD	1.80	1.20
20:U:90:TYR:CE2	20:U:92:LYS:HB2	1.76	1.20
47:Ac:128:PHE:CD1	70:Ac:404:U10:C4M	2.24	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
49:AE:127:TYR:CD1	53:AJ:33:GLU:HA	1.78	1.19
7:G:571:HIS:HD2	7:G:572:HIS:CD2	1.60	1.19
4:D:360:ASP:OD1	4:D:360:ASP:O	1.60	1.18
3:C:87:ILE:HG13	3:C:144:THR:HG22	1.25	1.18
46:Ab:297:PRO:HG3	46:Ab:304:ASN:ND2	1.57	1.18
7:G:544:MET:HE3	7:G:546:PHE:CZ	1.78	1.17
49:AE:80:HIS:CD2	49:AE:81:THR:HG23	1.78	1.17
3:C:223:VAL:CG2	3:C:225:LEU:CD1	2.22	1.16
25:Z:89:GLU:HG2	30:e:97:HIS:NE2	1.58	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:128:PHE:CE1	70:Ac:404:U10:C4M	2.28	1.16
12:L:141:PHE:CE2	13:M:375:LEU:HD21	1.81	1.16
8:H:260:MET:HE3	26:a:13:GLY:O	1.43	1.16
3:C:229:PHE:CE1	9:I:126:GLN:HG3	1.80	1.15
49:Ae:164:ASN:HA	49:Ae:177:ARG:HA	1.28	1.15
10:J:125:MET:O	25:Z:121:ILE:HD12	1.47	1.15
12:L:466:PHE:HB2	35:j:68:TRP:HZ2	1.11	1.15
10:J:132:GLY:HA2	25:Z:68:ARG:NH1	1.62	1.14
1:A:66:ASP:OD2	10:J:58:ILE:HD13	1.43	1.14
47:Ac:199:PHE:HZ	47:Ac:8:HIS:CE1	1.63	1.14
49:Ae:130:LYS:HD3	53:Aj:33:GLU:HG2	1.16	1.14
12:L:247:LEU:CD1	12:L:248:HIS:CD2	2.30	1.14
25:Z:97:ILE:CG2	30:e:92:TYR:HE1	1.59	1.14
19:S:95:LEU:HD12	19:S:95:LEU:O	1.46	1.14
47:Ac:128:PHE:CE1	70:Ac:404:U10:H4M2	1.83	1.14
52:Ah:32:ARG:HD3	52:Ah:76:ARG:NH1	1.60	1.14
1:A:35:ASN:OD1	1:A:36:PRO:HD2	1.49	1.12
12:L:261:VAL:O	12:L:264:HIS:CD2	2.02	1.12
14:N:215:MET:CE	14:N:248:LEU:HD21	1.79	1.12
49:Ae:239:HIS:CG	49:Ae:253:PRO:HG3	1.83	1.12
10:J:124:LEU:CD2	25:Z:137:ASN:HD21	1.61	1.12
48:AD:157:GLY:HA3	48:AD:167:ARG:HB3	1.32	1.11
1:A:18:ILE:CD1	8:H:76:THR:CG2	2.27	1.11
9:I:152:CYS:SG	56:I:302:SF4:FE1	1.41	1.11
9:I:210:LEU:HD13	43:r:39:PRO:O	1.47	1.11
15:O:80:GLN:HG3	15:O:270:VAL:HG21	1.25	1.11
29:d:14:LEU:O	29:d:14:LEU:HD12	1.49	1.11
51:AG:9:ALA:HB3	51:AG:11:ILE:HD11	1.33	1.11
4:D:47:PHE:HB3	14:N:227:ILE:HD11	1.25	1.11
20:U:90:TYR:OH	20:U:92:LYS:HD2	1.48	1.11
46:Ab:297:PRO:HG3	46:Ab:304:ASN:HD21	1.07	1.11
4:D:144:MET:SD	4:D:222:MET:HA	1.91	1.11
7:G:611:THR:HG21	17:Q:105:GLU:HA	1.14	1.11
12:L:229:LEU:HD12	12:L:229:LEU:O	1.51	1.11
12:L:365:ILE:HD12	12:L:366:MET:HG3	1.32	1.11
1:A:67:LEU:HD11	11:K:68:ALA:CB	1.80	1.10
6:F:266:GLY:CA	6:F:271:SER:HA	1.79	1.10
12:L:466:PHE:HB2	35:j:68:TRP:CZ2	1.85	1.10
3:C:229:PHE:HE1	9:I:126:GLN:HG3	0.99	1.10
1:A:18:ILE:HD12	8:H:76:THR:CG2	1.82	1.10
13:M:127:ILE:CD1	14:N:256:PRO:HG3	1.82	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:263:TYR:HA	49:Ae:273:VAL:HA	1.13	1.10
12:L:141:PHE:CE2	13:M:375:LEU:CD2	2.35	1.10
25:Z:120:LEU:HD23	25:Z:122:GLY:H	1.15	1.10
47:AC:144:THR:HG21	49:Ae:221:GLY:O	1.51	1.10
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.09
7:G:130:ILE:C	9:I:140:ARG:HH12	1.61	1.09
47:Ac:146:ILE:HG13	70:Ac:404:U10:C4M	1.83	1.09
1:A:79:ILE:HD11	8:H:155:LEU:HD22	1.27	1.09
12:L:121:LEU:HD22	12:L:246:LEU:HD21	1.32	1.09
45:Aa:402:HIS:CE1	45:Aa:403:LEU:CD1	2.36	1.09
48:AD:120:VAL:HG23	48:AD:253:LEU:HD11	1.21	1.09
25:Z:97:ILE:HG21	30:e:92:TYR:HE1	1.08	1.09
48:AD:153:GLU:HA	48:AD:168:PRO:HA	1.11	1.09
10:J:124:LEU:HD21	25:Z:137:ASN:ND2	1.68	1.08
45:AA:402:HIS:CE1	45:AA:403:LEU:CD1	2.36	1.08
48:AD:215:LEU:HD11	69:AD:401:HEC:HMB3	1.27	1.08
15:O:66:ILE:HD12	15:O:67:CYS:SG	1.94	1.08
49:AE:220:LEU:HD13	47:Ac:145:VAL:HG13	1.18	1.08
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
16:P:171:ASN:HB3	16:P:327:VAL:HB	1.26	1.08
46:Ab:297:PRO:CB	46:Ab:304:ASN:HD21	1.66	1.08
35:j:97:LEU:HB3	40:o:104:ARG:HB2	1.29	1.08
36:k:34:PRO:HG2	36:k:59:TYR:CE1	1.88	1.08
47:AC:266:PRO:O	49:Ae:237:PRO:HB2	1.52	1.08
52:AH:47:ARG:HH22	52:AH:71:ASP:HB2	1.01	1.08
47:Ac:128:PHE:CD1	70:Ac:404:U10:H4M2	1.85	1.08
12:L:141:PHE:HE2	13:M:375:LEU:CD2	1.67	1.07
47:AC:98:VAL:HG22	67:AC:402:HEM:HBC2	1.34	1.07
47:AC:268:ILE:CD1	49:Ae:238:CYS:SG	2.42	1.07
46:Ab:59:SER:HB2	46:Ab:224:GLY:HA3	1.29	1.07
2:B:92:PRO:HB2	2:B:122:ARG:NH1	1.68	1.07
6:F:266:GLY:HA3	6:F:271:SER:CA	1.84	1.07
12:L:141:PHE:CE2	13:M:370:PRO:HG3	1.87	1.07
47:Ac:146:ILE:HD11	70:Ac:404:U10:H3M2	1.15	1.07
43:r:27:ARG:HB3	43:r:31:ILE:HG23	1.32	1.07
71:Ad:402:3PH:H12	49:Ae:131:ASN:HD21	1.20	1.07
9:I:171:PRO:HB3	42:q:93:MET:HE1	1.08	1.07
12:L:466:PHE:CZ	35:j:72:ARG:NH2	2.22	1.07
48:Ad:295:MET:HB2	71:Ad:402:3PH:H341	1.34	1.07
51:Ag:11:ILE:HG21	51:Ag:14:VAL:HG21	1.36	1.07
52:Ah:45:ARG:HH11	52:Ah:48:LEU:HD23	1.00	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HB3	1:A:50:PRO:HD2	1.30	1.06
12:L:16:LEU:HD23	12:L:126:ILE:HD13	1.30	1.06
13:M:143:LEU:HD21	14:N:303:THR:CG2	1.85	1.06
52:AH:47:ARG:NH2	52:AH:71:ASP:CB	2.17	1.06
48:Ad:223:THR:HG22	52:Ah:65:CYS:HB2	1.36	1.06
7:G:571:HIS:CD2	7:G:572:HIS:CD2	2.44	1.06
12:L:550:LEU:HD12	13:M:275:ILE:HB	1.37	1.06
47:Ac:146:ILE:HD11	70:Ac:404:U10:C3M	1.84	1.06
4:D:267:ILE:HG22	8:H:278:PRO:HG2	1.32	1.05
3:C:120:THR:HG21	21:V:116:ILE:HG21	1.37	1.05
12:L:141:PHE:HB2	12:L:182:PHE:CE2	1.92	1.05
48:AD:153:GLU:HG2	48:AD:168:PRO:HB3	1.31	1.05
49:AE:127:TYR:HD1	53:AJ:33:GLU:HA	1.11	1.05
4:D:348:LEU:O	25:Z:11:PRO:HG3	1.57	1.05
5:E:131:ILE:HD11	5:E:185:VAL:HB	1.37	1.05
6:F:379:CYS:SG	56:F:502:SF4:FE4	1.46	1.05
12:L:141:PHE:HE2	13:M:375:LEU:HD22	1.22	1.05
8:H:111:LEU:HD11	10:J:56:PHE:CZ	1.92	1.05
16:P:350:ILE:HD11	16:P:366:ILE:HB	1.35	1.05
37:l:91:GLN:HE21	39:n:2:ALA:HB1	1.17	1.05
47:Ac:42:MET:HE1	68:Ac:405:UQ6:C21	1.86	1.05
47:Ac:146:ILE:HG13	70:Ac:404:U10:H4M3	1.36	1.05
4:D:36:GLN:HE22	13:M:135:ARG:NH1	1.55	1.04
10:J:9:SER:CB	11:K:7:ASN:HD22	1.68	1.04
15:O:227:MET:O	15:O:228:LYS:HG2	1.57	1.04
7:G:130:ILE:O	9:I:140:ARG:NH1	1.89	1.04
25:Z:85:GLN:OE1	30:e:105:ARG:HD3	1.57	1.04
52:AH:47:ARG:NH2	52:AH:71:ASP:HB2	1.70	1.04
49:Ae:239:HIS:ND1	49:Ae:253:PRO:CG	2.21	1.04
4:D:299:GLN:NE2	9:I:36:TYR:CE2	2.26	1.04
25:Z:93:GLU:CG	30:e:97:HIS:CE1	2.40	1.04
45:Aa:402:HIS:CE1	45:Aa:403:LEU:HD11	1.91	1.04
13:M:162:ILE:HG23	14:N:271:MET:HE3	1.33	1.04
14:N:233:LEU:HD23	14:N:241:LEU:HD12	1.36	1.04
49:AE:126:ALA:HB3	53:AJ:29:ALA:CB	1.87	1.04
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.36	1.03
45:AA:402:HIS:CE1	45:AA:403:LEU:HD11	1.91	1.03
12:L:466:PHE:CE1	35:j:72:ARG:NH2	2.27	1.03
12:L:466:PHE:CB	35:j:68:TRP:HZ2	1.70	1.03
13:M:249:ILE:O	13:M:250:LEU:HG	1.58	1.03
8:H:90:PRO:HD3	8:H:162:LEU:HD13	1.37	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:ILE:HG23	3:C:187:LEU:HG	1.35	1.03
4:D:238:LEU:HB3	43:r:36:GLN:HG3	1.37	1.03
15:O:168:VAL:HG21	15:O:241:TYR:CE1	1.92	1.03
4:D:256:ASP:HA	4:D:259:GLU:CB	1.89	1.02
12:L:131:LEU:HD12	12:L:140:LEU:HD12	1.36	1.02
47:AC:129:MET:HB3	47:AC:182:HIS:HB2	1.37	1.02
53:AJ:27:VAL:HG22	54:AK:30:VAL:HG11	1.36	1.02
7:G:130:ILE:CA	9:I:140:ARG:NH1	2.22	1.02
8:H:184:MET:HG2	8:H:293:PHE:CD2	1.95	1.02
10:J:132:GLY:HA2	25:Z:68:ARG:HH11	1.20	1.02
20:T:138:LEU:HD13	20:T:144:ILE:HG12	1.35	1.02
46:Ab:159:LYS:HA	46:Ab:162:LYS:HE2	1.38	1.02
47:Ac:98:VAL:HG22	67:Ac:402:HEM:HBC2	1.41	1.02
47:Ac:128:PHE:CD1	70:Ac:404:U10:H4M1	1.91	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
40:o:69:CYS:O	40:o:80:CYS:SG	2.17	1.02
51:AG:31:PHE:HA	51:AG:35:ILE:HD12	1.39	1.02
13:M:179:LEU:HB3	13:M:249:ILE:HD11	1.42	1.02
39:n:97:TYR:HB2	39:n:178:PRO:HG2	1.39	1.02
42:q:71:LYS:HB3	42:q:73:THR:HG23	1.40	1.02
52:AH:47:ARG:HH22	52:AH:71:ASP:CB	1.72	1.02
53:AJ:23:LEU:CB	54:AK:27:VAL:HG22	1.90	1.02
4:D:217:VAL:CG1	4:D:240:LEU:HD22	1.89	1.01
47:AC:266:PRO:O	49:Ae:237:PRO:CB	2.06	1.01
6:F:382:CYS:SG	56:F:502:SF4:FE3	1.50	1.01
12:L:123:LEU:HD21	62:L:704:CDL:H741	1.41	1.01
12:L:222:GLY:HA2	12:L:229:LEU:HD11	1.40	1.01
12:L:228:GLY:O	12:L:229:LEU:HG	1.61	1.01
48:AD:231:LEU:HD13	48:AD:241:ALA:HB1	1.40	1.01
1:A:18:ILE:CD1	8:H:76:THR:HG22	1.90	1.01
4:D:261:MET:HE1	9:I:73:THR:HG23	1.42	1.01
47:AC:199:PHE:CE1	47:Ac:8:HIS:NE2	2.28	1.01
10:J:60:LEU:HD13	10:J:60:LEU:C	1.86	1.00
13:M:172:GLY:O	13:M:173:THR:HG23	1.61	1.00
44:s:92:LEU:HB2	44:s:93:PRO:HD2	1.39	1.00
53:AJ:23:LEU:CD2	54:AK:23:MET:SD	2.49	1.00
12:L:553:LEU:HD11	38:m:93:ALA:HB3	1.44	1.00
67:Ac:402:HEM:HMA2	68:Ac:405:UQ6:H152	1.44	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
52:Ah:45:ARG:HH11	52:Ah:48:LEU:CD2	1.74	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:163:ARG:HG2	33:h:165:ASP:HB2	1.44	0.99
2:B:97:LEU:HD13	4:D:94:VAL:HG13	1.42	0.99
3:C:223:VAL:HG22	3:C:225:LEU:CD1	1.90	0.99
15:O:209:VAL:HG12	15:O:260:SER:HB2	1.43	0.99
1:A:66:ASP:OD2	10:J:58:ILE:CD1	2.08	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.42	0.99
47:AC:199:PHE:CZ	47:Ac:8:HIS:HE1	1.77	0.99
13:M:196:TRP:CD1	13:M:250:LEU:HD13	1.96	0.99
15:O:168:VAL:HG11	15:O:241:TYR:CD1	1.97	0.99
47:Ac:244:LEU:HD13	48:Ad:289:GLY:HA2	1.41	0.99
8:H:184:MET:HG2	8:H:293:PHE:CE2	1.98	0.99
37:l:184:TYR:HA	40:o:36:GLU:HA	1.45	0.99
22:W:74:ALA:HA	66:W:201:EHZ:O4	1.61	0.99
42:q:142:THR:OG1	42:q:143:PRO:HD2	1.62	0.99
40:o:8:ARG:HB2	40:o:16:GLU:HG2	1.45	0.98
49:AE:220:LEU:HD13	47:Ac:145:VAL:CG1	1.92	0.98
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.98
12:L:141:PHE:HB2	12:L:182:PHE:HE2	1.27	0.98
25:Z:97:ILE:CG2	30:e:92:TYR:CE1	2.46	0.98
25:Z:97:ILE:HG21	30:e:92:TYR:CE1	1.98	0.98
3:C:149:LEU:HD21	17:Q:64:LEU:CD2	1.93	0.98
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.28	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
4:D:376:GLU:HG3	7:G:121:LEU:HD12	1.46	0.98
47:AC:199:PHE:HZ	47:Ac:8:HIS:HE1	1.07	0.98
49:AE:119:ALA:HA	53:AJ:25:ILE:HD11	1.46	0.98
42:q:78:ASP:HB2	42:q:81:MET:HG3	1.42	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
13:M:275:ILE:HD11	13:M:288:TYR:CG	1.98	0.98
14:N:307:THR:HB	15:O:319:ILE:CD1	1.93	0.98
52:Ah:45:ARG:NH1	52:Ah:48:LEU:HD23	1.79	0.98
3:C:223:VAL:CG2	3:C:225:LEU:HD11	1.92	0.98
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.43	0.98
13:M:173:THR:CG2	33:h:147:ALA:HB2	1.94	0.98
48:AD:189:ASN:HB3	69:AD:401:HEC:HMD2	1.44	0.98
4:D:181:LEU:HD12	4:D:210:MET:SD	2.00	0.97
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.45	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.41	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:126:ALA:HB3	53:AJ:29:ALA:HB1	1.47	0.97
6:F:118:ASP:HA	6:F:159:ARG:HG3	1.45	0.97
3:C:152:ILE:HD11	3:C:177:PHE:CE2	1.99	0.97
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.05	0.97
10:J:122:ASP:OD2	25:Z:122:GLY:HA2	1.64	0.96
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.44	0.96
25:Z:93:GLU:CD	30:e:97:HIS:HE1	1.73	0.96
1:A:80:GLN:C	27:b:46:ASN:HD21	1.73	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
12:L:174:TYR:HD2	12:L:232:TRP:CD1	1.82	0.96
1:A:68:GLU:CG	1:A:98:LEU:HD13	1.93	0.96
25:Z:98:MET:CE	30:e:83:ARG:HB2	1.96	0.96
45:AA:463:GLU:OE1	51:AG:8:LEU:HB2	1.66	0.96
7:G:75:CYS:SG	59:G:803:FES:FE1	1.57	0.96
49:AE:89:SER:HA	49:AE:92:ARG:HB2	1.46	0.96
9:I:171:PRO:CB	42:q:93:MET:HE1	1.96	0.96
13:M:250:LEU:HD12	13:M:250:LEU:O	1.65	0.96
12:L:174:TYR:CD2	12:L:232:TRP:HD1	1.83	0.96
10:J:9:SER:HB3	11:K:7:ASN:HD22	1.27	0.96
26:a:58:ASN:HD22	26:a:60:TYR:HE1	1.10	0.96
37:l:38:PRO:HB2	38:m:75:ASN:HD22	1.23	0.96
7:G:611:THR:HG21	17:Q:105:GLU:CA	1.95	0.96
20:U:90:TYR:HE2	20:U:92:LYS:HB2	1.25	0.96
48:AD:247:PRO:HB3	69:AD:401:HEC:HMC2	1.48	0.96
4:D:256:ASP:HA	4:D:259:GLU:HB3	1.45	0.96
6:F:196:PHE:CE1	44:s:91:ARG:HD3	2.00	0.96
12:L:247:LEU:HD12	12:L:248:HIS:CD2	1.98	0.96
12:L:363:THR:HG23	12:L:431:THR:HB	1.48	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
46:Ab:146:PHE:HD2	46:Ab:202:SER:HB3	1.28	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
48:AD:242:ILE:HD11	48:AD:244:MET:HE3	1.44	0.95
53:AJ:23:LEU:HD13	54:AK:27:VAL:HG22	1.45	0.95
46:Ab:215:SER:HA	46:Ab:218:MET:HE2	1.48	0.95
12:L:466:PHE:CE1	35:j:72:ARG:CZ	2.49	0.95
20:T:138:LEU:HD12	20:T:138:LEU:O	1.66	0.95
49:AE:130:LYS:HD3	53:AJ:33:GLU:CG	1.96	0.95
2:B:166:ASN:O	9:I:150:THR:HB	1.66	0.95
12:L:319:MET:HE1	12:L:399:ILE:HA	1.47	0.95
52:Ah:32:ARG:HD3	52:Ah:76:ARG:HH12	1.28	0.95
1:A:18:ILE:HD12	8:H:76:THR:HG22	1.43	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:200:HIS:CD2	49:Ae:201:ASP:OD1	2.19	0.95
2:B:122:ARG:HB2	57:B:302:UQ1:H72	1.47	0.95
49:AE:119:ALA:HA	53:AJ:25:ILE:CD1	1.95	0.95
7:G:130:ILE:C	9:I:140:ARG:NH1	2.25	0.95
47:AC:30:TRP:HB3	47:AC:100:ARG:HD3	1.46	0.95
51:Ag:19:LEU:HD23	51:Ag:24:GLN:HB3	1.49	0.95
6:F:382:CYS:HG	56:F:502:SF4:FE3	0.77	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
12:L:174:TYR:HD2	12:L:232:TRP:HD1	1.02	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
7:G:114:GLU:OE2	43:r:53:TYR:HA	1.66	0.95
53:AJ:30:LEU:HG	54:AK:34:TRP:HB2	1.48	0.94
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.94
5:E:134:CYS:HG	59:E:301:FES:FE1	0.65	0.94
13:M:4:ILE:HG22	13:M:107:ILE:HD13	1.47	0.94
13:M:216:LEU:HG	13:M:220:HIS:CE1	2.02	0.94
20:T:99:SER:HB2	20:T:102:SER:HB3	1.48	0.94
53:AJ:23:LEU:CD1	54:AK:27:VAL:HG22	1.96	0.94
12:L:246:LEU:HD12	12:L:247:LEU:N	1.81	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:117:LEU:CD2	8:H:136:VAL:HG11	1.97	0.94
8:H:260:MET:HE2	26:a:17:VAL:HG13	1.47	0.94
1:A:68:GLU:HG2	1:A:98:LEU:HD13	1.49	0.94
4:D:259:GLU:HG3	25:Z:25:LEU:HD21	1.50	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
12:L:173:LEU:HD23	55:L:702:3PE:H321	1.47	0.94
45:Aa:100:GLY:O	45:Aa:101:THR:HG23	1.68	0.94
49:Ae:263:TYR:HA	49:Ae:273:VAL:CA	1.97	0.94
1:A:79:ILE:HA	1:A:87:MET:SD	2.06	0.94
12:L:274:LEU:HA	12:L:277:MET:HE3	1.49	0.94
12:L:362:ILE:HD12	12:L:430:VAL:HG12	1.50	0.94
13:M:1:MET:HG3	13:M:4:ILE:HD13	1.50	0.94
20:U:140:CYS:HB2	20:U:143:GLU:HG2	1.49	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.93
6:F:196:PHE:HE1	44:s:91:ARG:HD3	1.31	0.93
7:G:382:ARG:NE	7:G:652:ASN:HD21	1.67	0.93
12:L:13:ILE:HD11	55:i:201:3PE:H2C2	1.49	0.93
12:L:247:LEU:HD11	12:L:248:HIS:NE2	1.83	0.93
27:b:78:LEU:HD22	27:b:80:TRP:HE1	1.33	0.93
45:Aa:110:GLU:HB2	46:Ab:299:ILE:HD13	1.50	0.93
2:B:170:TYR:HE2	4:D:135:TYR:CG	1.87	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.50	0.93
47:AC:144:THR:CG2	49:Ae:221:GLY:O	2.15	0.93
49:AE:238:CYS:SG	47:Ac:268:ILE:HD12	2.09	0.93
13:M:453:LEU:CD1	13:M:454:ILE:HG23	1.99	0.93
4:D:238:LEU:HD23	43:r:36:GLN:HB2	1.47	0.93
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.82	0.93
49:Ae:188:ALA:HA	49:Ae:200:HIS:NE2	1.83	0.93
7:G:544:MET:HE3	7:G:546:PHE:CE1	2.03	0.93
9:I:152:CYS:HG	56:I:302:SF4:FE1	0.62	0.93
16:P:220:TYR:HD2	16:P:226:VAL:HG13	1.32	0.93
25:Z:97:ILE:HG23	25:Z:98:MET:HG3	1.51	0.93
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.51	0.93
46:AB:85:LEU:HD23	49:AI:68:VAL:HG21	1.50	0.93
47:AC:145:VAL:HG13	49:Ae:220:LEU:HB3	1.51	0.93
54:Ak:6:LEU:HA	54:Ak:11:ARG:HH12	1.32	0.93
49:AE:218:THR:HG21	49:AE:256:LEU:O	1.68	0.93
7:G:674:LEU:HD11	19:S:46:LYS:HE2	1.49	0.93
48:Ad:181:ASN:HB3	48:Ad:183:GLU:HG2	1.49	0.93
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
15:O:314:LEU:CD1	15:O:315:PRO:HD2	2.00	0.92
23:X:18:VAL:HG21	25:Z:74:LEU:HD11	1.51	0.92
13:M:127:ILE:CD1	14:N:256:PRO:CG	2.47	0.92
45:AA:384:THR:HG23	45:AA:387:GLU:H	1.31	0.92
7:G:338:VAL:CG1	7:G:546:PHE:HE1	1.81	0.92
4:D:267:ILE:HG21	8:H:278:PRO:O	1.67	0.92
12:L:41:LYS:HG3	12:L:98:TRP:CZ2	2.04	0.92
46:Ab:212:HIS:CE1	46:Ab:246:LEU:CD2	2.52	0.92
8:H:121:TRP:HE1	10:J:76:GLU:CD	1.77	0.92
46:Ab:297:PRO:CG	46:Ab:304:ASN:ND2	2.23	0.92
7:G:182:CYS:SG	56:G:802:SF4:FE2	1.61	0.92
7:G:661:GLU:O	7:G:661:GLU:HG2	1.68	0.92
16:P:306:GLY:HA2	16:P:312:PRO:HB3	1.48	0.92
46:Ab:212:HIS:HE1	46:Ab:246:LEU:HD23	1.03	0.92
13:M:127:ILE:HD12	14:N:256:PRO:HG3	1.50	0.92
47:AC:74:ASN:HB2	49:AE:139:SER:HA	1.51	0.92
48:AD:264:SER:HB3	52:AH:28:LEU:HB2	1.50	0.92
8:H:17:MET:HE1	61:H:400:UQ9:H17	1.50	0.92
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.52	0.91
51:Ag:46:ILE:CG2	55:Ag:103:3PE:H3H1	2.00	0.91
24:Y:19:GLN:HE21	24:Y:22:ARG:HG2	1.32	0.91
12:L:136:ASN:HD21	62:h:201:CDL:H273	1.33	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:260:MET:HE3	26:a:13:GLY:C	1.95	0.91
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.00	0.91
2:B:98:ALA:HB2	2:B:134:ALA:O	1.69	0.91
3:C:87:ILE:HG13	3:C:144:THR:CG2	2.00	0.91
4:D:256:ASP:HB2	25:Z:25:LEU:HD12	1.52	0.91
7:G:611:THR:CG2	17:Q:105:GLU:HA	1.99	0.91
9:I:113:CYS:HG	56:I:303:SF4:FE3	0.61	0.91
37:l:91:GLN:NE2	39:n:2:ALA:HB1	1.86	0.91
20:U:87:LEU:HB2	20:U:98:LEU:CD2	1.99	0.91
6:F:379:CYS:HG	56:F:502:SF4:FE4	0.61	0.91
12:L:245:ALA:O	12:L:249:SER:HB3	1.70	0.91
45:Aa:120:LEU:N	46:Ab:298:HIS:O	2.04	0.91
46:Ab:84:ARG:HG2	49:Ai:68:VAL:HG22	1.51	0.91
4:D:361:ALA:O	4:D:384:LEU:HD11	1.71	0.91
4:D:376:GLU:HG3	7:G:121:LEU:CD1	2.00	0.91
12:L:202:MET:HE3	12:L:265:PRO:HG3	1.53	0.91
48:Ad:302:LEU:HD13	49:Ae:121:THR:HA	1.49	0.91
26:a:64:LYS:HE2	26:a:66:LEU:HB2	1.51	0.90
47:AC:199:PHE:HE1	47:Ac:8:HIS:NE2	1.68	0.90
15:O:106:ILE:HG12	15:O:111:SER:HA	1.50	0.90
49:AE:118:THR:OG1	53:AJ:21:PHE:HZ	1.53	0.90
2:B:141:MET:HE2	4:D:115:LEU:HB3	1.54	0.90
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.53	0.90
7:G:662:THR:HG23	7:G:662:THR:O	1.71	0.90
15:O:316:GLU:OE2	32:g:51:MET:HG3	1.72	0.90
16:P:168:SER:O	16:P:202:ARG:HA	1.71	0.90
47:AC:190:ALA:HB1	68:AC:403:UQ6:H203	1.51	0.90
52:Ah:72:PHE:CZ	52:Ah:76:ARG:HD3	2.06	0.90
12:L:364:LYS:HE2	36:k:67:ILE:CD1	2.02	0.90
13:M:231:LEU:HD12	13:M:235:LEU:CD1	2.00	0.90
15:O:347:VAL:O	15:O:347:VAL:HG12	1.71	0.90
47:Ac:42:MET:CE	68:Ac:405:UQ6:C21	2.50	0.90
3:C:234:LEU:O	3:C:234:LEU:CD1	2.20	0.90
15:O:314:LEU:CG	15:O:315:PRO:HD2	2.02	0.90
45:Aa:109:LEU:CD1	45:Aa:110:GLU:N	2.35	0.90
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.85	0.89
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.89
13:M:453:LEU:HD12	13:M:454:ILE:N	1.87	0.89
16:P:268:PRO:HG3	16:P:342:PRO:HB2	1.54	0.89
51:AG:9:ALA:HB3	51:AG:11:ILE:CD1	2.02	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
12:L:123:LEU:HD22	12:L:150:MET:SD	2.12	0.89
13:M:2:LEU:HA	13:M:5:ILE:HG12	1.53	0.89
43:r:12:ARG:NH2	43:r:21:GLN:HE22	1.69	0.89
46:Ab:59:SER:HB3	46:Ab:224:GLY:HA3	1.54	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
12:L:455:LYS:NZ	35:j:57:GLN:OE1	2.04	0.89
25:Z:98:MET:HE3	30:e:83:ARG:HB2	1.52	0.89
7:G:404:GLY:HA2	7:G:684:LEU:HD13	1.52	0.89
13:M:380:PHE:HA	13:M:383:MET:HE2	1.55	0.89
45:Aa:96:LEU:HD21	45:Aa:161:ILE:HA	1.54	0.89
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.37	0.89
48:AD:153:GLU:HA	48:AD:168:PRO:CA	2.02	0.89
8:H:111:LEU:CD2	10:J:60:LEU:HD11	2.02	0.89
10:J:12:PHE:CE2	11:K:42:ILE:HD13	2.07	0.89
53:AJ:23:LEU:HB2	54:AK:27:VAL:HG22	1.55	0.89
13:M:50:LYS:HE2	13:M:52:PHE:HE1	1.36	0.89
48:AD:113:GLY:CA	48:AD:270:VAL:HA	2.03	0.89
46:Ab:305:THR:HG23	46:Ab:306:THR:H	1.36	0.89
16:P:292:PRO:O	16:P:293:LEU:HG	1.72	0.89
47:Ac:119:LEU:HD22	67:Ac:402:HEM:HBB2	1.55	0.89
4:D:269:ARG:O	4:D:273:VAL:HG12	1.72	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
8:H:19:PHE:CE2	26:a:11:ILE:HG21	2.08	0.88
47:Ac:146:ILE:CG1	70:Ac:404:U10:H4M3	2.02	0.88
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.88
7:G:176:CYS:HG	56:G:802:SF4:FE4	0.62	0.88
13:M:8:SER:HA	13:M:11:LEU:HD13	1.54	0.88
15:O:59:VAL:HA	15:O:157:VAL:CG2	2.02	0.88
23:X:20:VAL:HG23	23:X:25:LEU:CD1	2.03	0.88
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.39	0.88
1:A:79:ILE:HD11	8:H:155:LEU:CD2	2.01	0.88
12:L:261:VAL:O	12:L:264:HIS:HD2	1.51	0.88
13:M:173:THR:HG21	33:h:147:ALA:HB2	1.55	0.88
26:a:58:ASN:HB3	26:a:60:TYR:CD1	2.08	0.88
39:n:101:GLU:O	39:n:122:ARG:NH2	2.06	0.88
47:Ac:214:ASP:HB3	51:Ag:9:ALA:HB2	1.54	0.88
48:Ad:302:LEU:HB3	49:Ae:121:THR:OG1	1.74	0.88
2:B:194:CYS:SG	56:B:301:SF4:FE4	1.65	0.88
49:AE:140:MET:O	47:Ac:177:ARG:NH2	2.07	0.88
4:D:120:THR:HG23	4:D:135:TYR:CD1	2.09	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AJ:23:LEU:HD13	54:AK:27:VAL:CG2	2.03	0.88
12:L:428:TYR:HA	12:L:432:MET:HG2	1.56	0.88
13:M:310:MET:SD	13:M:455:THR:HB	2.13	0.88
42:q:60:ARG:HH12	42:q:95:ASP:HA	1.37	0.88
3:C:223:VAL:HG21	3:C:225:LEU:HD11	1.56	0.87
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.56	0.87
12:L:594:ASN:ND2	14:N:110:PRO:HB2	1.88	0.87
13:M:368:ALA:HB1	13:M:375:LEU:HD13	1.56	0.87
45:AA:402:HIS:CE1	45:AA:403:LEU:HD12	2.07	0.87
12:L:362:ILE:HD12	12:L:430:VAL:CG1	2.04	0.87
2:B:82:ILE:HD11	58:B:304:PC1:H362	1.54	0.87
13:M:447:LEU:HD11	13:M:454:ILE:HG21	1.55	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.87
3:C:229:PHE:HE1	9:I:126:GLN:CG	1.86	0.87
7:G:608:VAL:HG23	17:Q:103:THR:HB	1.57	0.87
12:L:496:LEU:HD12	12:L:497:GLY:N	1.90	0.87
30:e:17:HIS:CD2	30:e:18:PHE:HD1	1.92	0.87
47:AC:199:PHE:CE1	47:Ac:8:HIS:CE1	2.63	0.87
52:AH:58:ARG:HD3	52:AH:61:THR:HB	1.56	0.87
13:M:102:LEU:HD13	13:M:230:ILE:HG12	1.57	0.87
6:F:266:GLY:HA3	6:F:271:SER:HA	0.89	0.87
12:L:79:SER:HB2	12:L:135:ASN:HB2	1.55	0.87
49:AE:238:CYS:SG	47:Ac:268:ILE:CD1	2.63	0.87
53:Aj:30:LEU:HA	54:Ak:34:TRP:CD1	2.10	0.87
6:F:110:PRO:HB3	6:F:152:ARG:HE	1.40	0.87
7:G:615:LEU:HG	16:P:41:ILE:HG23	1.56	0.86
15:O:295:ARG:NH1	15:O:299:GLN:HB2	1.90	0.86
43:r:12:ARG:HH21	43:r:21:GLN:HE22	1.18	0.86
51:Ag:11:ILE:HG21	51:Ag:14:VAL:CG2	2.05	0.86
4:D:256:ASP:HB2	25:Z:25:LEU:CD1	2.05	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
17:Q:52:LEU:HD22	22:W:19:SER:HB3	1.58	0.86
48:AD:135:LEU:HA	48:AD:276:TRP:HH2	1.40	0.86
25:Z:58:ARG:HG2	27:b:45:ILE:HG12	1.57	0.86
13:M:1:MET:HE1	13:M:111:SER:HB2	1.58	0.86
14:N:307:THR:HB	15:O:319:ILE:HD11	1.57	0.86
3:C:87:ILE:CG1	3:C:144:THR:HG22	2.05	0.86
10:J:12:PHE:CE2	11:K:42:ILE:CD1	2.57	0.86
34:i:14:GLN:HB3	39:n:164:PRO:HG3	1.57	0.86
37:l:156:VAL:HG11	40:o:95:TYR:CZ	2.10	0.86
1:A:18:ILE:CD1	8:H:76:THR:HG23	2.04	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:552:LEU:HD12	37:l:70:MET:HE1	1.56	0.86
46:AB:300:LYS:HG2	46:AB:301:ARG:HG3	1.56	0.86
45:Aa:402:HIS:CE1	45:Aa:403:LEU:HD12	2.07	0.86
4:D:451:ILE:HG23	4:D:456:ILE:HD11	1.57	0.86
47:AC:148:ASN:HB2	49:Ae:220:LEU:HA	1.56	0.86
4:D:137:ASP:OD2	4:D:223:HIS:HA	1.76	0.86
23:X:17:GLU:OE2	30:e:105:ARG:NH2	2.08	0.86
25:Z:120:LEU:HD23	25:Z:122:GLY:N	1.90	0.86
46:Ab:84:ARG:HG2	49:Ai:68:VAL:CG2	2.06	0.86
51:Ag:29:SER:HB2	51:Ag:32:SER:HB2	1.57	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.85
8:H:19:PHE:HE2	26:a:11:ILE:HG21	1.39	0.85
10:J:37:PHE:CE2	10:J:41:LEU:HD11	2.10	0.85
43:r:27:ARG:HB3	43:r:31:ILE:CG2	2.05	0.85
46:AB:45:ASN:ND2	46:AB:239:ASN:HA	1.90	0.85
52:AH:47:ARG:NH2	52:AH:71:ASP:HB3	1.89	0.85
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
1:A:80:GLN:CA	27:b:46:ASN:HD21	1.90	0.85
37:l:167:TYR:HD2	37:l:168:LEU:HD12	1.41	0.85
45:Aa:109:LEU:HD12	45:Aa:110:GLU:CA	2.05	0.85
8:H:45:ILE:HD11	26:a:11:ILE:HD11	1.57	0.85
49:AE:127:TYR:HH	53:AJ:36:PHE:HD1	0.87	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
12:L:417:SER:HB3	12:L:493:ILE:HG13	1.58	0.85
15:O:176:GLN:HG3	15:O:177:GLY:H	1.41	0.85
16:P:55:VAL:HG21	18:R:43:TYR:HB2	1.58	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
7:G:662:THR:O	7:G:662:THR:CG2	2.25	0.85
46:AB:304:ASN:HB3	46:AB:307:SER:CB	2.07	0.85
4:D:261:MET:O	4:D:265:ASN:ND2	2.10	0.85
13:M:29:SER:HB3	32:g:91:PHE:CD2	2.12	0.85
49:Ae:200:HIS:HD2	49:Ae:201:ASP:H	1.21	0.85
20:T:117:GLU:HA	20:T:120:MET:HE2	1.58	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
6:F:300:ILE:HD13	6:F:307:VAL:H	1.40	0.85
9:I:123:CYS:HG	56:I:302:SF4:FE2	0.60	0.85
45:AA:384:THR:CG2	45:AA:387:GLU:HB3	2.07	0.85
4:D:137:ASP:OD2	4:D:223:HIS:CA	2.24	0.85
4:D:266:ARG:HH21	9:I:60:ILE:HA	1.42	0.85
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.58	0.85
7:G:388:ASN:H	7:G:514:ASN:CB	1.90	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:54:PHE:O	12:L:58:ASN:N	2.10	0.85
49:AE:220:LEU:CD1	47:Ac:145:VAL:HG13	2.06	0.85
47:Ac:41:LEU:HD23	68:Ac:405:UQ6:H201	1.56	0.85
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.59	0.84
26:a:52:ARG:HG3	26:a:57:VAL:O	1.76	0.84
49:Ae:163:LYS:H	49:Ae:178:HIS:HB3	1.42	0.84
1:A:7:ILE:HD13	55:H:401:3PE:H371	1.56	0.84
8:H:114:TYR:CE1	10:J:65:VAL:CG2	2.60	0.84
12:L:128:MET:HG2	12:L:251:THR:HB	1.59	0.84
33:h:96:ALA:HB3	41:p:63:TYR:HD1	1.40	0.84
12:L:247:LEU:HD11	12:L:248:HIS:CD2	2.11	0.84
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.59	0.84
15:O:237:ILE:HG22	15:O:241:TYR:HE2	1.42	0.84
53:AJ:30:LEU:CG	54:AK:34:TRP:HB2	2.06	0.84
4:D:192:LEU:HD11	4:D:200:PHE:HB2	1.59	0.84
13:M:142:ARG:HH21	14:N:303:THR:HG22	1.40	0.84
15:O:314:LEU:HD12	15:O:315:PRO:HD2	1.56	0.84
7:G:544:MET:CE	7:G:546:PHE:CZ	2.60	0.84
13:M:447:LEU:HD11	13:M:454:ILE:CG2	2.07	0.84
47:AC:45:ILE:HA	67:AC:401:HEM:HAB	1.56	0.84
48:Ad:154:VAL:HG12	48:Ad:155:GLN:HG2	1.57	0.84
49:Ae:123:VAL:HG13	53:Aj:29:ALA:HA	1.59	0.84
2:B:98:ALA:HB2	2:B:134:ALA:C	2.02	0.84
4:D:96:ARG:HG3	4:D:115:LEU:HD11	1.59	0.84
13:M:391:PHE:CE2	55:m:202:3PE:H261	2.12	0.84
15:O:238:GLU:HA	15:O:241:TYR:HD2	1.43	0.84
20:U:110:LEU:CD1	20:U:118:ILE:HD11	2.06	0.84
30:e:14:LEU:HD12	30:e:15:ASP:HB2	1.57	0.84
13:M:196:TRP:NE1	13:M:250:LEU:HD13	1.92	0.84
48:AD:113:GLY:HA3	48:AD:270:VAL:HA	1.59	0.84
12:L:445:GLU:HB2	12:L:450:LEU:HD23	1.59	0.84
14:N:215:MET:SD	14:N:248:LEU:HD21	2.18	0.84
37:l:167:TYR:CD2	37:l:168:LEU:HD12	2.13	0.84
1:A:18:ILE:HD11	8:H:76:THR:CG2	2.07	0.84
7:G:377:ALA:HB3	7:G:384:ASN:HD21	1.43	0.84
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.84
16:P:220:TYR:CD2	16:P:226:VAL:HG13	2.13	0.84
20:U:100:VAL:HA	20:U:141:PRO:HG2	1.59	0.84
47:AC:145:VAL:CG1	49:Ae:220:LEU:HD13	2.08	0.84
49:AE:130:LYS:CD	53:AJ:33:GLU:HG2	2.04	0.84
48:AD:242:ILE:CD1	48:AD:244:MET:HE3	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:127:TYR:CZ	53:AJ:36:PHE:HB3	2.11	0.84
50:AF:99:ILE:HG23	50:AF:102:ARG:HH21	1.39	0.84
53:AJ:23:LEU:HD22	54:AK:23:MET:CG	2.08	0.84
47:Ac:128:PHE:CE1	70:Ac:404:U10:H4M1	2.05	0.84
12:L:20:LEU:HD12	12:L:21:ILE:N	1.92	0.83
49:AE:118:THR:HG1	53:AJ:21:PHE:HZ	0.84	0.83
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HA	1.59	0.83
15:O:314:LEU:HG	15:O:315:PRO:HD2	1.58	0.83
16:P:96:LEU:C	16:P:96:LEU:HD12	2.03	0.83
2:B:94:THR:H	57:B:302:UQ1:H113	1.43	0.83
12:L:16:LEU:HD23	12:L:126:ILE:CD1	2.08	0.83
19:S:95:LEU:O	19:S:95:LEU:CD1	2.26	0.83
25:Z:93:GLU:CD	30:e:97:HIS:CE1	2.56	0.83
34:i:94:PRO:HG3	41:p:10:TYR:CE2	2.13	0.83
13:M:361:MET:HB3	13:M:441:MET:HE3	1.60	0.83
16:P:293:LEU:HB2	16:P:298:TYR:CZ	2.14	0.83
47:AC:145:VAL:HG13	49:Ae:220:LEU:CD1	2.08	0.83
46:Ab:167:GLN:HG2	49:Ai:43:LEU:HD13	1.59	0.83
3:C:223:VAL:CG2	3:C:225:LEU:HD12	2.08	0.83
4:D:67:ASN:HB3	4:D:69:VAL:HG12	1.58	0.83
12:L:364:LYS:HE2	36:k:67:ILE:HD11	1.58	0.83
13:M:373:ILE:HG12	13:M:454:ILE:HD11	1.60	0.83
49:AE:130:LYS:HB3	53:AJ:33:GLU:OE1	1.79	0.83
4:D:144:MET:SD	4:D:222:MET:HG3	2.19	0.83
48:AD:262:THR:HG21	52:AH:27:PRO:HD3	1.58	0.83
53:AJ:23:LEU:HB2	54:AK:27:VAL:CG2	2.07	0.83
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.61	0.83
15:O:99:GLY:HA2	28:c:30:TYR:HD1	1.42	0.83
47:AC:199:PHE:CZ	47:Ac:8:HIS:NE2	2.46	0.83
48:AD:295:MET:HG2	53:AJ:36:PHE:CZ	2.14	0.83
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.83
10:J:33:ILE:HG23	10:J:60:LEU:CD2	2.09	0.83
48:Ad:117:TYR:HA	48:Ad:121:CYS:SG	2.19	0.83
6:F:425:CYS:SG	56:F:502:SF4:FE1	1.70	0.83
7:G:75:CYS:HG	59:G:803:FES:FE1	0.90	0.83
18:R:47:ARG:HB2	42:q:125:VAL:HG11	1.61	0.83
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.14	0.83
10:J:135:LEU:HD12	11:K:54:MET:CE	2.09	0.83
32:g:53:TRP:CD1	32:g:53:TRP:H	1.95	0.83
7:G:617:ARG:HH12	22:W:128:GLY:C	1.86	0.82
13:M:269:MET:HE1	13:M:396:MET:HA	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:293:LEU:HB2	16:P:298:TYR:CE2	2.14	0.82
1:A:68:GLU:CD	1:A:98:LEU:HD13	2.04	0.82
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.10	0.82
8:H:203:GLY:O	8:H:207:LEU:O	1.96	0.82
12:L:131:LEU:CD1	12:L:140:LEU:HD12	2.09	0.82
20:U:87:LEU:HB2	20:U:98:LEU:HD21	1.61	0.82
49:AE:127:TYR:CE1	53:AJ:36:PHE:HB3	2.15	0.82
4:D:236:LEU:HD22	4:D:240:LEU:HD23	1.59	0.82
4:D:256:ASP:CA	4:D:259:GLU:HB3	2.09	0.82
7:G:403:VAL:HG23	7:G:432:ILE:HB	1.61	0.82
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.59	0.82
52:AH:44:ALA:HA	52:AH:47:ARG:HD3	1.61	0.82
2:B:194:CYS:HG	56:B:301:SF4:FE4	0.54	0.82
14:N:335:MET:HG3	14:N:335:MET:O	1.79	0.82
51:AG:74:ASN:HB3	51:AG:77:MET:HG2	1.61	0.82
49:Ae:234:TYR:HB2	49:Ae:243:TYR:HB2	1.62	0.82
8:H:80:THR:HG21	55:H:401:3PE:H3D2	1.62	0.82
12:L:222:GLY:HA2	12:L:229:LEU:CD1	2.08	0.82
17:Q:154:LYS:HB2	17:Q:155:PRO:HD2	1.61	0.82
4:D:36:GLN:HE22	13:M:135:ARG:HH12	1.26	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.44	0.82
10:J:22:LYS:HD2	11:K:23:ARG:HG2	1.62	0.82
16:P:104:THR:HG21	18:R:46:VAL:HG12	1.60	0.82
53:AJ:23:LEU:HD13	54:AK:27:VAL:HA	1.59	0.82
4:D:129:TYR:HE1	4:D:411:LEU:HD21	1.43	0.82
12:L:493:ILE:HD12	12:L:496:LEU:HD21	1.62	0.82
46:Ab:341:ILE:HD12	49:Ai:59:ALA:HB2	1.61	0.82
8:H:114:TYR:CE1	10:J:65:VAL:HG22	2.15	0.82
8:H:199:ASP:HB2	8:H:279:ARG:HD3	1.59	0.82
12:L:432:MET:HG3	12:L:432:MET:O	1.78	0.82
53:AJ:23:LEU:CD1	54:AK:27:VAL:HA	2.09	0.82
49:Ae:142:ALA:CB	49:Ae:147:LEU:HD23	2.08	0.82
2:B:92:PRO:HB2	2:B:122:ARG:HH12	1.45	0.82
4:D:390:GLN:OE1	7:G:145:MET:HE1	1.80	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
47:AC:198:LEU:HD21	47:Ac:9:PRO:C	2.04	0.82
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.60	0.82
2:B:170:TYR:HE2	4:D:135:TYR:CD1	1.97	0.81
17:Q:131:LYS:HG2	17:Q:135:ILE:CD1	2.09	0.81
25:Z:58:ARG:HG2	27:b:45:ILE:CG1	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:227:LEU:HD22	48:AD:231:LEU:HB3	1.62	0.81
3:C:149:LEU:HD21	17:Q:64:LEU:HD22	1.62	0.81
39:n:97:TYR:HB2	39:n:178:PRO:CG	2.10	0.81
52:Ah:32:ARG:CD	52:Ah:76:ARG:HH12	1.92	0.81
49:Ai:46:LYS:HG2	49:Ai:47:ARG:N	1.93	0.81
2:B:122:ARG:CB	57:B:302:UQ1:H72	2.11	0.81
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
9:I:89:GLU:HG2	42:q:61:TRP:HB3	1.62	0.81
13:M:336:ARG:NH2	13:M:429:SER:HA	1.95	0.81
36:k:34:PRO:HD2	36:k:59:TYR:CD1	2.16	0.81
46:AB:304:ASN:HB3	46:AB:307:SER:OG	1.79	0.81
48:AD:146:LYS:HD3	48:AD:171:LEU:HG	1.63	0.81
48:AD:213:SER:HB3	48:AD:236:TYR:CG	2.15	0.81
49:AE:126:ALA:CB	53:AJ:29:ALA:HB1	2.10	0.81
45:Aa:100:GLY:O	45:Aa:101:THR:CG2	2.28	0.81
46:Ab:163:ALA:C	49:Ai:43:LEU:HD22	2.04	0.81
48:Ad:222:PRO:HB2	52:Ah:65:CYS:HB3	1.59	0.81
2:B:92:PRO:HD2	2:B:119:VAL:HG13	1.61	0.81
12:L:16:LEU:CD2	12:L:126:ILE:HD13	2.10	0.81
48:AD:262:THR:HB	52:AH:26:ASP:HA	1.63	0.81
4:D:192:LEU:HD11	4:D:200:PHE:CB	2.10	0.81
36:k:30:ILE:HD11	36:k:39:GLN:HB2	1.61	0.81
47:Ac:146:ILE:CD1	70:Ac:404:U10:H3M2	2.07	0.81
1:A:25:PRO:O	1:A:26:GLN:HB2	1.78	0.81
6:F:228:PRO:HG2	17:Q:160:TYR:HD2	1.45	0.81
10:J:76:GLU:OE1	10:J:76:GLU:O	1.99	0.81
12:L:73:SER:HB3	41:p:100:GLN:NE2	1.96	0.81
47:AC:145:VAL:CA	49:Ae:220:LEU:O	2.25	0.81
49:AE:122:THR:CG2	53:AJ:25:ILE:HG21	2.10	0.81
46:Ab:305:THR:HG23	46:Ab:306:THR:N	1.92	0.81
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.63	0.81
8:H:54:LYS:HE2	8:H:58:LYS:HD2	1.62	0.81
8:H:316:PRO:HG3	25:Z:57:ARG:HB3	1.61	0.81
12:L:428:TYR:OH	39:n:33:HIS:CE1	2.34	0.81
45:AA:403:LEU:HD21	46:AB:56:ALA:HB1	1.62	0.81
47:Ac:18:PHE:HE1	68:Ac:405:UQ6:H71	1.45	0.81
1:A:67:LEU:CD1	11:K:68:ALA:HB3	2.11	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
8:H:121:TRP:NE1	10:J:76:GLU:OE2	2.12	0.81
21:V:72:LEU:HD13	21:V:80:VAL:HG11	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:93:GLU:HG3	30:e:97:HIS:CE1	2.15	0.81
25:Z:120:LEU:CD2	25:Z:122:GLY:H	1.94	0.81
37:l:115:ASN:OD1	37:l:115:ASN:O	1.98	0.81
38:m:125:PHE:CE1	41:p:133:THR:HG22	2.16	0.81
41:p:6:ASP:HB3	41:p:9:VAL:HG22	1.61	0.81
48:AD:120:VAL:CG2	48:AD:253:LEU:HD11	2.07	0.81
49:Ae:239:HIS:CE1	49:Ae:253:PRO:HB3	2.16	0.81
8:H:114:TYR:OH	10:J:60:LEU:O	1.97	0.81
8:H:229:THR:O	8:H:229:THR:HG22	1.81	0.81
10:J:33:ILE:HG23	10:J:60:LEU:HD21	1.61	0.81
12:L:229:LEU:O	12:L:229:LEU:CD1	2.28	0.81
12:L:506:ASN:HA	12:L:509:MET:HE2	1.63	0.81
14:N:277:ILE:HG23	14:N:278:MET:N	1.96	0.81
46:AB:51:SER:HB2	46:AB:230:LEU:HD12	1.61	0.81
48:Ad:223:THR:CG2	52:Ah:65:CYS:HB2	2.11	0.81
6:F:425:CYS:HG	56:F:502:SF4:FE1	0.53	0.81
7:G:388:ASN:H	7:G:514:ASN:HB3	1.45	0.80
12:L:424:MET:HE2	12:L:502:LEU:HB2	1.62	0.80
13:M:172:GLY:O	13:M:173:THR:CG2	2.28	0.80
13:M:453:LEU:HD12	13:M:454:ILE:HG23	1.63	0.80
16:P:171:ASN:HB3	16:P:327:VAL:CB	2.10	0.80
48:Ad:202:ARG:HG3	48:Ad:278:SER:HB3	1.63	0.80
46:Ab:59:SER:CB	46:Ab:224:GLY:CA	2.56	0.80
46:Ab:59:SER:HB2	46:Ab:224:GLY:CA	2.10	0.80
46:Ab:297:PRO:CB	46:Ab:304:ASN:ND2	2.41	0.80
49:Ae:204:ARG:HB3	49:Ae:260:VAL:HG21	1.64	0.80
2:B:92:PRO:HG3	2:B:130:VAL:CG1	2.10	0.80
2:B:170:TYR:CE1	4:D:134:PRO:HB2	2.17	0.80
6:F:109:ARG:NH1	6:F:237:GLY:O	2.13	0.80
7:G:89:VAL:HB	7:G:94:MET:HG3	1.62	0.80
7:G:667:GLN:HE21	19:S:38:VAL:HA	1.45	0.80
8:H:117:LEU:HD21	8:H:136:VAL:HG11	1.60	0.80
14:N:200:LEU:HD21	14:N:265:ILE:HG12	1.63	0.80
14:N:277:ILE:CG2	14:N:278:MET:H	1.93	0.80
15:O:227:MET:O	15:O:228:LYS:CG	2.30	0.80
55:i:201:3PE:H2E1	55:i:201:3PE:H342	1.63	0.80
52:AH:42:VAL:HG13	52:AH:45:ARG:HH21	1.46	0.80
45:Aa:68:THR:HG21	46:Ab:384:MET:HG3	1.62	0.80
6:F:234:GLY:HA3	6:F:238:CYS:O	1.81	0.80
7:G:617:ARG:HH12	22:W:129:HIS:N	1.79	0.80
38:m:18:LEU:HD21	39:n:69:GLU:HA	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:255:TYR:OH	48:AD:266:VAL:HA	1.81	0.80
4:D:241:LEU:HB3	25:Z:16:TYR:OH	1.82	0.80
8:H:90:PRO:HG2	8:H:240:ILE:HD13	1.61	0.80
13:M:216:LEU:HD12	13:M:236:LEU:HD21	1.60	0.80
49:AE:126:ALA:CB	53:AJ:29:ALA:CB	2.60	0.80
47:Ac:128:PHE:HD1	70:Ac:404:U10:H4M1	1.43	0.80
1:A:33:LYS:HA	2:B:150:ASP:O	1.81	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
13:M:127:ILE:HD11	14:N:256:PRO:CG	2.09	0.80
23:X:18:VAL:HG12	23:X:20:VAL:HG22	1.63	0.80
25:Z:97:ILE:HG23	30:e:92:TYR:CE1	2.14	0.80
48:AD:158:PRO:HB2	48:AD:162:GLY:HA2	1.64	0.80
71:Ad:402:3PH:H12	49:Ae:131:ASN:ND2	1.97	0.80
1:A:72:LEU:HD21	1:A:94:LEU:HD23	1.64	0.80
3:C:147:ASP:OD1	3:C:148:GLU:OE1	2.00	0.80
4:D:253:LEU:HB2	43:r:23:LYS:HD2	1.63	0.80
13:M:29:SER:HB3	32:g:91:PHE:HD2	1.47	0.80
19:S:62:GLN:HB2	19:S:80:ASN:HB2	1.64	0.80
20:T:82:ARG:HD2	20:T:125:GLU:HG3	1.61	0.80
46:AB:323:VAL:HG22	46:AB:340:THR:HG22	1.64	0.80
51:AG:9:ALA:CB	51:AG:11:ILE:HD11	2.11	0.80
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.22	0.80
10:J:124:LEU:CD2	25:Z:137:ASN:ND2	2.32	0.80
62:L:704:CDL:HA62	33:h:68:LEU:HD13	1.63	0.80
13:M:173:THR:HG23	33:h:147:ALA:CB	2.11	0.80
15:O:117:PHE:CE1	15:O:173:MET:HE3	2.17	0.80
16:P:363:SER:HA	22:W:54:GLN:HE22	1.46	0.80
45:AA:74:TRP:CZ2	45:AA:411:GLU:HA	2.16	0.80
1:A:94:LEU:HD22	10:J:152:MET:CE	2.12	0.80
12:L:553:LEU:HD11	38:m:93:ALA:CB	2.10	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
47:AC:145:VAL:HG13	49:Ae:220:LEU:HD13	1.64	0.80
12:L:456:ARG:HG2	55:L:701:3PE:H241	1.62	0.79
15:O:199:LEU:HD11	15:O:294:LEU:HD22	1.64	0.79
30:e:38:LYS:HE3	33:h:181:HIS:HD2	1.45	0.79
42:q:43:LYS:HZ3	42:q:44:TYR:HE2	1.28	0.79
48:AD:227:LEU:HD22	48:AD:231:LEU:CB	2.13	0.79
49:Ae:200:HIS:CD2	49:Ae:201:ASP:H	1.99	0.79
4:D:177:ILE:O	4:D:181:LEU:HD13	1.81	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.62	0.79
38:m:125:PHE:HE1	41:p:133:THR:HG22	1.47	0.79
48:Ad:153:GLU:HG2	48:Ad:168:PRO:HA	1.64	0.79
12:L:552:LEU:HD21	38:m:90:GLY:HA2	1.62	0.79
15:O:59:VAL:HA	15:O:157:VAL:HG23	1.63	0.79
20:U:93:ILE:HD11	20:U:110:LEU:HD11	1.64	0.79
46:Ab:109:LYS:HB2	49:Ai:71:ASN:OD1	1.82	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:73:GLY:HA2	59:G:803:FES:S1	2.22	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
12:L:130:ILE:HG23	12:L:139:GLN:HE21	1.46	0.79
13:M:122:PHE:CZ	13:M:206:LYS:HD3	2.18	0.79
45:Aa:338:CYS:HB3	45:Aa:368:MET:SD	2.22	0.79
47:Ac:253:PRO:HG2	48:Ad:205:HIS:CE1	2.17	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
13:M:367:LEU:HD21	13:M:408:MET:HE2	1.63	0.79
16:P:51:VAL:HG22	16:P:53:GLY:H	1.48	0.79
47:Ac:138:MET:HE1	47:Ac:268:ILE:HA	1.64	0.79
10:J:9:SER:CB	11:K:7:ASN:ND2	2.45	0.79
7:G:338:VAL:HG13	7:G:546:PHE:HE1	1.47	0.79
8:H:28:LEU:HD21	8:H:274:ARG:HD3	1.65	0.79
20:T:106:LYS:H	20:T:106:LYS:HD2	1.48	0.79
39:n:20:TYR:CE2	39:n:24:LEU:HD11	2.18	0.79
48:Ad:146:LYS:HD3	48:Ad:171:LEU:HG	1.63	0.79
3:C:170:TRP:CG	3:C:183:LEU:HD21	2.18	0.79
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.98	0.79
16:P:88:VAL:HG13	16:P:91:ILE:HD11	1.63	0.79
16:P:225:ALA:CB	16:P:289:ILE:HB	2.13	0.79
7:G:544:MET:HE3	7:G:546:PHE:HZ	1.39	0.78
9:I:211:TYR:CZ	43:r:39:PRO:HG3	2.17	0.78
12:L:131:LEU:HD12	12:L:140:LEU:CD1	2.12	0.78
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.63	0.78
48:Ad:291:LYS:CB	71:Ad:402:3PH:H32	2.12	0.78
7:G:130:ILE:HA	9:I:140:ARG:HH11	1.45	0.78
7:G:284:GLU:OE2	17:Q:84:ARG:NH2	2.15	0.78
13:M:231:LEU:HD12	13:M:235:LEU:HD13	1.64	0.78
14:N:123:PRO:HG2	14:N:126:MET:HG2	1.63	0.78
16:P:188:GLU:HG2	16:P:200:ILE:HD13	1.64	0.78
20:U:90:TYR:HH	20:U:92:LYS:HD2	1.43	0.78
4:D:137:ASP:OD1	4:D:138:ARG:HG3	1.83	0.78
6:F:224:ARG:HD3	17:Q:164:PHE:CE1	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:173:THR:HG23	33:h:147:ALA:HB2	1.65	0.78
13:M:370:PRO:HA	13:M:375:LEU:CD2	2.13	0.78
15:O:66:ILE:HD11	15:O:218:ILE:CG1	2.13	0.78
15:O:117:PHE:HE1	15:O:173:MET:CE	1.96	0.78
48:AD:215:LEU:HD21	69:AD:401:HEC:C2B	2.14	0.78
45:Aa:74:TRP:CZ2	45:Aa:411:GLU:HA	2.16	0.78
49:Ae:142:ALA:HB3	49:Ae:147:LEU:HD23	1.65	0.78
8:H:196:ALA:HB1	8:H:197:PRO:CD	2.13	0.78
13:M:9:LEU:HD23	13:M:104:ILE:HD13	1.65	0.78
15:O:314:LEU:HD12	15:O:315:PRO:CD	2.13	0.78
25:Z:82:ARG:HD3	30:e:106:PRO:O	1.83	0.78
48:AD:215:LEU:HD23	48:AD:244:MET:CE	2.13	0.78
12:L:3:ILE:H	12:L:3:ILE:HD12	1.48	0.78
12:L:136:ASN:HA	12:L:197:GLU:HA	1.66	0.78
12:L:534:HIS:O	12:L:538:PRO:HG3	1.83	0.78
13:M:143:LEU:HD21	14:N:303:THR:HG23	1.63	0.78
13:M:248:ILE:HG13	13:M:249:ILE:HD12	1.64	0.78
37:l:44:THR:OG1	37:l:45:PRO:HD2	1.83	0.78
45:AA:182:VAL:CG1	45:AA:186:TYR:CE2	2.67	0.78
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.13	0.78
16:P:226:VAL:HG12	16:P:228:LEU:HG	1.64	0.78
1:A:72:LEU:CD2	1:A:94:LEU:HD23	2.13	0.78
13:M:319:HIS:HA	13:M:322:THR:HG22	1.66	0.78
14:N:215:MET:CE	14:N:248:LEU:CD2	2.62	0.78
1:A:52:SER:HB2	1:A:55:PHE:CE2	2.14	0.78
3:C:160:ILE:HD12	4:D:285:ASN:HD22	1.49	0.78
13:M:162:ILE:HG23	14:N:271:MET:CE	2.14	0.78
46:AB:113:THR:OG1	49:AI:65:VAL:CG1	2.32	0.78
47:AC:8:HIS:CE1	47:Ac:199:PHE:CZ	2.71	0.78
47:AC:69:ILE:HA	47:AC:73:VAL:HB	1.65	0.78
46:Ab:297:PRO:HA	46:Ab:304:ASN:OD1	1.83	0.78
48:Ad:156:ASP:HB3	48:Ad:167:ARG:HB3	1.64	0.78
2:B:136:THR:HG21	4:D:118:ARG:HD3	1.66	0.78
3:C:103:THR:HG21	21:V:55:LYS:HE3	1.66	0.78
6:F:424:ILE:HD11	7:G:73:GLY:O	1.84	0.78
15:O:305:LEU:HD12	15:O:305:LEU:O	1.83	0.78
46:AB:100:THR:HG23	49:AI:70:LEU:CD1	2.14	0.78
48:AD:249:TYR:H	48:AD:252:VAL:HB	1.49	0.78
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.66	0.77
46:AB:63:LEU:HD11	46:AB:238:LEU:HD21	1.65	0.77
48:AD:233:PHE:HA	48:AD:240:GLN:O	1.82	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
9:I:210:LEU:HD12	43:r:39:PRO:HD2	1.66	0.77
55:L:703:3PE:H361	14:N:164:MET:HE1	1.66	0.77
48:Ad:114:PHE:HE1	48:Ad:175:PHE:HE2	1.28	0.77
1:A:68:GLU:HG2	1:A:98:LEU:CD1	2.13	0.77
4:D:256:ASP:HA	4:D:259:GLU:HB2	1.63	0.77
14:N:170:LEU:HD11	14:N:288:LEU:HG	1.65	0.77
15:O:206:TYR:CD2	15:O:257:VAL:HG13	2.19	0.77
15:O:256:LEU:HD11	15:O:276:LEU:HD23	1.64	0.77
37:l:89:TRP:CZ2	39:n:86:PRO:HD2	2.20	0.77
49:Ae:176:VAL:HG13	49:Ae:212:ILE:HG12	1.64	0.77
1:A:73:LEU:O	1:A:76:PRO:HD2	1.84	0.77
5:E:196:THR:H	5:E:199:ASP:HB2	1.47	0.77
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.66	0.77
4:D:47:PHE:CB	14:N:227:ILE:HD11	2.12	0.77
8:H:184:MET:CG	8:H:293:PHE:CD2	2.66	0.77
8:H:227:GLU:O	8:H:231:ILE:HG13	1.83	0.77
13:M:274:SER:O	13:M:277:LEU:HB2	1.85	0.77
14:N:254:LEU:HD12	14:N:255:PRO:CD	2.14	0.77
20:T:123:GLU:HG2	20:T:130:ILE:HG12	1.65	0.77
30:e:17:HIS:CD2	30:e:18:PHE:CD1	2.72	0.77
47:AC:141:TRP:CD1	47:AC:265:PRO:HD3	2.19	0.77
48:AD:221:PRO:HB2	48:AD:225:VAL:HG11	1.65	0.77
8:H:102:ILE:HG21	8:H:150:LEU:HD21	1.65	0.77
13:M:204:LEU:HD22	13:M:209:LEU:HD12	1.65	0.77
13:M:453:LEU:HD11	13:M:454:ILE:HG23	1.65	0.77
14:N:45:ILE:O	14:N:45:ILE:HG13	1.83	0.77
51:AG:45:ARG:HG2	51:AG:48:ARG:NH2	1.98	0.77
45:Aa:104:ARG:HB3	45:Aa:108:ALA:HB3	1.65	0.77
1:A:3:LEU:HD23	55:H:401:3PE:H31	1.66	0.77
4:D:137:ASP:CG	4:D:223:HIS:HA	2.09	0.77
13:M:98:MET:CE	13:M:128:PRO:HA	2.14	0.77
16:P:266:THR:HG21	16:P:329:PRO:HG3	1.67	0.77
18:R:95:LEU:HD21	18:R:111:PHE:HB3	1.66	0.77
25:Z:101:VAL:HB	25:Z:102:PRO:HD2	1.67	0.77
51:Ag:11:ILE:CG2	51:Ag:14:VAL:CG2	2.63	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
25:Z:98:MET:HG3	30:e:92:TYR:CE1	2.20	0.77
37:l:169:GLU:C	37:l:171:GLY:H	1.92	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:27:ARG:HD2	43:r:31:ILE:HG22	1.67	0.77
1:A:94:LEU:HD22	10:J:152:MET:HE1	1.65	0.77
3:C:89:PRO:O	3:C:92:VAL:HG23	1.85	0.77
12:L:419:THR:HA	12:L:422:TYR:CE2	2.20	0.77
15:O:168:VAL:HG21	15:O:241:TYR:OH	1.83	0.77
19:S:25:GLN:HG3	19:S:57:GLU:OE1	1.84	0.77
32:g:70:ASP:OD1	39:n:108:HIS:NE2	2.17	0.77
47:AC:215:ALA:HB2	50:AF:60:MET:HE3	1.67	0.77
51:Ag:19:LEU:HD11	51:Ag:23:GLU:HG2	1.65	0.77
8:H:117:LEU:HD23	8:H:136:VAL:HG11	1.67	0.77
12:L:56:HIS:HA	40:o:74:PHE:CD1	2.19	0.77
13:M:208:PRO:HG2	13:M:216:LEU:HD13	1.67	0.77
46:AB:407:MET:HG2	46:AB:411:THR:OG1	1.85	0.77
50:AF:110:LYS:HG2	54:Ak:10:TYR:CE1	2.20	0.77
51:AG:25:ARG:HH12	51:AG:28:PRO:HA	1.49	0.77
45:Aa:68:THR:HG22	45:Aa:136:LEU:HD23	1.67	0.77
3:C:70:LYS:HD3	21:V:101:GLU:HB2	1.67	0.76
4:D:299:GLN:NE2	9:I:36:TYR:CD2	2.53	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
11:K:1:MET:HA	11:K:4:THR:HG22	1.67	0.76
15:O:99:GLY:HA2	28:c:30:TYR:CD1	2.20	0.76
23:X:20:VAL:HG23	23:X:25:LEU:HD11	1.66	0.76
49:AE:93:ARG:HB3	51:AG:25:ARG:HA	1.65	0.76
49:Ae:200:HIS:NE2	49:Ae:201:ASP:OD1	2.18	0.76
4:D:259:GLU:HB3	25:Z:25:LEU:HD11	1.66	0.76
13:M:42:LEU:HG	13:M:67:ILE:HD11	1.68	0.76
13:M:171:VAL:HG11	13:M:179:LEU:HD21	1.65	0.76
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.65	0.76
15:O:66:ILE:CD1	15:O:218:ILE:HD11	2.14	0.76
45:AA:190:THR:HB	45:AA:275:ILE:HD12	1.67	0.76
49:AE:126:ALA:HB3	53:AJ:29:ALA:HB2	1.66	0.76
51:Ag:46:ILE:HG23	55:Ag:103:3PE:H3H1	1.66	0.76
8:H:86:TRP:HE1	8:H:229:THR:HG22	1.48	0.76
16:P:225:ALA:HB1	16:P:289:ILE:HB	1.68	0.76
20:U:123:GLU:HG2	20:U:130:ILE:HG12	1.67	0.76
34:i:22:TRP:CE2	39:n:172:THR:HG22	2.20	0.76
48:Ad:193:LEU:HD12	48:Ad:194:PRO:HD2	1.66	0.76
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.67	0.76
42:q:39:VAL:HG21	42:q:89:TRP:CZ2	2.21	0.76
48:Ad:292:MET:HA	71:Ad:402:3PH:H331	1.66	0.76
2:B:202:LEU:HD23	9:I:86:TYR:CG	2.20	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:496:LEU:HD12	12:L:496:LEU:C	2.09	0.76
13:M:60:PRO:O	13:M:64:PRO:HD3	1.85	0.76
52:Ah:69:LEU:HD21	52:Ah:73:LEU:HD11	1.67	0.76
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.66	0.76
6:F:109:ARG:CZ	6:F:237:GLY:O	2.34	0.76
7:G:652:ASN:HB3	7:G:655:ARG:NH2	2.01	0.76
14:N:211:LEU:HD23	14:N:333:SER:HB2	1.68	0.76
16:P:221:ARG:HD2	16:P:286:ARG:HD2	1.68	0.76
32:g:145:ILE:HG23	41:p:160:LYS:HE2	1.66	0.76
43:r:12:ARG:HH21	43:r:21:GLN:NE2	1.82	0.76
46:Ab:407:MET:HG2	46:Ab:411:THR:OG1	1.85	0.76
33:h:175:GLU:HB3	33:h:177:GLU:HG2	1.65	0.76
51:AG:31:PHE:HA	51:AG:35:ILE:CD1	2.16	0.76
2:B:170:TYR:HE2	4:D:135:TYR:CD2	2.03	0.76
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
13:M:344:MET:HE1	38:m:59:HIS:NE2	1.99	0.76
14:N:319:LYS:HA	15:O:302:THR:HG21	1.67	0.76
49:Ae:167:PHE:HB2	49:Ae:174:LEU:HB3	1.66	0.76
8:H:92:PRO:HG3	8:H:255:TYR:HB3	1.68	0.76
10:J:122:ASP:OD2	25:Z:122:GLY:CA	2.33	0.76
12:L:232:TRP:CZ3	12:L:233:LEU:CD2	2.69	0.76
12:L:605:ASN:OD1	12:L:605:ASN:O	2.03	0.76
15:O:168:VAL:HG11	15:O:241:TYR:CE1	2.19	0.76
23:X:36:CYS:O	23:X:40:ASN:ND2	2.19	0.76
37:l:38:PRO:HB2	38:m:75:ASN:ND2	2.00	0.76
3:C:160:ILE:HD12	4:D:285:ASN:ND2	1.99	0.76
10:J:40:CYS:SG	10:J:56:PHE:HB2	2.26	0.76
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.67	0.76
46:Ab:228:SER:HA	46:Ab:231:LYS:HE2	1.68	0.76
48:Ad:291:LYS:HB3	71:Ad:402:3PH:H32	1.66	0.76
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
16:P:226:VAL:HG11	16:P:277:VAL:HG11	1.68	0.75
19:S:22:HIS:C	19:S:58:CYS:SG	2.69	0.75
48:AD:223:THR:HG21	52:AH:64:ASP:HA	1.66	0.75
48:AD:242:ILE:CD1	48:AD:244:MET:HB3	2.15	0.75
49:AE:127:TYR:CE1	53:AJ:33:GLU:HA	2.21	0.75
12:L:16:LEU:HD21	62:L:704:CDL:H591	1.68	0.75
12:L:480:LEU:HD21	35:j:82:GLY:HA3	1.65	0.75
13:M:458:THR:CG2	41:p:148:ALA:HB1	2.16	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:314:MET:HB2	15:O:305:LEU:HD11	1.68	0.75
17:Q:64:LEU:HG	22:W:84:LEU:HD12	1.68	0.75
25:Z:24:ASN:OD1	25:Z:24:ASN:O	2.04	0.75
28:c:68:GLU:HG3	29:d:19:ARG:HH21	1.52	0.75
39:n:20:TYR:CZ	39:n:24:LEU:HD11	2.21	0.75
8:H:260:MET:SD	26:a:13:GLY:HA2	2.25	0.75
12:L:387:THR:HG23	12:L:461:SER:O	1.85	0.75
12:L:513:MET:HE3	12:L:515:LYS:HG3	1.68	0.75
49:AE:127:TYR:HD1	53:AJ:33:GLU:CA	1.95	0.75
46:Ab:126:ILE:H	46:Ab:126:ILE:HD12	1.51	0.75
51:Ag:11:ILE:HG22	51:Ag:14:VAL:HG22	1.69	0.75
10:J:60:LEU:C	10:J:60:LEU:CD1	2.59	0.75
45:AA:192:PHE:O	45:AA:198:ALA:HB2	1.85	0.75
45:Aa:62:GLU:OE1	45:Aa:423:ARG:NH1	2.19	0.75
49:Ae:191:GLU:HB2	49:Ae:194:GLN:HB2	1.66	0.75
2:B:94:THR:O	57:B:302:UQ1:H111	1.86	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75
15:O:121:PRO:O	15:O:122:LYS:HG2	1.86	0.75
49:AE:175:PHE:CE2	49:AE:224:PRO:HD2	2.22	0.75
6:F:184:LYS:HB3	44:s:92:LEU:HD22	1.67	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
12:L:446:ASN:ND2	35:j:51:THR:HG21	2.01	0.75
14:N:227:ILE:HA	14:N:230:ILE:HG22	1.66	0.75
25:Z:93:GLU:HG3	30:e:97:HIS:ND1	2.00	0.75
45:Aa:68:THR:OG1	46:Ab:387:GLU:OE1	2.04	0.75
47:Ac:128:PHE:HD1	70:Ac:404:U10:C4M	1.93	0.75
49:Ae:142:ALA:HB3	49:Ae:147:LEU:CD2	2.15	0.75
51:Ag:43:ARG:HG3	55:Ag:103:3PE:H382	1.68	0.75
4:D:34:ALA:HB3	13:M:86:LYS:NZ	2.01	0.75
4:D:97:LEU:O	4:D:97:LEU:HG	1.85	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
24:Y:83:ARG:NH1	24:Y:90:LEU:HD22	2.00	0.75
42:q:25:ARG:HB3	42:q:29:ARG:HH12	1.52	0.75
45:Aa:55:ASN:HB3	45:Aa:226:ALA:CB	2.16	0.75
1:A:80:GLN:HA	27:b:46:ASN:ND2	2.00	0.75
4:D:36:GLN:NE2	13:M:135:ARG:NH1	2.34	0.75
7:G:127:ASP:HA	18:R:106:TYR:OH	1.86	0.75
8:H:304:HIS:O	8:H:308:PRO:HD3	1.87	0.75
12:L:393:ASP:OD1	12:L:394:LEU:N	2.19	0.75
12:L:482:MET:HE2	12:L:486:LEU:HB3	1.68	0.75
16:P:217:PHE:HB2	16:P:280:ILE:HD13	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:104:CYS:SG	18:R:107:CYS:HB2	2.27	0.75
47:AC:145:VAL:HG13	49:Ae:220:LEU:CB	2.17	0.75
49:Ae:218:THR:HG21	49:Ae:256:LEU:O	1.86	0.75
57:B:302:UQ1:HM22	57:B:302:UQ1:HM33	1.67	0.75
14:N:277:ILE:HG23	14:N:278:MET:H	1.50	0.75
15:O:206:TYR:HD2	15:O:257:VAL:HG13	1.52	0.75
46:Ab:115:THR:HG23	46:Ab:118:ASN:H	1.52	0.75
52:Ah:32:ARG:CD	52:Ah:76:ARG:NH1	2.44	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
12:L:362:ILE:HG23	12:L:366:MET:HE3	1.68	0.74
12:L:475:THR:HA	40:o:55:GLN:NE2	2.01	0.74
16:P:228:LEU:HD21	16:P:277:VAL:HG21	1.68	0.74
21:V:35:LEU:HD13	21:V:48:THR:HG23	1.68	0.74
23:X:128:VAL:O	23:X:128:VAL:HG23	1.87	0.74
25:Z:89:GLU:HG2	30:e:97:HIS:CD2	2.21	0.74
34:i:127:HIS:HB3	40:o:89:TYR:HE2	1.52	0.74
9:I:90:LYS:HB2	42:q:90:LEU:CD2	2.17	0.74
9:I:180:HIS:CD2	16:P:100:LEU:HD21	2.21	0.74
11:K:95:LEU:HG	14:N:54:GLU:OE2	1.87	0.74
13:M:314:MET:HA	13:M:454:ILE:HD12	1.69	0.74
15:O:66:ILE:HD11	15:O:218:ILE:HD11	1.67	0.74
15:O:117:PHE:CE1	15:O:128:SER:HB2	2.22	0.74
15:O:333:GLU:O	15:O:333:GLU:CD	2.30	0.74
18:R:31:ILE:HG12	18:R:37:VAL:HB	1.70	0.74
24:Y:71:MET:HG3	24:Y:102:THR:HG21	1.68	0.74
45:AA:62:GLU:OE1	45:AA:423:ARG:NH1	2.19	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
16:P:359:TYR:O	16:P:360:ARG:HB3	1.86	0.74
49:Ae:159:ILE:HB	49:Ae:210:TRP:CH2	2.23	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
15:O:66:ILE:CD1	15:O:67:CYS:SG	2.76	0.74
47:AC:185:LEU:HD23	47:AC:188:ILE:HD12	1.69	0.74
49:AE:123:VAL:HG13	53:AJ:29:ALA:HA	1.69	0.74
10:J:52:GLY:O	10:J:55:VAL:HG12	1.87	0.74
12:L:136:ASN:ND2	62:h:201:CDL:H273	2.01	0.74
16:P:272:LEU:HG	16:P:375:VAL:HG21	1.68	0.74
17:Q:69:GLU:O	17:Q:72:ILE:HG22	1.86	0.74
23:X:49:GLU:HG3	23:X:50:GLU:HG3	1.70	0.74
34:i:22:TRP:CD2	39:n:172:THR:HG22	2.21	0.74
45:AA:55:ASN:HB3	45:AA:226:ALA:HB1	1.68	0.74
46:AB:304:ASN:HB3	46:AB:307:SER:HB2	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Ac:402:HEM:HMA2	68:Ac:405:UQ6:C15	2.17	0.74
2:B:170:TYR:CE2	4:D:135:TYR:CG	2.75	0.74
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.01	0.74
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.70	0.74
45:Aa:55:ASN:HB3	45:Aa:226:ALA:HB1	1.68	0.74
46:Ab:429:LYS:HA	46:Ab:432:VAL:HG12	1.67	0.74
49:Ae:218:THR:HG21	49:Ae:256:LEU:C	2.13	0.74
4:D:261:MET:HE1	9:I:73:THR:CG2	2.16	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
8:H:200:LEU:HD21	8:H:282:TYR:HA	1.69	0.74
23:X:162:LYS:HB3	23:X:166:ARG:HH21	1.53	0.74
24:Y:76:THR:HG23	24:Y:95:GLY:HA3	1.70	0.74
50:AF:42:GLU:HA	50:AF:45:LYS:HD3	1.68	0.74
5:E:176:LEU:HD12	5:E:184:MET:HE3	1.69	0.74
48:AD:105:LEU:HB3	48:AD:110:ILE:HD11	1.69	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
13:M:310:MET:HG3	13:M:455:THR:HA	1.70	0.74
33:h:57:VAL:HG12	39:n:99:VAL:HG21	1.68	0.74
49:AE:220:LEU:HB3	47:Ac:145:VAL:HG22	1.68	0.74
46:Ab:297:PRO:CA	46:Ab:304:ASN:HD21	2.01	0.74
4:D:259:GLU:HG3	25:Z:25:LEU:CD2	2.17	0.74
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.22	0.74
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.69	0.74
12:L:525:LEU:HD21	39:n:77:PRO:HB3	1.68	0.74
55:L:703:3PE:H272	14:N:164:MET:HE3	1.67	0.74
16:P:55:VAL:HG21	18:R:43:TYR:CB	2.18	0.74
28:c:72:ARG:HH11	29:d:19:ARG:HD3	1.53	0.74
45:AA:55:ASN:HB3	45:AA:226:ALA:CB	2.16	0.74
1:A:67:LEU:HD11	11:K:68:ALA:HB1	1.69	0.73
3:C:118:VAL:HG12	3:C:120:THR:HG22	1.69	0.73
4:D:67:ASN:HB2	15:O:193:LEU:CD2	2.16	0.73
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.22	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.73
10:J:151:MET:HE2	14:N:28:LEU:HD13	1.70	0.73
55:L:705:3PE:H272	14:N:288:LEU:HD13	1.70	0.73
13:M:1:MET:HB2	13:M:52:PHE:CD2	2.23	0.73
13:M:260:PRO:O	13:M:264:LEU:HG	1.88	0.73
33:h:96:ALA:HB3	41:p:63:TYR:CD1	2.22	0.73
48:Ad:202:ARG:HH21	48:Ad:279:GLU:HG3	1.53	0.73
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:202:LEU:O	14:N:206:MET:HG2	1.87	0.73
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.23	0.73
19:S:42:VAL:HG13	19:S:43:GLU:CD	2.13	0.73
46:Ab:146:PHE:CD2	46:Ab:202:SER:HB3	2.18	0.73
71:Ad:402:3PH:C1	49:Ae:131:ASN:HD21	1.99	0.73
4:D:368:ARG:NH2	9:I:165:ASP:OD1	2.21	0.73
12:L:174:TYR:HE1	55:L:702:3PE:H362	1.53	0.73
13:M:200:MET:HE1	13:M:247:SER:HB2	1.69	0.73
13:M:263:LEU:HD11	38:m:102:TYR:HD1	1.53	0.73
15:O:117:PHE:HE1	15:O:173:MET:HE3	1.53	0.73
45:Aa:171:GLU:O	45:Aa:174:GLU:HG2	1.88	0.73
3:C:223:VAL:HG22	3:C:225:LEU:HD12	1.69	0.73
4:D:36:GLN:NE2	13:M:135:ARG:HH12	1.84	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.12	0.73
33:h:175:GLU:HB2	33:h:178:PHE:HD2	1.53	0.73
55:m:201:3PE:H242	55:m:201:3PE:H362	1.69	0.73
51:AG:21:PRO:HA	51:AG:24:GLN:HE21	1.54	0.73
53:AJ:23:LEU:HD13	54:AK:27:VAL:CA	2.17	0.73
8:H:92:PRO:CG	8:H:255:TYR:HB3	2.17	0.73
13:M:167:ILE:HD11	13:M:195:LEU:HD21	1.70	0.73
20:U:110:LEU:HD11	20:U:118:ILE:HD11	1.69	0.73
46:Ab:214:THR:O	46:Ab:218:MET:HG3	1.89	0.73
2:B:161:MET:HG2	2:B:196:PRO:HG2	1.70	0.73
4:D:65:PRO:HG3	4:D:70:ASP:OD1	1.88	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.52	0.73
12:L:20:LEU:HD12	12:L:20:LEU:C	2.13	0.73
20:T:119:ILE:HD12	20:T:138:LEU:HD11	1.70	0.73
24:Y:143:VAL:HG23	33:h:157:ARG:HG2	1.69	0.73
45:AA:171:GLU:O	45:AA:174:GLU:HG2	1.89	0.73
1:A:99:SER:HB3	55:A:201:3PE:H392	1.71	0.73
3:C:149:LEU:CD2	17:Q:64:LEU:CD2	2.67	0.73
10:J:75:THR:HG21	11:K:27:MET:CB	2.19	0.73
12:L:174:TYR:CD2	12:L:232:TRP:CD1	2.68	0.73
12:L:232:TRP:CZ3	12:L:233:LEU:HD23	2.23	0.73
12:L:428:TYR:OH	39:n:33:HIS:HE1	1.69	0.73
31:f:38:ARG:HH12	31:f:54:VAL:HG21	1.54	0.73
53:AJ:30:LEU:HA	54:AK:34:TRP:CD1	2.23	0.73
48:Ad:121:CYS:HA	69:Ad:401:HEC:HMC3	1.71	0.73
6:F:67:GLU:HG3	6:F:71:LYS:HE3	1.70	0.73
9:I:61:LEU:O	55:I:301:3PE:H362	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:7:LEU:HD12	25:Z:91:LEU:HD22	1.69	0.73
55:m:203:3PE:H261	55:m:203:3PE:H371	1.69	0.73
48:AD:126:SER:HB3	48:AD:178:PRO:HD2	1.70	0.73
49:Ae:239:HIS:CE1	49:Ae:253:PRO:HG3	2.23	0.73
7:G:226:CYS:HG	56:G:802:SF4:FE1	1.05	0.73
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.73
12:L:466:PHE:HE1	35:j:72:ARG:CZ	1.99	0.73
13:M:122:PHE:CD1	13:M:238:LEU:HG	2.23	0.73
48:AD:252:VAL:HG13	48:AD:253:LEU:N	2.03	0.73
49:AE:80:HIS:HD2	49:AE:81:THR:HG23	1.49	0.73
4:D:203:MET:HE1	4:D:254:ARG:HB3	1.70	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
10:J:67:PHE:CE2	11:K:75:LEU:HD21	2.24	0.73
12:L:445:GLU:OE2	35:j:54:GLN:HG3	1.89	0.73
12:L:579:ASN:OD1	12:L:579:ASN:O	2.06	0.73
13:M:441:MET:SD	13:M:444:LEU:HD23	2.29	0.73
16:P:96:LEU:HD12	16:P:97:MET:N	2.01	0.73
46:AB:173:ILE:HG21	46:AB:339:TYR:HE1	1.54	0.73
47:AC:141:TRP:CH2	49:Ae:223:VAL:HG23	2.23	0.73
48:AD:215:LEU:CD1	69:AD:401:HEC:HMB3	2.16	0.73
47:Ac:41:LEU:HD23	68:Ac:405:UQ6:C20	2.19	0.73
2:B:115:ASP:HA	2:B:119:VAL:O	1.88	0.72
12:L:9:LEU:HD22	34:i:82:VAL:HG13	1.71	0.72
30:e:95:PRO:HB2	30:e:97:HIS:HD1	1.53	0.72
32:g:106:TYR:CE2	33:h:86:ILE:HD12	2.24	0.72
68:AC:403:UQ6:H13	68:AC:403:UQ6:H101	1.71	0.72
2:B:90:LEU:O	2:B:92:PRO:HD3	1.89	0.72
8:H:111:LEU:CD2	10:J:60:LEU:CD1	2.66	0.72
10:J:71:THR:HG22	10:J:76:GLU:HB2	1.71	0.72
14:N:277:ILE:CG2	14:N:278:MET:N	2.52	0.72
15:O:80:GLN:HG3	15:O:270:VAL:CG2	2.11	0.72
16:P:134:TRP:HB3	16:P:312:PRO:HG3	1.71	0.72
36:k:34:PRO:HG2	36:k:59:TYR:HE1	1.54	0.72
41:p:7:LYS:O	41:p:11:PRO:HA	1.89	0.72
50:AF:106:GLU:O	50:AF:109:ALA:HB3	1.89	0.72
46:Ab:305:THR:CG2	46:Ab:306:THR:H	2.02	0.72
4:D:215:GLU:OE2	9:I:94:SER:HB3	1.89	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
10:J:32:LEU:HG	10:J:64:LEU:HD21	1.71	0.72
16:P:274:PHE:HE1	16:P:290:PRO:HG3	1.54	0.72
25:Z:129:THR:HB	25:Z:132:GLU:HG3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:173:ILE:HG21	46:AB:339:TYR:CE1	2.24	0.72
52:Ah:72:PHE:HZ	52:Ah:76:ARG:HD3	1.49	0.72
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.23	0.72
13:M:216:LEU:HG	13:M:220:HIS:HE1	1.48	0.72
13:M:243:MET:HE1	13:M:302:MET:HE3	1.71	0.72
14:N:215:MET:SD	14:N:248:LEU:CD2	2.77	0.72
16:P:263:PHE:CD1	16:P:333:PRO:HB2	2.24	0.72
16:P:270:ARG:HH21	16:P:327:VAL:C	1.98	0.72
37:l:152:SER:HA	40:o:5:LEU:HD21	1.69	0.72
45:Aa:478:LEU:HD23	53:Aj:18:THR:HG21	1.72	0.72
48:Ad:154:VAL:HA	48:Ad:166:MET:HA	1.70	0.72
49:Ae:187:GLU:HB3	49:Ae:201:ASP:HB3	1.71	0.72
58:B:303:PC1:H341	58:B:303:PC1:H222	1.70	0.72
3:C:45:THR:HG22	4:D:358:VAL:CG2	2.20	0.72
8:H:260:MET:HE1	26:a:16:LEU:HB2	1.70	0.72
10:J:159:LEU:HD23	11:K:69:CYS:SG	2.29	0.72
12:L:141:PHE:HD2	13:M:370:PRO:HB3	1.54	0.72
14:N:59:TYR:CE2	14:N:63:GLN:HG3	2.23	0.72
20:T:104:PHE:HB3	20:T:110:LEU:HD22	1.71	0.72
33:h:163:ARG:HG2	33:h:165:ASP:CB	2.19	0.72
45:AA:68:THR:HG21	46:AB:384:MET:HG3	1.71	0.72
1:A:65:PHE:O	1:A:68:GLU:HB2	1.90	0.72
5:E:185:VAL:HG22	5:E:195:LEU:HD13	1.72	0.72
7:G:544:MET:CE	7:G:546:PHE:HZ	2.01	0.72
9:I:154:TYR:HA	9:I:169:GLU:OE2	1.89	0.72
12:L:316:THR:CG2	12:L:325:ALA:HB2	2.18	0.72
16:P:73:LEU:HA	16:P:76:MET:HE2	1.71	0.72
21:V:28:TYR:OH	21:V:55:LYS:HD3	1.89	0.72
45:AA:384:THR:HG22	45:AA:387:GLU:HB3	1.69	0.72
48:AD:110:ILE:HG23	48:AD:273:PHE:HA	1.72	0.72
4:D:67:ASN:HB2	15:O:193:LEU:HD23	1.70	0.72
4:D:217:VAL:HG11	4:D:240:LEU:HD22	1.72	0.72
4:D:320:ILE:HD11	9:I:38:TYR:CE1	2.25	0.72
16:P:64:PHE:HE1	16:P:209:ARG:O	1.72	0.72
16:P:124:ASN:OD1	16:P:125:VAL:HG23	1.89	0.72
45:AA:249:HIS:O	45:AA:250:LEU:HB2	1.89	0.72
46:Ab:322:ASP:OD2	49:Ai:59:ALA:HB3	1.88	0.72
4:D:144:MET:SD	4:D:222:MET:CA	2.73	0.72
4:D:267:ILE:CG2	8:H:278:PRO:HG2	2.15	0.72
4:D:320:ILE:HD11	9:I:38:TYR:CD1	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.20	0.72
25:Z:93:GLU:HG2	30:e:97:HIS:CE1	2.23	0.72
26:a:58:ASN:ND2	26:a:60:TYR:HE1	1.84	0.72
28:c:72:ARG:HD2	29:d:20:SER:HA	1.70	0.72
1:A:52:SER:O	10:J:73:MET:HE1	1.90	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.72	0.72
12:L:576:LEU:HD12	12:L:577:THR:N	2.05	0.72
15:O:351:TRP:HB3	28:c:39:PRO:HG3	1.70	0.72
26:a:64:LYS:HE2	26:a:66:LEU:CB	2.19	0.72
48:AD:193:LEU:HD12	48:AD:194:PRO:HD2	1.71	0.72
51:AG:56:VAL:HA	51:AG:59:ILE:HD12	1.72	0.72
48:Ad:124:CYS:SG	69:Ad:401:HEC:HAC	2.29	0.72
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.90	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
12:L:299:LYS:HB2	12:L:354:GLN:HE21	1.55	0.72
48:AD:218:TYR:HE1	48:AD:242:ILE:HG21	1.55	0.72
46:Ab:59:SER:HB3	46:Ab:224:GLY:CA	2.20	0.72
49:Ae:176:VAL:HG22	49:Ae:212:ILE:HG23	1.71	0.72
2:B:97:LEU:HD22	2:B:141:MET:HG2	1.72	0.71
2:B:170:TYR:CE2	4:D:135:TYR:CD1	2.77	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
12:L:247:LEU:HD12	12:L:248:HIS:N	2.04	0.71
14:N:308:ASN:HB3	15:O:317:ILE:HG22	1.71	0.71
38:m:9:ALA:HB1	38:m:10:PRO:HD2	1.71	0.71
45:AA:182:VAL:HG12	45:AA:186:TYR:CE2	2.25	0.71
45:Aa:74:TRP:HZ2	45:Aa:411:GLU:HA	1.54	0.71
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.71	0.71
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.71	0.71
55:K:101:3PE:H2A2	55:K:101:3PE:H262	1.69	0.71
13:M:106:LEU:HD13	13:M:234:ILE:HG22	1.72	0.71
13:M:373:ILE:CG1	13:M:454:ILE:HD11	2.19	0.71
14:N:232:LEU:HD23	14:N:307:THR:HG23	1.70	0.71
15:O:100:ASP:OD1	15:O:101:GLY:N	2.24	0.71
48:Ad:181:ASN:HB3	48:Ad:183:GLU:CG	2.19	0.71
49:Ae:93:ARG:HD2	49:Ae:110:ARG:HD2	1.72	0.71
4:D:97:LEU:HD11	4:D:109:CYS:HB3	1.70	0.71
4:D:146:CYS:SG	4:D:178:THR:OG1	2.48	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
13:M:173:THR:HB	33:h:143:GLU:OE2	1.90	0.71
14:N:146:TYR:CD1	14:N:147:PRO:HD3	2.26	0.71
16:P:276:LEU:HD23	16:P:280:ILE:HD12	1.72	0.71
19:S:79:LEU:HA	19:S:82:LEU:HG	1.73	0.71
23:X:7:LEU:HD22	25:Z:87:LEU:CD1	2.19	0.71
46:Ab:109:LYS:HG2	46:Ab:124:GLU:HB3	1.70	0.71
1:A:22:PHE:HA	8:H:60:PRO:HG3	1.71	0.71
1:A:52:SER:OG	1:A:55:PHE:HB2	1.90	0.71
4:D:238:LEU:HB3	43:r:36:GLN:CG	2.16	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.71
8:H:45:ILE:CD1	26:a:11:ILE:HD11	2.19	0.71
8:H:51:ASP:HA	8:H:54:LYS:HB3	1.73	0.71
13:M:370:PRO:HA	13:M:375:LEU:HD23	1.72	0.71
53:AJ:23:LEU:HA	54:AK:27:VAL:HG13	1.73	0.71
45:Aa:340:SER:HB2	49:Ai:45:VAL:HG21	1.72	0.71
49:Ai:46:LYS:CG	49:Ai:47:ARG:N	2.53	0.71
12:L:141:PHE:CD2	13:M:370:PRO:HB3	2.25	0.71
13:M:313:THR:HG21	13:M:456:GLY:HA3	1.71	0.71
37:l:106:HIS:CD2	37:l:107:TRP:H	2.08	0.71
46:Ab:297:PRO:HA	46:Ab:304:ASN:CG	2.16	0.71
48:Ad:249:TYR:CZ	48:Ad:252:VAL:HA	2.25	0.71
4:D:202:TRP:HH2	4:D:261:MET:CE	2.03	0.71
7:G:266:ARG:HH12	9:I:131:GLU:HG2	1.54	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
8:H:157:ASN:ND2	8:H:165:LEU:HD11	2.06	0.71
15:O:336:GLY:H	15:O:344:ASN:ND2	1.89	0.71
15:O:354:LEU:HD21	28:c:44:VAL:HG11	1.72	0.71
47:AC:181:PHE:HA	47:AC:184:ILE:HG22	1.71	0.71
47:AC:266:PRO:O	49:Ae:237:PRO:HB3	1.90	0.71
1:A:84:THR:HG22	27:b:43:SER:HB2	1.72	0.71
3:C:120:THR:HG23	3:C:121:ARG:N	2.05	0.71
3:C:152:ILE:HD11	3:C:177:PHE:HE2	1.50	0.71
4:D:386:THR:CG2	9:I:118:LEU:HD13	2.21	0.71
7:G:651:PRO:HB2	19:S:57:GLU:O	1.89	0.71
12:L:466:PHE:CB	35:j:68:TRP:CZ2	2.57	0.71
13:M:220:HIS:CE1	13:M:231:LEU:HD23	2.26	0.71
15:O:237:ILE:HG22	15:O:241:TYR:CE2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:144:ILE:O	20:U:148:ILE:HG12	1.91	0.71
62:a:101:CDL:HA32	42:q:10:GLY:HA3	1.72	0.71
48:AD:232:TYR:CE1	48:AD:245:ALA:HA	2.24	0.71
49:Ae:207:LYS:HB2	49:Ae:210:TRP:HB2	1.73	0.71
8:H:288:LEU:HD11	55:I:301:3PE:H2	1.71	0.71
38:m:45:ARG:O	38:m:45:ARG:HG2	1.90	0.71
49:Ae:241:SER:HA	49:Ae:252:GLY:HA3	1.70	0.71
8:H:18:ALA:O	8:H:21:THR:OG1	2.07	0.71
10:J:124:LEU:HD11	25:Z:138:PHE:CZ	2.25	0.71
12:L:73:SER:HB3	41:p:100:GLN:HE21	1.55	0.71
15:O:209:VAL:HG23	15:O:214:VAL:HG13	1.72	0.71
33:h:87:THR:HA	62:h:201:CDL:H512	1.73	0.71
48:AD:145:ALA:HA	48:AD:148:LEU:HD12	1.73	0.71
48:Ad:185:ALA:HB1	48:Ad:193:LEU:HA	1.72	0.71
5:E:240:PRO:HB3	6:F:60:GLY:HA3	1.73	0.71
8:H:196:ALA:HB1	8:H:197:PRO:HD3	1.73	0.71
12:L:556:ILE:HG21	38:m:80:PHE:CE1	2.25	0.71
42:q:25:ARG:O	42:q:29:ARG:HB3	1.91	0.71
42:q:26:VAL:HG12	42:q:32:ASP:O	1.91	0.71
48:AD:313:VAL:HA	51:AG:24:GLN:HE22	1.56	0.71
45:Aa:249:HIS:O	45:Aa:250:LEU:HB2	1.89	0.71
46:Ab:167:GLN:HE22	49:Ai:46:LYS:HA	1.56	0.71
5:E:71:GLU:HG3	44:s:94:GLN:HE21	1.54	0.70
5:E:131:ILE:HD13	5:E:187:ILE:HG12	1.72	0.70
7:G:382:ARG:CZ	7:G:652:ASN:HD21	2.03	0.70
8:H:265:LEU:O	8:H:269:THR:N	2.24	0.70
12:L:368:PHE:HB3	12:L:445:GLU:CD	2.15	0.70
13:M:373:ILE:HG12	13:M:454:ILE:CD1	2.20	0.70
23:X:47:ARG:NH2	25:Z:80:ASP:OD1	2.24	0.70
47:AC:141:TRP:NE1	47:AC:263:ASN:O	2.24	0.70
50:Af:24:ALA:O	51:Ag:48:ARG:NH2	2.24	0.70
4:D:129:TYR:CE1	4:D:411:LEU:HD21	2.25	0.70
4:D:436:ASP:OD1	4:D:437:LYS:N	2.24	0.70
7:G:671:LEU:HD21	19:S:45:LYS:HG2	1.71	0.70
10:J:95:GLY:HA2	10:J:98:MET:HB3	1.73	0.70
16:P:64:PHE:CZ	16:P:242:VAL:HG21	2.26	0.70
1:A:18:ILE:HD11	8:H:76:THR:HG22	1.69	0.70
14:N:237:THR:HG23	14:N:237:THR:O	1.88	0.70
23:X:167:PHE:HB3	23:X:170:TRP:CD1	2.25	0.70
45:AA:147:LEU:HD23	45:AA:150:ILE:HD12	1.73	0.70
48:AD:215:LEU:HD11	69:AD:401:HEC:CMB	2.16	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:164:ASN:HA	49:Ae:177:ARG:CA	2.16	0.70
7:G:359:ASN:OD1	19:S:68:ARG:NH1	2.24	0.70
8:H:121:TRP:HH2	10:J:27:TYR:CE1	2.09	0.70
12:L:436:ARG:HA	36:k:58:ARG:NH1	2.07	0.70
15:O:135:LEU:HB3	15:O:139:ARG:HH12	1.57	0.70
16:P:157:LYS:HB2	16:P:195:PHE:HD1	1.55	0.70
46:Ab:106:VAL:HG11	46:Ab:132:ILE:HD11	1.72	0.70
46:Ab:167:GLN:HG2	49:Ai:43:LEU:CD1	2.20	0.70
71:Ad:402:3PH:C35	49:Ae:128:ALA:HB1	2.22	0.70
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.21	0.70
8:H:114:TYR:CE1	10:J:65:VAL:HG23	2.25	0.70
12:L:510:LYS:HE3	12:L:512:SER:HB3	1.72	0.70
16:P:174:MET:O	16:P:175:LYS:HG2	1.91	0.70
49:AE:80:HIS:CD2	49:AE:81:THR:CG2	2.69	0.70
4:D:94:VAL:HG11	4:D:116:LEU:HB2	1.73	0.70
4:D:202:TRP:HH2	4:D:261:MET:HE2	1.57	0.70
7:G:617:ARG:NH1	22:W:128:GLY:C	2.50	0.70
12:L:306:THR:HA	12:L:336:LYS:HZ2	1.57	0.70
12:L:428:TYR:HA	12:L:432:MET:CG	2.20	0.70
12:L:559:GLU:O	12:L:564:LYS:HB2	1.92	0.70
13:M:446:LEU:HD13	32:g:101:THR:HG21	1.73	0.70
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.74	0.70
45:AA:378:ARG:O	45:AA:382:SER:N	2.23	0.70
67:AC:402:HEM:HMA1	68:AC:403:UQ6:H72	1.72	0.70
46:Ab:60:ARG:N	46:Ab:223:LEU:O	2.24	0.70
1:A:80:GLN:HA	27:b:46:ASN:HD21	1.53	0.70
4:D:359:ASP:C	4:D:359:ASP:OD1	2.34	0.70
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.70
8:H:100:LEU:HD22	10:J:49:SER:HB2	1.74	0.70
11:K:1:MET:HG3	11:K:50:ASN:HD22	1.57	0.70
48:AD:126:SER:HB3	48:AD:178:PRO:CD	2.21	0.70
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.15	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:221:ARG:NH2	5:E:227:ALA:HB2	2.07	0.70
8:H:111:LEU:HD11	10:J:56:PHE:HZ	1.54	0.70
8:H:260:MET:CE	26:a:17:VAL:HG13	2.20	0.70
15:O:161:ARG:HH22	63:O:401:ADP:H5'2	1.55	0.70
19:S:42:VAL:HG22	19:S:46:LYS:HE3	1.72	0.70
23:X:130:LYS:HD3	27:b:63:MET:HG3	1.74	0.70
46:AB:293:LEU:HB3	46:AB:309:LEU:HG	1.73	0.70
48:AD:227:LEU:HD13	48:AD:231:LEU:C	2.17	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:137:GLN:HG3	47:Ac:265:PRO:HD3	1.73	0.70
48:Ad:201:VAL:HG22	48:Ad:278:SER:OG	1.91	0.70
4:D:277:VAL:HA	4:D:324:GLY:O	1.91	0.70
4:D:304:LYS:HG3	4:D:316:PHE:CZ	2.26	0.70
9:I:54:THR:HA	27:b:13:TRP:HE1	1.57	0.70
10:J:132:GLY:CA	25:Z:68:ARG:HH11	1.99	0.70
24:Y:19:GLN:HG3	24:Y:22:ARG:HB2	1.74	0.70
42:q:26:VAL:CG1	42:q:32:ASP:O	2.40	0.70
47:Ac:99:GLY:HA3	55:Ac:403:3PE:H272	1.73	0.70
18:R:70:ASN:HB2	18:R:111:PHE:HD1	1.55	0.70
25:Z:89:GLU:CG	30:e:97:HIS:NE2	2.45	0.70
31:f:56:TRP:CE3	33:h:131:LYS:HG3	2.26	0.70
48:AD:121:CYS:SG	69:AD:401:HEC:CAB	2.80	0.70
48:AD:153:GLU:HG2	48:AD:168:PRO:CB	2.17	0.70
48:AD:227:LEU:HB3	48:AD:231:LEU:HB2	1.74	0.70
46:Ab:65:VAL:HG13	46:Ab:218:MET:HG2	1.73	0.70
46:Ab:177:LEU:HD11	46:Ab:272:VAL:HG22	1.72	0.70
49:Ae:235:TYR:CE1	49:Ae:240:GLY:HA2	2.27	0.70
1:A:35:ASN:CG	1:A:36:PRO:HD2	2.16	0.69
6:F:228:PRO:CG	17:Q:160:TYR:HD2	2.05	0.69
7:G:83:GLU:O	7:G:84:LYS:HG2	1.90	0.69
12:L:285:THR:HG22	12:L:415:ALA:CB	2.21	0.69
12:L:594:ASN:CG	14:N:110:PRO:HB2	2.17	0.69
13:M:134:THR:O	13:M:142:ARG:HD2	1.91	0.69
14:N:254:LEU:HD12	14:N:255:PRO:HD3	1.72	0.69
22:W:87:ILE:HG22	22:W:91:MET:HE3	1.73	0.69
33:h:57:VAL:HG12	39:n:99:VAL:CG2	2.21	0.69
46:Ab:106:VAL:HG23	46:Ab:108:GLY:H	1.56	0.69
49:Ae:202:LEU:HA	49:Ae:205:VAL:HG22	1.74	0.69
7:G:628:GLU:OE1	22:W:122:LEU:HB2	1.92	0.69
12:L:480:LEU:HD23	12:L:480:LEU:O	1.93	0.69
13:M:447:LEU:HD21	13:M:454:ILE:HD13	1.73	0.69
15:O:206:TYR:HB3	15:O:257:VAL:HA	1.72	0.69
28:c:34:PRO:HG2	28:c:37:ALA:HB2	1.74	0.69
52:Ah:76:ARG:O	52:Ah:80:VAL:HG23	1.93	0.69
8:H:67:SER:HB2	10:J:27:TYR:OH	1.92	0.69
8:H:197:PRO:HD3	8:H:273:ILE:HG21	1.74	0.69
10:J:79:PRO:C	16:P:360:ARG:HD3	2.16	0.69
23:X:142:TYR:HA	25:Z:115:ARG:HE	1.57	0.69
32:g:106:TYR:OH	33:h:86:ILE:HG23	1.92	0.69
47:AC:147:THR:HG22	47:AC:161:VAL:HG13	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AJ:23:LEU:CG	54:AK:27:VAL:HG22	2.22	0.69
45:Aa:109:LEU:HD12	45:Aa:109:LEU:C	2.15	0.69
48:Ad:146:LYS:HE3	48:Ad:170:LYS:HA	1.75	0.69
48:Ad:159:ASN:HB2	48:Ad:164:MET:H	1.57	0.69
1:A:33:LYS:HE2	8:H:61:MET:HE2	1.74	0.69
16:P:165:ILE:HD13	16:P:253:THR:HG22	1.73	0.69
46:Ab:183:LYS:HG3	46:Ab:254:ARG:HB3	1.74	0.69
47:Ac:128:PHE:HE1	70:Ac:404:U10:C4M	2.01	0.69
49:Ae:192:VAL:HA	49:Ae:195:LEU:HD12	1.73	0.69
2:B:97:LEU:HD13	4:D:94:VAL:CG1	2.20	0.69
4:D:35:ARG:O	4:D:36:GLN:C	2.35	0.69
8:H:287:HIS:CD2	8:H:291:LYS:HD2	2.28	0.69
12:L:556:ILE:HD11	38:m:76:ILE:HG22	1.74	0.69
15:O:59:VAL:HA	15:O:157:VAL:HG22	1.71	0.69
16:P:91:ILE:HG13	16:P:95:ARG:HH12	1.57	0.69
16:P:236:VAL:CG2	16:P:270:ARG:HG2	2.22	0.69
21:V:113:LYS:O	21:V:116:ILE:HG13	1.93	0.69
44:s:89:LYS:NZ	44:s:90:PHE:CZ	2.60	0.69
45:AA:74:TRP:HZ2	45:AA:411:GLU:HA	1.54	0.69
67:Ac:402:HEM:HBA1	68:Ac:405:UQ6:C4	2.22	0.69
48:Ad:121:CYS:HB3	69:Ad:401:HEC:CAB	2.22	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
14:N:248:LEU:HD13	14:N:296:LEU:HD23	1.75	0.69
48:AD:308:ARG:HD3	51:AG:27:PHE:CE2	2.27	0.69
52:Ah:69:LEU:HD21	52:Ah:73:LEU:CD1	2.23	0.69
1:A:35:ASN:OD1	1:A:36:PRO:CD	2.36	0.69
4:D:259:GLU:HG2	25:Z:23:ARG:HD2	1.74	0.69
5:E:185:VAL:HG22	5:E:195:LEU:CD1	2.23	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
12:L:305:SER:HB2	12:L:422:TYR:HE1	1.57	0.69
16:P:226:VAL:CG1	16:P:228:LEU:HG	2.22	0.69
21:V:19:THR:HB	21:V:22:GLU:HG3	1.74	0.69
23:X:59:GLU:HA	23:X:62:LEU:HG	1.73	0.69
35:j:97:LEU:HB3	40:o:104:ARG:CB	2.16	0.69
37:l:122:THR:HG21	37:l:129:MET:HE1	1.73	0.69
37:l:158:PRO:HD3	40:o:22:ILE:HB	1.74	0.69
46:AB:183:LYS:HG3	46:AB:254:ARG:HB3	1.74	0.69
48:Ad:295:MET:CB	71:Ad:402:3PH:H341	2.18	0.69
1:A:35:ASN:HA	8:H:64:LEU:HD12	1.75	0.69
3:C:87:ILE:CG1	3:C:144:THR:CG2	2.69	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:220:ALA:HB2	9:I:98:ARG:HH21	1.58	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
10:J:76:GLU:CD	10:J:76:GLU:O	2.36	0.69
12:L:153:LEU:HD11	13:M:360:LEU:HD11	1.73	0.69
13:M:216:LEU:HD11	13:M:236:LEU:HD11	1.72	0.69
20:T:82:ARG:HD2	20:T:125:GLU:CG	2.23	0.69
20:U:87:LEU:HB2	20:U:98:LEU:HD22	1.72	0.69
23:X:7:LEU:HD22	25:Z:87:LEU:HD11	1.74	0.69
48:AD:159:ASN:HB3	48:AD:166:MET:HE2	1.75	0.69
48:AD:242:ILE:HG12	48:AD:244:MET:H	1.57	0.69
49:AE:220:LEU:HD12	49:AE:239:HIS:CE1	2.27	0.69
48:Ad:146:LYS:HD2	48:Ad:149:ALA:HB3	1.74	0.69
48:Ad:158:PRO:HG3	48:Ad:167:ARG:HB2	1.73	0.69
49:Ae:127:TYR:HE1	53:Aj:33:GLU:HG3	1.57	0.69
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.58	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
13:M:50:LYS:HE2	13:M:52:PHE:CE1	2.25	0.69
13:M:151:PHE:CZ	14:N:291:PHE:HB2	2.27	0.69
25:Z:116:TRP:O	33:h:188:ASP:OD2	2.10	0.69
36:k:34:PRO:CD	36:k:59:TYR:CD1	2.76	0.69
40:o:19:PRO:HA	40:o:22:ILE:HD11	1.74	0.69
49:AE:93:ARG:HB3	51:Ag:25:ARG:CA	2.23	0.69
51:Ag:40:ARG:HA	51:Ag:43:ARG:HD2	1.75	0.69
3:C:120:THR:CG2	21:V:116:ILE:HG21	2.18	0.69
12:L:332:HIS:NE2	12:L:336:LYS:HG3	2.07	0.69
14:N:215:MET:HE2	14:N:248:LEU:CD2	2.23	0.69
17:Q:99:MET:HE2	17:Q:126:LEU:HD12	1.73	0.69
34:i:104:ILE:HG13	40:o:48:ASP:HB3	1.75	0.69
44:s:92:LEU:HB2	44:s:93:PRO:CD	2.22	0.69
46:AB:412:VAL:HG13	46:AB:415:GLN:HE21	1.58	0.69
47:AC:48:GLY:HA3	67:AC:401:HEM:C1B	2.28	0.69
48:AD:228:ARG:HG2	48:AD:229:GLU:HG3	1.74	0.69
49:AE:122:THR:HB	53:Aj:25:ILE:HG21	1.75	0.69
47:Ac:41:LEU:CD2	68:Ac:405:UQ6:H201	2.23	0.69
49:Ae:200:HIS:CD2	49:Ae:201:ASP:N	2.59	0.69
53:Aj:30:LEU:HD12	54:Ak:34:TRP:HB2	1.73	0.69
4:D:255:ILE:HG12	4:D:337:MET:HE2	1.74	0.68
6:F:194:ASP:OD2	44:s:91:ARG:HB3	1.93	0.68
7:G:617:ARG:NH1	22:W:129:HIS:N	2.39	0.68
8:H:203:GLY:O	8:H:207:LEU:HB2	1.93	0.68
12:L:312:LEU:HD21	12:L:395:ILE:HG21	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:113:GLY:HA2	48:AD:270:VAL:HA	1.74	0.68
45:Aa:310:ILE:HG21	45:Aa:379:LEU:HD21	1.73	0.68
49:Ae:159:ILE:HB	49:Ae:210:TRP:HH2	1.57	0.68
5:E:178:ALA:HB3	5:E:184:MET:SD	2.34	0.68
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.68
8:H:121:TRP:CH2	10:J:27:TYR:CE1	2.81	0.68
8:H:196:ALA:C	8:H:198:PHE:N	2.47	0.68
12:L:18:PRO:O	12:L:21:ILE:HG22	1.92	0.68
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.75	0.68
15:O:140:LEU:HG	15:O:304:VAL:HG12	1.74	0.68
24:Y:77:CYS:SG	24:Y:78:VAL:N	2.66	0.68
46:AB:115:THR:HG22	49:AI:65:VAL:HG22	1.76	0.68
49:Ae:162:GLY:H	49:Ae:178:HIS:CD2	2.12	0.68
8:H:155:LEU:O	8:H:315:PRO:HG2	1.94	0.68
11:K:1:MET:HG3	11:K:50:ASN:ND2	2.08	0.68
13:M:369:LEU:HD12	13:M:370:PRO:HD3	1.74	0.68
14:N:215:MET:HE1	14:N:248:LEU:HD21	1.71	0.68
20:T:111:ASP:H	20:T:114:ASP:HB2	1.58	0.68
21:V:106:GLU:HG3	21:V:107:PRO:HD2	1.74	0.68
38:m:48:LEU:HB3	39:n:166:LEU:HD23	1.75	0.68
1:A:84:THR:O	1:A:87:MET:HG2	1.93	0.68
12:L:211:ILE:N	12:L:212:PRO:HD2	2.08	0.68
13:M:255:LYS:NZ	29:d:117:HIS:HB3	2.08	0.68
20:U:110:LEU:CD1	20:U:118:ILE:CD1	2.71	0.68
37:l:78:LEU:HD11	37:l:104:PRO:HB2	1.74	0.68
45:AA:464:GLN:HA	51:AG:5:PHE:HB3	1.75	0.68
48:AD:135:LEU:HA	48:AD:276:TRP:CH2	2.26	0.68
47:Ac:146:ILE:HG13	70:Ac:404:U10:H4M2	1.74	0.68
47:Ac:244:LEU:CD1	48:Ad:289:GLY:HA2	2.21	0.68
52:Ah:38:LEU:HB2	52:Ah:41:CYS:SG	2.32	0.68
7:G:652:ASN:HB3	7:G:655:ARG:HH22	1.57	0.68
10:J:9:SER:HB2	11:K:7:ASN:ND2	2.09	0.68
13:M:446:LEU:HD13	32:g:101:THR:CG2	2.23	0.68
15:O:60:ILE:HD12	15:O:203:ALA:HB3	1.73	0.68
20:U:134:ASP:OD2	39:n:2:ALA:N	2.26	0.68
25:Z:98:MET:CG	30:e:92:TYR:CE1	2.76	0.68
47:AC:114:ASN:HA	47:AC:117:VAL:HG22	1.74	0.68
50:AF:33:MET:O	50:AF:36:ASP:HB2	1.93	0.68
46:Ab:412:VAL:HG13	46:Ab:415:GLN:HE21	1.58	0.68
49:Ae:127:TYR:CE1	53:Aj:33:GLU:HG3	2.29	0.68
1:A:66:ASP:CG	10:J:58:ILE:HD13	2.18	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
8:H:111:LEU:HD23	10:J:60:LEU:HD11	1.72	0.68
24:Y:96:GLY:HA3	24:Y:121:GLY:HA2	1.75	0.68
25:Z:92:GLU:O	25:Z:96:ILE:N	2.26	0.68
51:AG:35:ILE:O	51:AG:39:LEU:HG	1.92	0.68
48:Ad:158:PRO:HB2	48:Ad:164:MET:HB3	1.75	0.68
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.68
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.75	0.68
12:L:383:MET:SD	12:L:384:PRO:HD2	2.33	0.68
12:L:446:ASN:HD21	35:j:51:THR:HG21	1.56	0.68
55:M:501:3PE:H241	14:N:277:ILE:HD12	1.75	0.68
15:O:323:GLN:HE22	32:g:54:GLN:HB3	1.58	0.68
16:P:61:ALA:HB3	16:P:82:ILE:HG23	1.76	0.68
16:P:252:ALA:HB2	16:P:338:LEU:HD21	1.76	0.68
23:X:48:TRP:CE2	27:b:55:VAL:HG22	2.29	0.68
24:Y:143:VAL:CG2	33:h:157:ARG:HG2	2.23	0.68
26:a:58:ASN:HB3	26:a:60:TYR:HD1	1.58	0.68
27:b:31:ILE:HA	27:b:34:MET:HE2	1.76	0.68
42:q:137:TRP:CH2	42:q:140:PRO:HD3	2.29	0.68
47:Ac:29:SER:HB2	62:Ag:102:CDL:H712	1.74	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
7:G:382:ARG:HH21	7:G:386:LEU:HD11	1.59	0.68
13:M:379:LEU:O	13:M:383:MET:HG3	1.93	0.68
15:O:224:PRO:HA	15:O:227:MET:HE3	1.74	0.68
15:O:246:LEU:HG	15:O:255:VAL:HG11	1.76	0.68
47:AC:287:LYS:NZ	49:Ae:255:PRO:HG2	2.07	0.68
47:AC:287:LYS:HZ1	49:Ae:255:PRO:HG2	1.57	0.68
49:AE:164:ASN:HB2	49:AE:234:TYR:OH	1.94	0.68
47:Ac:29:SER:OG	62:Ag:101:CDL:HA61	1.94	0.68
47:Ac:147:THR:HG22	47:Ac:161:VAL:HG13	1.75	0.68
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.76	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.74	0.68
13:M:311:GLY:HA2	13:M:314:MET:HE3	1.76	0.68
13:M:369:LEU:HD12	13:M:370:PRO:CD	2.24	0.68
26:a:18:ILE:N	26:a:19:PRO:CD	2.55	0.68
47:AC:256:TYR:CD2	48:AD:202:ARG:HB3	2.28	0.68
48:AD:149:ALA:HB1	48:AD:170:LYS:C	2.18	0.68
45:Aa:338:CYS:N	45:Aa:368:MET:SD	2.67	0.68
3:C:63:TYR:CZ	3:C:67:ILE:HD11	2.28	0.68
3:C:223:VAL:HG22	3:C:225:LEU:HD13	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:9:LEU:HD21	55:i:201:3PE:H2A1	1.76	0.68
13:M:39:LEU:HD23	13:M:67:ILE:HD13	1.74	0.68
13:M:388:TRP:CE2	38:m:109:ARG:HD2	2.29	0.68
15:O:38:TYR:HB3	15:O:299:GLN:HE22	1.58	0.68
46:Ab:123:VAL:HG21	46:Ab:133:LEU:HB3	1.76	0.68
46:Ab:297:PRO:CA	46:Ab:304:ASN:ND2	2.57	0.68
2:B:202:LEU:HD23	9:I:86:TYR:CD1	2.30	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
10:J:130:ASP:HB2	25:Z:79:LYS:CE	2.24	0.67
12:L:228:GLY:C	12:L:229:LEU:HG	2.19	0.67
25:Z:93:GLU:OE2	30:e:97:HIS:HE1	1.77	0.67
29:d:5:ARG:HD2	29:d:89:ASP:OD2	1.93	0.67
46:AB:233:VAL:HA	46:AB:236:GLN:HG2	1.76	0.67
47:AC:137:GLN:HG3	47:AC:265:PRO:HG3	1.76	0.67
48:AD:111:ARG:HG3	48:AD:140:TYR:CZ	2.29	0.67
52:AH:39:GLU:HA	52:AH:42:VAL:HB	1.75	0.67
47:Ac:16:HIS:CE1	47:Ac:201:HIS:NE2	2.62	0.67
48:Ad:164:MET:HE3	48:Ad:166:MET:HB2	1.76	0.67
2:B:171:TYR:CD1	4:D:135:TYR:HE1	2.12	0.67
9:I:89:GLU:OE1	42:q:58:ARG:HG2	1.94	0.67
9:I:123:CYS:SG	56:I:302:SF4:FE2	1.79	0.67
12:L:203:PHE:CZ	41:p:110:LEU:HD11	2.30	0.67
20:U:119:ILE:HD11	20:U:138:LEU:HB2	1.76	0.67
32:g:140:PHE:CE2	41:p:74:ILE:HG22	2.28	0.67
33:h:96:ALA:O	41:p:63:TYR:HE1	1.77	0.67
45:AA:397:ASN:HD21	46:AB:126:ILE:HD11	1.58	0.67
47:AC:16:HIS:CE1	47:AC:201:HIS:NE2	2.62	0.67
47:AC:137:GLN:HE21	47:AC:264:THR:HA	1.59	0.67
47:Ac:92:ILE:HG13	47:Ac:272:TRP:CH2	2.30	0.67
1:A:31:SER:HB2	1:A:33:LYS:HG3	1.76	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
12:L:80:PHE:C	12:L:135:ASN:ND2	2.52	0.67
13:M:275:ILE:HD11	13:M:288:TYR:CD1	2.29	0.67
14:N:26:LEU:HD23	14:N:29:MET:SD	2.35	0.67
16:P:266:THR:HG21	16:P:329:PRO:HB3	1.76	0.67
32:g:109:ASP:CB	32:g:114:GLU:HB3	2.24	0.67
32:g:140:PHE:CE2	41:p:74:ILE:CG2	2.76	0.67
37:l:122:THR:HG23	37:l:123:PRO:HD2	1.75	0.67
48:Ad:170:LYS:HD2	49:Ae:151:LYS:HE2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:121:TRP:HH2	10:J:27:TYR:HE1	1.43	0.67
14:N:25:ASN:ND2	30:e:18:PHE:CE2	2.63	0.67
14:N:149:LEU:HD13	14:N:154:ILE:HG21	1.75	0.67
15:O:114:LEU:HA	15:O:131:LEU:CD2	2.24	0.67
15:O:347:VAL:O	15:O:347:VAL:CG1	2.42	0.67
26:a:32:GLY:HA3	26:a:60:TYR:CD2	2.30	0.67
42:q:39:VAL:HG21	42:q:89:TRP:CH2	2.30	0.67
48:AD:242:ILE:HD11	48:AD:244:MET:HB3	1.76	0.67
45:Aa:281:ALA:HB2	51:Ag:10:ARG:HH22	1.59	0.67
51:Ag:19:LEU:HD11	51:Ag:23:GLU:CG	2.24	0.67
6:F:199:ARG:HD3	44:s:80:PHE:CE2	2.30	0.67
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
8:H:314:VAL:HG23	25:Z:58:ARG:HH21	1.59	0.67
13:M:30:TYR:O	13:M:34:ILE:HG12	1.95	0.67
14:N:342:GLN:HE21	29:d:30:ARG:HH11	1.41	0.67
16:P:266:THR:HG21	16:P:329:PRO:CG	2.25	0.67
28:c:72:ARG:HD2	29:d:20:SER:CA	2.25	0.67
47:AC:198:LEU:HD21	47:Ac:10:LEU:N	2.09	0.67
53:AJ:23:LEU:CA	54:AK:27:VAL:HG22	2.24	0.67
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HA	1.75	0.67
51:Ag:11:ILE:CG2	51:Ag:14:VAL:HG22	2.25	0.67
4:D:86:PRO:HG3	4:D:96:ARG:HG2	1.76	0.67
13:M:142:ARG:NH2	14:N:303:THR:HG22	2.08	0.67
36:k:55:GLU:CD	39:n:34:ARG:HD2	2.19	0.67
37:l:106:HIS:HD2	37:l:107:TRP:H	1.43	0.67
51:AG:79:GLU:HG3	52:AH:58:ARG:HD3	1.75	0.67
45:Aa:102:LYS:HB2	45:Aa:153:ASN:O	1.95	0.67
46:Ab:116:ARG:HH22	46:Ab:175:GLU:HA	1.59	0.67
48:Ad:186:ARG:HB3	48:Ad:191:GLY:HA2	1.76	0.67
49:Ae:239:HIS:CE1	49:Ae:253:PRO:CB	2.78	0.67
54:Ak:6:LEU:HA	54:Ak:11:ARG:NH1	2.09	0.67
4:D:36:GLN:HE21	4:D:38:GLN:NE2	1.93	0.67
5:E:129:TYR:HA	5:E:188:ASN:HD21	1.60	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.48	0.67
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.29	0.67
12:L:511:LEU:HD12	39:n:36:LYS:HA	1.75	0.67
13:M:98:MET:HE2	13:M:131:ILE:HB	1.77	0.67
15:O:124:ASN:O	32:g:51:MET:SD	2.53	0.67
19:S:40:ARG:HA	19:S:43:GLU:OE1	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:105:LYS:HD3	25:Z:108:GLU:OE1	1.94	0.67
45:Aa:342:GLN:HE21	45:Aa:357:HIS:HB3	1.59	0.67
48:Ad:232:TYR:CD1	48:Ad:245:ALA:HA	2.30	0.67
49:Ae:273:VAL:O	49:Ae:274:GLY:C	2.38	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
8:H:317:TYR:CD2	10:J:134:MET:HE1	2.30	0.67
9:I:171:PRO:HB3	42:q:93:MET:CE	2.04	0.67
12:L:81:LYS:N	12:L:135:ASN:ND2	2.43	0.67
13:M:11:LEU:HB3	13:M:100:ILE:HD13	1.77	0.67
16:P:166:HIS:CD2	16:P:191:VAL:HG21	2.29	0.67
48:AD:179:TYR:HB3	48:AD:184:ALA:HB3	1.77	0.67
52:AH:82:HIS:HB3	52:AH:83:LYS:HZ2	1.60	0.67
48:Ad:93:SER:HA	48:Ad:209:ASP:OD2	1.95	0.67
1:A:68:GLU:OE2	1:A:98:LEU:HD22	1.95	0.67
2:B:169:GLY:O	2:B:170:TYR:C	2.36	0.67
2:B:195:PRO:O	2:B:196:PRO:C	2.35	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:117:ALA:HB1	6:F:131:MET:SD	2.35	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
12:L:552:LEU:CD2	12:L:553:LEU:HD12	2.25	0.67
14:N:313:MET:CG	15:O:305:LEU:HD22	2.25	0.67
29:d:14:LEU:O	29:d:14:LEU:CD1	2.37	0.67
30:e:14:LEU:CD1	30:e:15:ASP:HB2	2.25	0.67
3:C:223:VAL:HG21	3:C:225:LEU:CD1	2.17	0.67
5:E:131:ILE:HG23	5:E:170:LEU:HA	1.77	0.67
5:E:197:PRO:HA	5:E:200:ILE:HD12	1.77	0.67
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.67
9:I:210:LEU:CD1	43:r:39:PRO:O	2.35	0.67
10:J:59:TYR:OH	11:K:34:GLU:HB3	1.94	0.67
11:K:66:PHE:HZ	14:N:35:PHE:CZ	2.12	0.67
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.60	0.67
15:O:66:ILE:HD12	15:O:67:CYS:HG	1.59	0.67
24:Y:76:THR:HG22	24:Y:92:TYR:HA	1.77	0.67
43:r:8:ILE:O	43:r:11:LEU:HB2	1.95	0.67
49:AE:177:ARG:HD2	49:AE:234:TYR:OH	1.95	0.67
51:AG:9:ALA:C	51:AG:11:ILE:HD12	2.20	0.67
1:A:52:SER:O	10:J:73:MET:CE	2.43	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
55:L:703:3PE:C36	14:N:164:MET:HE1	2.24	0.66
13:M:114:GLU:HG3	23:X:169:PHE:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:270:ILE:HG22	13:M:271:MET:HE2	1.76	0.66
13:M:285:LEU:HD13	13:M:342:MET:HE1	1.76	0.66
33:h:102:PRO:HD2	33:h:105:TYR:HB2	1.77	0.66
48:AD:249:TYR:CE1	48:AD:252:VAL:HG23	2.30	0.66
46:Ab:45:ASN:HD22	46:Ab:239:ASN:HA	1.59	0.66
48:Ad:121:CYS:HB3	69:Ad:401:HEC:HAB	1.77	0.66
2:B:107:MET:HE3	2:B:114:MET:HE2	1.77	0.66
5:E:192:TYR:HB3	5:E:195:LEU:HD21	1.78	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.95	0.66
13:M:361:MET:CB	13:M:441:MET:HE3	2.25	0.66
15:O:66:ILE:HD11	15:O:218:ILE:CD1	2.24	0.66
55:i:201:3PE:H342	55:i:201:3PE:H2B1	1.77	0.66
55:m:201:3PE:H2	55:m:201:3PE:H241	1.78	0.66
40:o:89:TYR:CE2	40:o:93:LEU:HD11	2.30	0.66
45:AA:87:ASN:HB3	45:AA:204:PRO:HD2	1.77	0.66
45:AA:116:ILE:HG21	45:AA:142:LYS:HG2	1.77	0.66
45:AA:342:GLN:HE21	45:AA:357:HIS:HB3	1.59	0.66
45:Aa:341:PHE:CZ	45:Aa:372:LEU:HD13	2.31	0.66
47:Ac:346:PRO:HG3	51:Ag:66:GLU:HG2	1.78	0.66
1:A:26:GLN:HG3	58:B:304:PC1:H232	1.77	0.66
2:B:113:ASP:OD1	8:H:34:ARG:HD3	1.94	0.66
8:H:121:TRP:HE1	10:J:76:GLU:CG	2.08	0.66
8:H:230:ASN:CB	8:H:233:LEU:HD12	2.25	0.66
12:L:201:ILE:HG22	12:L:266:LEU:HD11	1.76	0.66
13:M:173:THR:CG2	33:h:147:ALA:CB	2.69	0.66
14:N:307:THR:O	15:O:319:ILE:N	2.28	0.66
16:P:176:SER:H	16:P:182:ARG:HG2	1.60	0.66
20:U:128:PHE:CZ	20:U:148:ILE:HD12	2.31	0.66
24:Y:71:MET:HG3	24:Y:102:THR:CG2	2.26	0.66
29:d:106:LYS:HB3	41:p:79:GLU:HB3	1.77	0.66
46:AB:109:LYS:HD2	49:AI:71:ASN:HD22	1.60	0.66
47:AC:169:SER:HB3	49:Ae:172:LYS:HD2	1.78	0.66
48:AD:155:GLN:NE2	48:AD:164:MET:O	2.28	0.66
46:Ab:89:LEU:HD22	46:Ab:150:GLU:HB3	1.77	0.66
48:Ad:155:GLN:H	48:Ad:165:PHE:C	2.03	0.66
49:Ae:166:ALA:HA	49:Ae:175:PHE:HA	1.77	0.66
1:A:25:PRO:CG	8:H:60:PRO:HD3	2.26	0.66
2:B:92:PRO:HB3	2:B:130:VAL:HG13	1.78	0.66
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.76	0.66
2:B:170:TYR:CE2	4:D:135:TYR:CD2	2.84	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:385:PHE:CD1	35:j:72:ARG:HG3	2.30	0.66
12:L:407:TRP:CE3	12:L:410:LEU:HD11	2.29	0.66
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.78	0.66
19:S:44:LEU:HD11	19:S:95:LEU:HD21	1.78	0.66
30:e:38:LYS:HG2	33:h:179:ILE:HG21	1.78	0.66
48:AD:110:ILE:HG12	48:AD:272:THR:HG22	1.77	0.66
47:Ac:270:PRO:HG2	47:Ac:275:LEU:HD23	1.76	0.66
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HB2	1.78	0.66
8:H:87:VAL:HG22	8:H:88:PRO:HD3	1.78	0.66
8:H:203:GLY:O	8:H:207:LEU:C	2.38	0.66
15:O:343:TYR:HD1	15:O:352:ILE:HG23	1.59	0.66
34:i:101:LYS:HG2	41:p:116:ARG:O	1.95	0.66
1:A:2:ASN:HB2	25:Z:143:TYR:HE1	1.60	0.66
2:B:164:CYS:HA	2:B:168:GLY:O	1.95	0.66
2:B:202:LEU:CD2	9:I:86:TYR:CG	2.79	0.66
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.26	0.66
10:J:165:ILE:HG23	14:N:42:PRO:HG3	1.78	0.66
16:P:227:PRO:HB2	16:P:298:TYR:CE1	2.30	0.66
18:R:97:LYS:HE3	18:R:100:LYS:HD3	1.78	0.66
31:f:41:SER:O	31:f:45:GLN:HB2	1.96	0.66
37:l:38:PRO:HG2	38:m:71:ALA:HB2	1.77	0.66
41:p:70:ARG:CZ	41:p:91:GLN:HE21	2.09	0.66
43:r:6:ARG:O	43:r:9:GLN:HG2	1.96	0.66
45:AA:196:PRO:O	45:AA:199:GLN:HG2	1.95	0.66
2:B:168:GLY:HA3	2:B:172:HIS:CD2	2.30	0.66
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.66
8:H:92:PRO:HG3	8:H:255:TYR:CB	2.25	0.66
12:L:141:PHE:CD2	13:M:375:LEU:HD21	2.30	0.66
13:M:318:ALA:HB2	13:M:373:ILE:HG23	1.75	0.66
16:P:187:GLY:HA2	16:P:190:GLU:HG2	1.78	0.66
20:T:93:ILE:HG13	20:T:110:LEU:HG	1.78	0.66
23:X:133:THR:HG22	23:X:134:ASP:H	1.60	0.66
30:e:86:LEU:HB3	30:e:91:LYS:HB2	1.78	0.66
46:AB:229:VAL:O	46:AB:232:GLN:HG2	1.95	0.66
48:Ad:177:LYS:HE3	48:Ad:180:PRO:HB3	1.77	0.66
4:D:266:ARG:HH21	9:I:60:ILE:CA	2.08	0.66
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.61	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.66
12:L:25:ASN:OD1	12:L:25:ASN:O	2.14	0.66
12:L:116:ARG:HG2	12:L:120:TYR:CE2	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:243:MET:HG2	29:d:44:MET:HE2	1.77	0.66
15:O:200:PRO:HG3	15:O:282:PRO:HD2	1.77	0.66
16:P:171:ASN:CB	16:P:327:VAL:HB	2.16	0.66
45:AA:397:ASN:HD21	46:AB:126:ILE:CD1	2.08	0.66
47:AC:141:TRP:HD1	47:AC:265:PRO:HD3	1.59	0.66
46:Ab:305:THR:HG23	46:Ab:306:THR:HG23	1.77	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
12:L:552:LEU:HD23	12:L:553:LEU:HD12	1.77	0.66
15:O:40:LEU:HG	15:O:292:HIS:CE1	2.31	0.66
16:P:209:ARG:HA	16:P:352:VAL:HG12	1.78	0.66
20:T:123:GLU:CD	20:T:130:ILE:H	2.03	0.66
26:a:7:PRO:O	26:a:11:ILE:HD12	1.95	0.66
46:Ab:341:ILE:CD1	49:Ai:59:ALA:HB2	2.25	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
8:H:10:LEU:HD22	8:H:83:LEU:HG	1.78	0.66
8:H:111:LEU:HD23	10:J:60:LEU:CD1	2.25	0.66
16:P:301:ILE:HG22	16:P:305:PHE:HE2	1.61	0.66
30:e:38:LYS:CE	33:h:181:HIS:HD2	2.09	0.66
48:AD:128:ASP:HA	48:AD:177:LYS:HE2	1.78	0.66
1:A:60:ILE:HD13	10:J:166:ILE:HG21	1.78	0.65
58:B:303:PC1:H112	42:q:75:TRP:CE3	2.31	0.65
8:H:184:MET:HA	8:H:293:PHE:HE2	1.62	0.65
9:I:90:LYS:HD3	42:q:91:HIS:CE1	2.31	0.65
11:K:22:PHE:HB2	12:L:585:LYS:HG2	1.76	0.65
12:L:553:LEU:HD21	38:m:93:ALA:C	2.21	0.65
13:M:373:ILE:CD1	13:M:454:ILE:HD11	2.25	0.65
37:l:101:TRP:NE1	38:m:62:ASP:HA	2.11	0.65
48:AD:249:TYR:CZ	48:AD:252:VAL:HA	2.31	0.65
53:AJ:30:LEU:CD1	54:AK:34:TRP:HB2	2.26	0.65
5:E:151:LEU:CD1	5:E:200:ILE:HG21	2.26	0.65
6:F:227:PRO:HG3	7:G:94:MET:SD	2.35	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
8:H:99:ASN:O	8:H:100:LEU:HB2	1.96	0.65
9:I:89:GLU:HG2	42:q:61:TRP:CB	2.26	0.65
12:L:66:TRP:HZ3	12:L:68:TRP:CD1	2.14	0.65
12:L:142:ILE:HA	13:M:370:PRO:HB2	1.78	0.65
13:M:175:ASN:HD22	33:h:143:GLU:HG2	1.61	0.65
13:M:350:MET:HG2	39:n:99:VAL:HG12	1.77	0.65
15:O:73:LEU:HD22	15:O:207:ILE:HD11	1.78	0.65
23:X:18:VAL:HA	23:X:68:LEU:HD21	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:92:THR:O	41:p:4:SER:HB2	1.96	0.65
47:AC:8:HIS:CE1	47:Ac:199:PHE:HZ	2.14	0.65
13:M:47:GLU:OE2	41:p:93:ARG:HB3	1.96	0.65
13:M:367:LEU:CD2	13:M:408:MET:HE2	2.25	0.65
23:X:24:VAL:HG12	23:X:86:TRP:CD1	2.31	0.65
42:q:67:GLU:HG2	42:q:72:ASN:HA	1.78	0.65
45:AA:388:VAL:HG21	45:AA:438:ALA:HB2	1.78	0.65
48:AD:164:MET:HG3	48:AD:165:PHE:H	1.60	0.65
48:Ad:184:ALA:HA	48:Ad:187:ALA:HB3	1.77	0.65
2:B:100:CYS:HB2	2:B:134:ALA:HB1	1.77	0.65
2:B:170:TYR:HD1	9:I:153:ILE:HD13	1.60	0.65
8:H:114:TYR:CZ	10:J:65:VAL:HG23	2.31	0.65
12:L:190:SER:HB2	12:L:196:TRP:HE1	1.60	0.65
15:O:38:TYR:CE2	15:O:292:HIS:HD2	2.14	0.65
16:P:64:PHE:CZ	16:P:242:VAL:CG2	2.79	0.65
20:T:87:LEU:HD13	20:T:98:LEU:HD11	1.79	0.65
20:T:105:MET:HE2	20:T:139:MET:HG2	1.79	0.65
38:m:15:PRO:CG	38:m:18:LEU:HD12	2.27	0.65
40:o:25:PHE:HB3	40:o:26:PRO:HD2	1.78	0.65
48:AD:189:ASN:CB	69:AD:401:HEC:HMD2	2.23	0.65
52:AH:58:ARG:CD	52:AH:61:THR:HB	2.26	0.65
2:B:98:ALA:HB3	2:B:101:ALA:H	1.61	0.65
4:D:192:LEU:CD1	4:D:200:PHE:HB2	2.25	0.65
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.78	0.65
7:G:338:VAL:CG1	7:G:546:PHE:CE1	2.72	0.65
12:L:141:PHE:CE2	13:M:370:PRO:CG	2.73	0.65
12:L:387:THR:HG22	12:L:465:GLY:H	1.61	0.65
55:M:502:3PE:H2A1	62:h:201:CDL:H202	1.78	0.65
14:N:258:THR:HB	14:N:333:SER:O	1.96	0.65
18:R:70:ASN:HB2	18:R:111:PHE:CD1	2.31	0.65
23:X:132:LYS:HB3	27:b:59:ASP:HB3	1.78	0.65
23:X:147:ARG:HH12	30:e:39:GLU:HG3	1.62	0.65
30:e:38:LYS:HE3	33:h:181:HIS:CD2	2.31	0.65
45:AA:463:GLU:CD	51:AG:8:LEU:HB2	2.21	0.65
46:Ab:307:SER:HB2	46:Ab:310:SER:HB2	1.78	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
7:G:652:ASN:CB	7:G:655:ARG:NH2	2.60	0.65
14:N:220:MET:C	14:N:223:ASN:H	2.04	0.65
32:g:108:PRO:O	32:g:109:ASP:OD1	2.13	0.65
45:AA:463:GLU:OE2	51:AG:8:LEU:HG	1.97	0.65
46:AB:117:GLU:OE2	46:AB:331:SER:N	2.22	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:177:LEU:HD11	46:AB:272:VAL:HG22	1.77	0.65
48:AD:122:SER:HA	48:AD:125:HIS:O	1.97	0.65
48:AD:140:TYR:HA	48:AD:144:GLU:OE1	1.97	0.65
49:AE:118:THR:OG1	53:AJ:21:PHE:CZ	2.35	0.65
10:J:33:ILE:CG2	10:J:60:LEU:HD21	2.26	0.65
25:Z:127:LEU:HD22	30:e:83:ARG:HH21	1.61	0.65
31:f:38:ARG:NH1	31:f:54:VAL:HG21	2.11	0.65
37:l:38:PRO:CB	38:m:75:ASN:HD22	2.03	0.65
49:AE:122:THR:CB	53:AJ:25:ILE:HG21	2.27	0.65
45:Aa:74:TRP:HH2	45:Aa:410:CYS:HG	1.41	0.65
45:Aa:341:PHE:CE1	45:Aa:372:LEU:HD13	2.32	0.65
2:B:109:ALA:HB1	2:B:110:PRO:HD2	1.79	0.65
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.78	0.65
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.77	0.65
7:G:614:GLY:O	22:W:129:HIS:HE1	1.80	0.65
8:H:92:PRO:HG3	8:H:255:TYR:CG	2.32	0.65
8:H:303:TRP:HE3	27:b:29:ALA:HB2	1.61	0.65
12:L:88:LEU:HD23	12:L:326:PHE:CE2	2.32	0.65
17:Q:75:ARG:HH22	17:Q:104:ARG:HG3	1.61	0.65
35:j:92:TRP:CZ3	40:o:100:LYS:HA	2.32	0.65
36:k:34:PRO:CG	36:k:59:TYR:CE1	2.72	0.65
40:o:71:ARG:HB3	40:o:71:ARG:HH11	1.61	0.65
1:A:17:LEU:HD13	8:H:225:MET:HE1	1.78	0.65
12:L:13:ILE:HD11	55:i:201:3PE:C2C	2.26	0.65
12:L:368:PHE:HB3	12:L:445:GLU:OE2	1.97	0.65
12:L:594:ASN:HD21	14:N:110:PRO:HB2	1.57	0.65
15:O:38:TYR:HB3	15:O:299:GLN:NE2	2.12	0.65
15:O:343:TYR:CE1	15:O:355:LYS:HB2	2.32	0.65
36:k:38:VAL:HG13	39:n:39:TYR:HB2	1.76	0.65
45:AA:403:LEU:HD12	45:AA:403:LEU:N	2.12	0.65
46:AB:299:ILE:H	46:AB:299:ILE:HD12	1.62	0.65
48:AD:127:MET:HE3	48:AD:198:SER:HA	1.79	0.65
49:Ae:239:HIS:CD2	49:Ae:239:HIS:O	2.49	0.65
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.27	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
8:H:198:PHE:HD1	8:H:285:LEU:HD13	1.61	0.65
8:H:311:THR:HG22	25:Z:51:MET:HG3	1.79	0.65
13:M:122:PHE:HD1	13:M:238:LEU:HG	1.62	0.65
24:Y:137:LEU:HD23	24:Y:138:PHE:CG	2.31	0.65
32:g:106:TYR:OH	33:h:86:ILE:HD12	1.97	0.65
34:i:110:ILE:HD13	41:p:16:ARG:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:24:THR:HG22	41:p:26:LEU:H	1.62	0.65
45:Aa:403:LEU:HD12	45:Aa:403:LEU:N	2.12	0.65
47:Ac:238:ILE:HD12	62:Ag:102:CDL:H772	1.79	0.65
48:Ad:315:LYS:O	50:Af:72:ARG:NH1	2.26	0.65
2:B:126:ARG:NH2	8:H:63:PRO:HB3	2.12	0.64
4:D:47:PHE:HB3	14:N:227:ILE:CD1	2.16	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:90:PRO:CG	8:H:240:ILE:HD13	2.27	0.64
13:M:300:SER:HB3	13:M:381:ILE:HG23	1.78	0.64
33:h:127:ASP:OD1	33:h:127:ASP:O	2.15	0.64
49:Ae:166:ALA:HB2	49:Ae:175:PHE:CD1	2.31	0.64
49:Ae:199:GLN:O	49:Ae:248:ARG:HD3	1.96	0.64
3:C:152:ILE:HD12	3:C:153:ASP:O	1.97	0.64
4:D:259:GLU:CG	25:Z:25:LEU:HD11	2.27	0.64
10:J:109:TYR:O	10:J:110:ASP:C	2.40	0.64
11:K:70:GLU:HA	14:N:38:LEU:HD21	1.78	0.64
11:K:96:LEU:O	11:K:97:GLN:C	2.40	0.64
12:L:141:PHE:CE2	13:M:375:LEU:HD22	2.12	0.64
13:M:167:ILE:O	13:M:171:VAL:HG12	1.98	0.64
13:M:307:TRP:CD1	13:M:459:MET:SD	2.91	0.64
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.78	0.64
47:AC:266:PRO:C	49:Ae:237:PRO:HB2	2.22	0.64
71:Ad:402:3PH:H382	49:Ae:128:ALA:HB1	1.79	0.64
49:Ae:122:THR:HG21	53:Aj:25:ILE:HD13	1.79	0.64
4:D:136:PHE:HA	4:D:139:LEU:HD12	1.80	0.64
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.62	0.64
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.80	0.64
12:L:81:LYS:N	12:L:135:ASN:HD21	1.96	0.64
13:M:119:TYR:CD1	13:M:160:LEU:HD22	2.32	0.64
15:O:117:PHE:CE1	15:O:173:MET:CE	2.77	0.64
15:O:194:THR:HG23	15:O:307:TYR:HB2	1.79	0.64
37:l:122:THR:CG2	37:l:123:PRO:HD2	2.27	0.64
41:p:74:ILE:HD13	41:p:85:ILE:HG13	1.80	0.64
48:Ad:290:LEU:O	48:Ad:294:LEU:HG	1.97	0.64
48:Ad:299:LEU:HD12	71:Ad:402:3PH:C37	2.27	0.64
1:A:60:ILE:CD1	10:J:166:ILE:HG21	2.26	0.64
2:B:169:GLY:C	2:B:171:TYR:N	2.51	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
7:G:572:HIS:HB2	7:G:699:SER:OG	1.97	0.64
12:L:247:LEU:CD1	12:L:248:HIS:NE2	2.52	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:366:MET:CG	12:L:443:ILE:HG21	2.28	0.64
33:h:175:GLU:HB2	33:h:178:PHE:CD2	2.31	0.64
35:j:97:LEU:O	40:o:104:ARG:NH1	2.29	0.64
43:r:68:ILE:HG13	43:r:68:ILE:O	1.97	0.64
47:AC:145:VAL:CG1	49:Ae:220:LEU:HB3	2.27	0.64
45:Aa:463:GLU:OE1	51:Ag:8:LEU:HB2	1.98	0.64
4:D:113:ILE:HG21	4:D:432:LEU:CD2	2.27	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
8:H:98:LEU:HD21	55:H:401:3PE:H2	1.78	0.64
12:L:174:TYR:CE1	55:L:702:3PE:H331	2.32	0.64
12:L:246:LEU:HD12	12:L:246:LEU:C	2.22	0.64
16:P:114:ASP:HA	16:P:117:ARG:HB2	1.80	0.64
23:X:133:THR:HG21	23:X:135:ARG:CZ	2.26	0.64
29:d:60:ARG:O	29:d:61:GLN:C	2.40	0.64
29:d:109:TYR:HA	29:d:112:ILE:CG2	2.28	0.64
33:h:57:VAL:HG22	39:n:104:LEU:HD11	1.78	0.64
46:AB:426:LYS:O	46:AB:429:LYS:HG2	1.97	0.64
46:Ab:171:THR:HA	49:Ai:64:LEU:HD21	1.78	0.64
52:Ah:39:GLU:HG2	52:Ah:40:LYS:N	2.12	0.64
52:Ah:45:ARG:NH1	52:Ah:48:LEU:CD2	2.48	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:401:LEU:HD21	7:G:432:ILE:CD1	2.28	0.64
10:J:122:ASP:CG	25:Z:122:GLY:HA2	2.22	0.64
13:M:458:THR:HG22	41:p:148:ALA:HB1	1.79	0.64
14:N:179:MET:HG3	14:N:216:PHE:HE1	1.63	0.64
25:Z:59:ARG:HG2	27:b:81:LEU:HG	1.79	0.64
35:j:47:PHE:HA	36:k:63:PHE:CZ	2.33	0.64
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.33	0.64
8:H:145:THR:O	8:H:149:ILE:HG12	1.97	0.64
12:L:40:ILE:HD13	12:L:97:THR:HG22	1.79	0.64
14:N:37:LEU:HD12	14:N:63:GLN:HB3	1.79	0.64
32:g:139:TYR:HB2	41:p:142:ARG:CZ	2.28	0.64
41:p:5:TRP:HH2	41:p:12:GLU:OE1	1.81	0.64
47:AC:144:THR:HG22	49:Ae:221:GLY:HA3	1.80	0.64
48:AD:235:PRO:HA	48:AD:240:GLN:HG3	1.78	0.64
51:AG:9:ALA:CB	51:AG:11:ILE:CD1	2.74	0.64
51:Ag:64:ASN:O	51:Ag:68:GLU:HG2	1.97	0.64
2:B:92:PRO:CB	2:B:122:ARG:HH12	2.11	0.64
2:B:138:THR:HG21	4:D:116:LEU:HA	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:ARG:HD2	3:C:148:GLU:OE2	1.98	0.64
4:D:266:ARG:HH22	9:I:63:TRP:HA	1.62	0.64
5:E:176:LEU:HB2	5:E:184:MET:HE1	1.80	0.64
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.80	0.64
10:J:104:CYS:HA	10:J:107:ASN:HB2	1.80	0.64
12:L:41:LYS:HG3	12:L:98:TRP:CE2	2.33	0.64
15:O:99:GLY:CA	28:c:30:TYR:HD1	2.11	0.64
18:R:112:LYS:O	18:R:113:GLN:C	2.40	0.64
34:i:89:HIS:HB3	55:i:201:3PE:H122	1.79	0.64
47:AC:211:LEU:CD2	50:AF:37:THR:HA	2.28	0.64
45:Aa:182:VAL:HG12	45:Aa:186:TYR:CE2	2.33	0.64
46:Ab:426:LYS:O	46:Ab:429:LYS:HG2	1.97	0.64
48:Ad:114:PHE:HE1	48:Ad:175:PHE:CE2	2.15	0.64
48:Ad:222:PRO:CB	52:Ah:65:CYS:HB3	2.28	0.64
1:A:24:LEU:CD1	58:B:304:PC1:H3B2	2.28	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
7:G:571:HIS:CD2	7:G:572:HIS:HD2	2.11	0.64
13:M:160:LEU:HD11	13:M:203:PHE:CZ	2.33	0.64
13:M:196:TRP:HZ3	13:M:261:PHE:HE2	1.44	0.64
15:O:168:VAL:CG2	15:O:241:TYR:CE1	2.77	0.64
15:O:168:VAL:CG2	15:O:241:TYR:CZ	2.62	0.64
18:R:36:GLN:NE2	42:q:127:TYR:HB3	2.13	0.64
24:Y:143:VAL:O	33:h:158:ARG:NH2	2.31	0.64
32:g:139:TYR:CD1	41:p:142:ARG:NH2	2.65	0.64
48:Ad:158:PRO:HG2	48:Ad:164:MET:HG3	1.79	0.64
3:C:63:TYR:CE2	3:C:67:ILE:HD11	2.33	0.64
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.77	0.64
6:F:224:ARG:NH1	17:Q:164:PHE:CD1	2.66	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.13	0.64
8:H:307:LEU:HD23	8:H:310:PHE:CZ	2.33	0.64
13:M:368:ALA:HB1	13:M:375:LEU:CD1	2.25	0.64
14:N:220:MET:HA	14:N:223:ASN:HA	1.79	0.64
14:N:313:MET:HG3	15:O:305:LEU:HD22	1.80	0.64
19:S:44:LEU:HD11	19:S:95:LEU:CD2	2.28	0.64
20:T:106:LYS:HD2	20:T:106:LYS:N	2.13	0.64
21:V:8:THR:HG23	21:V:8:THR:O	1.97	0.64
23:X:151:ASN:HD22	33:h:165:ASP:HA	1.62	0.64
34:i:29:SER:HB2	34:i:32:GLU:OE1	1.96	0.64
45:AA:101:THR:HG22	45:AA:154:SER:HA	1.78	0.64
48:AD:148:LEU:HA	48:AD:151:GLU:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:122:THR:HB	53:AJ:25:ILE:CG2	2.28	0.64
49:AE:122:THR:HG21	53:AJ:25:ILE:HG21	1.79	0.64
49:AE:218:THR:CG2	49:AE:256:LEU:O	2.45	0.64
47:Ac:99:GLY:HA3	55:Ac:403:3PE:H2A1	1.80	0.64
1:A:23:TRP:CZ3	1:A:24:LEU:HD23	2.33	0.63
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.80	0.63
14:N:143:ILE:HA	14:N:194:LEU:HD11	1.79	0.63
15:O:342:GLY:HA3	28:c:36:ASN:OD1	1.98	0.63
19:S:63:PRO:HB2	19:S:79:LEU:HD12	1.80	0.63
62:a:101:CDL:H521	42:q:3:LEU:HD13	1.80	0.63
31:f:41:SER:OG	33:h:134:GLU:HG2	1.99	0.63
37:l:106:HIS:CD2	37:l:107:TRP:N	2.67	0.63
37:l:119:THR:HG22	38:m:13:THR:HG23	1.79	0.63
55:m:201:3PE:H11	55:m:202:3PE:H331	1.81	0.63
47:AC:195:VAL:HG13	47:Ac:10:LEU:HD22	1.80	0.63
48:AD:107:HIS:CG	48:AD:138:VAL:HB	2.32	0.63
48:Ad:232:TYR:O	48:Ad:242:ILE:HG22	1.98	0.63
52:Ah:32:ARG:HG2	52:Ah:80:VAL:HG21	1.78	0.63
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.80	0.63
5:E:230:LEU:HD21	6:F:48:ARG:NE	2.13	0.63
6:F:174:ARG:HB2	44:s:87:LEU:HD11	1.80	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
12:L:305:SER:HB2	12:L:422:TYR:CE1	2.34	0.63
12:L:381:THR:HG21	12:L:498:PHE:CE2	2.33	0.63
13:M:220:HIS:NE2	13:M:231:LEU:HB3	2.13	0.63
13:M:250:LEU:O	13:M:250:LEU:CD1	2.44	0.63
20:U:72:PRO:HG3	35:j:42:PRO:HG2	1.79	0.63
30:e:38:LYS:HG2	33:h:179:ILE:CG2	2.28	0.63
47:AC:138:MET:HB2	47:AC:254:ASP:HB2	1.80	0.63
48:AD:221:PRO:HB3	48:AD:233:PHE:CD1	2.34	0.63
4:D:116:LEU:HG	4:D:116:LEU:O	1.97	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
12:L:100:ILE:HD13	12:L:341:MET:SD	2.38	0.63
12:L:202:MET:HE3	12:L:265:PRO:CG	2.25	0.63
62:L:704:CDL:H772	13:M:371:PRO:HG3	1.78	0.63
13:M:118:PHE:O	13:M:122:PHE:N	2.25	0.63
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.32	0.63
16:P:227:PRO:HB2	16:P:298:TYR:CZ	2.33	0.63
20:U:140:CYS:SG	20:U:143:GLU:OE2	2.53	0.63
23:X:83:THR:O	23:X:87:THR:OG1	2.10	0.63
30:e:75:ARG:O	30:e:79:ILE:HG13	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:63:ASN:OD1	39:n:106:TYR:HE1	1.82	0.63
47:AC:137:GLN:NE2	47:AC:141:TRP:HE1	1.94	0.63
47:AC:343:VAL:HG21	49:Ae:239:HIS:HD2	1.63	0.63
46:Ab:163:ALA:HB1	49:Ai:43:LEU:CD2	2.28	0.63
48:Ad:133:ARG:HD3	48:Ad:172:SER:HA	1.81	0.63
71:Ad:402:3PH:H262	71:Ad:402:3PH:H332	1.79	0.63
1:A:32:GLU:OE2	1:A:35:ASN:HB2	1.98	0.63
4:D:137:ASP:OD2	4:D:223:HIS:HB3	1.98	0.63
5:E:230:LEU:HD21	6:F:48:ARG:HE	1.63	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
7:G:449:PRO:HG3	7:G:483:ARG:HH22	1.62	0.63
12:L:80:PHE:C	12:L:135:ASN:HD21	2.06	0.63
12:L:410:LEU:HD12	12:L:411:ILE:N	2.13	0.63
12:L:433:THR:HG22	12:L:434:LYS:N	2.14	0.63
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.80	0.63
18:R:76:ILE:HD11	18:R:92:TYR:HB3	1.80	0.63
20:U:86:VAL:HB	20:U:122:MET:HE1	1.79	0.63
23:X:7:LEU:CD2	25:Z:87:LEU:CD1	2.77	0.63
43:r:6:ARG:HA	43:r:9:GLN:HG2	1.81	0.63
2:B:108:ALA:HA	2:B:114:MET:HG2	1.80	0.63
6:F:35:LEU:HD23	6:F:40:ARG:HG2	1.81	0.63
7:G:126:LEU:HD23	7:G:126:LEU:H	1.64	0.63
7:G:130:ILE:CA	9:I:140:ARG:HH12	2.01	0.63
8:H:95:LEU:HG	8:H:96:ILE:HG23	1.80	0.63
27:b:65:ASP:O	27:b:66:VAL:C	2.41	0.63
31:f:38:ARG:NH1	31:f:54:VAL:CG2	2.62	0.63
32:g:75:ASP:OD1	32:g:76:SER:N	2.32	0.63
36:k:34:PRO:HG2	36:k:59:TYR:CD1	2.34	0.63
39:n:95:GLU:HA	39:n:98:LYS:HG3	1.81	0.63
45:AA:468:TYR:HE1	45:AA:472:ARG:HH11	1.46	0.63
48:AD:233:PHE:CE2	48:AD:235:PRO:HD3	2.34	0.63
48:AD:237:PHE:CD1	48:AD:238:PRO:HD2	2.34	0.63
48:AD:263:MET:HE3	52:AH:28:LEU:HD23	1.80	0.63
10:J:116:LEU:HD23	10:J:123:TRP:CD2	2.34	0.63
12:L:56:HIS:O	40:o:71:ARG:HG3	1.99	0.63
13:M:1:MET:HB2	13:M:52:PHE:HD2	1.60	0.63
13:M:105:LEU:O	13:M:109:THR:HG23	1.98	0.63
14:N:149:LEU:HD13	14:N:154:ILE:CG2	2.28	0.63
14:N:308:ASN:CB	15:O:317:ILE:HG22	2.28	0.63
15:O:227:MET:C	15:O:228:LYS:HG2	2.23	0.63
15:O:305:LEU:HD12	15:O:305:LEU:C	2.24	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:217:VAL:HG11	4:D:240:LEU:CD2	2.29	0.63
4:D:315:GLU:HB3	4:D:346:GLN:HE22	1.62	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.33	0.63
13:M:129:THR:HG21	13:M:235:LEU:HD13	1.80	0.63
16:P:335:LEU:HB3	16:P:340:VAL:HB	1.81	0.63
44:s:87:LEU:HA	44:s:90:PHE:HD2	1.64	0.63
45:AA:467:ASP:OD2	47:AC:223:TYR:CE2	2.52	0.63
47:AC:128:PHE:CZ	47:AC:143:ALA:HA	2.34	0.63
45:Aa:80:ARG:NH2	45:Aa:268:CYS:SG	2.72	0.63
1:A:18:ILE:HD11	8:H:76:THR:HG23	1.73	0.63
7:G:617:ARG:HH11	22:W:129:HIS:HA	1.63	0.63
10:J:18:GLY:O	10:J:23:PRO:HD3	1.98	0.63
10:J:75:THR:HG21	11:K:27:MET:HB3	1.79	0.63
12:L:361:ASN:OD1	12:L:361:ASN:O	2.17	0.63
13:M:73:LEU:CD2	13:M:103:GLN:NE2	2.61	0.63
16:P:207:PHE:CE2	16:P:241:TYR:HD1	2.17	0.63
23:X:142:TYR:HB3	25:Z:115:ARG:HH21	1.62	0.63
33:h:155:GLU:O	33:h:159:LEU:HD13	1.99	0.63
34:i:28:LEU:HD22	34:i:32:GLU:HG2	1.79	0.63
47:Ac:77:TRP:HZ2	48:Ad:284:HIS:CD2	2.16	0.63
48:Ad:249:TYR:CE1	48:Ad:252:VAL:HA	2.34	0.63
1:A:52:SER:OG	1:A:55:PHE:CD2	2.52	0.63
2:B:137:LEU:HD22	2:B:145:LEU:CD2	2.29	0.63
3:C:189:ASP:OD1	3:C:190:TYR:N	2.32	0.63
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.81	0.63
4:D:386:THR:HG23	9:I:118:LEU:HD13	1.81	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.29	0.63
8:H:70:LEU:HA	8:H:73:ILE:HG22	1.79	0.63
12:L:357:ARG:NH1	39:n:78:GLN:O	2.32	0.63
12:L:556:ILE:HG23	38:m:80:PHE:CE2	2.34	0.63
13:M:391:PHE:HE2	55:m:202:3PE:H261	1.61	0.63
14:N:100:MET:HE3	14:N:111:PHE:CZ	2.34	0.63
14:N:131:LEU:O	14:N:135:LYS:HG2	1.98	0.63
14:N:158:ALA:O	14:N:162:ILE:HG12	1.98	0.63
20:T:102:SER:O	20:T:141:PRO:HD3	1.98	0.63
24:Y:19:GLN:NE2	24:Y:22:ARG:HG2	2.09	0.63
26:a:4:GLU:O	26:a:7:PRO:HD2	1.99	0.63
41:p:66:ARG:HD2	41:p:68:TYR:CZ	2.34	0.63
50:AF:78:LYS:HA	50:AF:81:TRP:CE2	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AJ:30:LEU:HA	54:AK:34:TRP:CG	2.33	0.63
5:E:183:PRO:HB2	5:E:195:LEU:N	2.14	0.62
10:J:125:MET:HE2	10:J:128:VAL:HG21	1.80	0.62
23:X:51:LYS:HB3	33:h:188:ASP:HA	1.80	0.62
43:r:5:THR:HG22	43:r:7:VAL:HG12	1.81	0.62
48:AD:152:VAL:HG11	48:AD:176:PRO:HG3	1.79	0.62
49:AE:175:PHE:HE2	49:AE:224:PRO:HD2	1.64	0.62
53:Aj:23:LEU:HD13	54:Ak:27:VAL:HG22	1.81	0.62
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:189:THR:HB	8:H:234:MET:HB3	1.80	0.62
10:J:77:GLU:OE1	11:K:87:THR:O	2.16	0.62
10:J:124:LEU:CG	25:Z:137:ASN:HD21	2.13	0.62
14:N:246:LEU:HD11	55:N:401:3PE:C3A	2.30	0.62
16:P:169:HIS:H	16:P:184:LYS:HE3	1.64	0.62
17:Q:59:LEU:N	17:Q:59:LEU:HD12	2.15	0.62
23:X:31:HIS:HB2	23:X:70:PHE:HZ	1.64	0.62
23:X:151:ASN:ND2	33:h:165:ASP:HA	2.14	0.62
37:l:38:PRO:C	38:m:75:ASN:ND2	2.58	0.62
38:m:49:LEU:HD12	38:m:49:LEU:O	1.99	0.62
39:n:141:GLN:O	39:n:144:THR:HG22	1.99	0.62
40:o:26:PRO:HB2	40:o:29:LEU:HB2	1.81	0.62
49:AE:234:TYR:HB2	49:AE:243:TYR:HB2	1.79	0.62
46:Ab:176:ASN:HB3	46:Ab:258:ILE:HD11	1.81	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.28	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
10:J:12:PHE:HE2	11:K:42:ILE:CD1	2.12	0.62
10:J:22:LYS:HB2	11:K:23:ARG:HD3	1.81	0.62
12:L:445:GLU:HB2	12:L:450:LEU:CD2	2.29	0.62
15:O:161:ARG:NH2	63:O:401:ADP:H5'2	2.15	0.62
19:S:20:ARG:HG2	19:S:66:TRP:HB2	1.81	0.62
30:e:101:ARG:NH2	30:e:104:PRO:HD2	2.14	0.62
45:AA:362:ALA:HB2	45:AA:461:PRO:HB2	1.81	0.62
47:AC:223:TYR:O	48:AD:311:TRP:NE1	2.32	0.62
48:AD:215:LEU:HD21	69:AD:401:HEC:CMB	2.29	0.62
49:AE:93:ARG:HB3	51:AG:25:ARG:N	2.14	0.62
52:AH:48:LEU:HD13	52:AH:69:LEU:HA	1.81	0.62
2:B:106:HIS:CE1	4:D:211:PHE:HE2	2.17	0.62
4:D:376:GLU:OE1	7:G:151:SER:HB2	1.99	0.62
6:F:254:ILE:HA	6:F:262:PHE:CE1	2.35	0.62
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:130:ASP:OD2	25:Z:79:LYS:HE2	1.99	0.62
12:L:9:LEU:HG	55:i:201:3PE:H2C1	1.80	0.62
13:M:123:GLU:HB3	14:N:255:PRO:HG2	1.81	0.62
13:M:307:TRP:CE3	13:M:383:MET:HE3	2.34	0.62
14:N:275:CYS:SG	24:Y:139:PRO:HG2	2.38	0.62
17:Q:82:PRO:HD3	17:Q:98:LYS:HG3	1.81	0.62
26:a:52:ARG:HG3	26:a:57:VAL:C	2.23	0.62
45:AA:74:TRP:HH2	45:AA:410:CYS:HG	1.44	0.62
45:AA:169:LEU:HD11	45:AA:209:ARG:HG2	1.81	0.62
47:AC:69:ILE:HG12	47:AC:73:VAL:HG21	1.82	0.62
48:AD:95:PRO:HA	48:AD:99:ARG:HH21	1.63	0.62
45:Aa:169:LEU:HD11	45:Aa:209:ARG:HG2	1.82	0.62
47:Ac:323:ILE:HD11	55:Ag:103:3PE:H12	1.80	0.62
52:Ah:44:ALA:O	52:Ah:48:LEU:N	2.32	0.62
3:C:126:GLU:OE2	3:C:143:LYS:HD3	1.99	0.62
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:136:GLU:HG2	17:Q:85:ASN:HD21	1.64	0.62
7:G:176:CYS:SG	56:G:802:SF4:FE4	1.78	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.62
12:L:211:ILE:HG13	55:m:201:3PE:H272	1.81	0.62
12:L:365:ILE:HD11	12:L:366:MET:HE2	1.82	0.62
13:M:307:TRP:HD1	13:M:459:MET:SD	2.23	0.62
13:M:318:ALA:CB	13:M:373:ILE:HG23	2.29	0.62
15:O:113:SER:HB3	15:O:116:LYS:HB2	1.80	0.62
16:P:244:ASP:HB3	16:P:335:LEU:HD13	1.82	0.62
16:P:266:THR:HG21	16:P:329:PRO:CB	2.29	0.62
16:P:276:LEU:HD23	16:P:280:ILE:CD1	2.30	0.62
23:X:86:TRP:CZ2	26:a:64:LYS:HA	2.34	0.62
27:b:78:LEU:HD22	27:b:80:TRP:NE1	2.10	0.62
31:f:56:TRP:CZ3	33:h:131:LYS:HG3	2.35	0.62
40:o:18:ASP:OD1	40:o:19:PRO:HD2	1.99	0.62
52:AH:69:LEU:O	52:AH:73:LEU:HG	2.00	0.62
45:Aa:100:GLY:C	45:Aa:101:THR:HG23	2.24	0.62
2:B:81:LEU:HG	8:H:53:MET:SD	2.39	0.62
6:F:228:PRO:HG2	17:Q:160:TYR:CD2	2.31	0.62
7:G:388:ASN:H	7:G:514:ASN:HB2	1.65	0.62
7:G:652:ASN:C	7:G:652:ASN:OD1	2.42	0.62
13:M:129:THR:HG21	13:M:235:LEU:CD1	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:121:PRO:O	15:O:122:LYS:CG	2.46	0.62
15:O:132:GLN:HE22	15:O:169:PHE:HB2	1.64	0.62
20:U:71:ALA:HB1	20:U:72:PRO:HD2	1.81	0.62
21:V:27:LEU:O	21:V:31:THR:HG23	2.00	0.62
23:X:7:LEU:HD13	25:Z:87:LEU:HD12	1.81	0.62
34:i:93:LYS:HD3	55:i:201:3PE:H121	1.81	0.62
39:n:168:TRP:O	39:n:172:THR:OG1	2.18	0.62
45:AA:114:GLU:HG2	46:AB:299:ILE:HD11	1.82	0.62
45:Aa:204:PRO:HB2	45:Aa:206:GLU:OE1	1.98	0.62
45:Aa:478:LEU:CD2	53:Aj:18:THR:HG21	2.28	0.62
71:Ad:402:3PH:H352	49:Ae:128:ALA:HB1	1.81	0.62
4:D:250:ASN:HA	43:r:23:LYS:HD3	1.82	0.62
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.82	0.62
11:K:4:THR:HG23	11:K:5:PHE:N	2.14	0.62
55:K:101:3PE:H3D2	12:L:593:ILE:HD13	1.81	0.62
14:N:109:ALA:CB	14:N:110:PRO:HD3	2.30	0.62
14:N:207:ILE:O	14:N:211:LEU:HG	2.00	0.62
14:N:307:THR:HB	15:O:319:ILE:CG1	2.30	0.62
23:X:8:PRO:HD2	25:Z:84:LEU:HD11	1.81	0.62
46:AB:176:ASN:HB3	46:AB:258:ILE:HD11	1.82	0.62
49:AE:130:LYS:HB3	53:AJ:33:GLU:CD	2.25	0.62
45:Aa:274:GLU:HG3	45:Aa:456:VAL:HB	1.80	0.62
46:Ab:65:VAL:HG22	46:Ab:218:MET:HG2	1.82	0.62
49:Ae:239:HIS:ND1	49:Ae:253:PRO:CB	2.62	0.62
2:B:97:LEU:HA	4:D:94:VAL:HG22	1.80	0.62
3:C:103:THR:HG21	21:V:55:LYS:CE	2.28	0.62
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:51:LYS:HA	25:Z:33:TYR:CE2	2.35	0.62
10:J:9:SER:HB3	11:K:7:ASN:ND2	2.06	0.62
16:P:297:VAL:O	16:P:301:ILE:HG12	2.00	0.62
16:P:363:SER:HB3	22:W:51:HIS:CE1	2.35	0.62
45:AA:99:LYS:HG3	45:AA:160:GLN:HG2	1.82	0.62
49:AE:132:VAL:HA	49:AE:135:GLN:HE21	1.65	0.62
52:AH:51:CYS:SG	52:AH:68:GLU:HB2	2.39	0.62
45:Aa:451:ASP:OD2	53:Aj:16:ARG:HG3	2.00	0.62
46:Ab:106:VAL:HG21	46:Ab:133:LEU:HD21	1.81	0.62
51:Ag:11:ILE:CG2	51:Ag:14:VAL:HG21	2.18	0.62
2:B:184:ILE:HG22	2:B:185:VAL:HG13	1.82	0.62
2:B:207:GLN:HG3	2:B:210:ARG:HH21	1.65	0.62
3:C:186:ILE:HG23	3:C:187:LEU:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:260:MET:CE	26:a:13:GLY:C	2.70	0.62
10:J:75:THR:HG21	11:K:27:MET:HB2	1.81	0.62
13:M:395:LEU:HD21	38:m:101:TRP:CE2	2.35	0.62
33:h:96:ALA:CB	41:p:63:TYR:HD1	2.12	0.62
38:m:127:ILE:CG2	41:p:136:THR:HG23	2.30	0.62
45:AA:399:LEU:HB3	45:AA:426:LEU:CD2	2.30	0.62
47:AC:148:ASN:CB	49:Ae:220:LEU:HA	2.28	0.62
45:Aa:362:ALA:HB2	45:Aa:461:PRO:HB2	1.81	0.62
47:Ac:223:TYR:O	48:Ad:311:TRP:NE1	2.33	0.62
49:Ae:229:GLY:HA2	49:Ae:242:HIS:ND1	2.14	0.62
52:Ah:47:ARG:HG2	52:Ah:50:LEU:HD12	1.82	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
4:D:202:TRP:CD2	9:I:76:TYR:HE2	2.18	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
12:L:187:VAL:HG22	13:M:383:MET:HG2	1.82	0.62
13:M:56:PHE:HE1	13:M:108:MET:HG2	1.64	0.62
14:N:335:MET:O	14:N:335:MET:CG	2.41	0.62
15:O:117:PHE:HE1	15:O:128:SER:HB2	1.63	0.62
16:P:263:PHE:HD1	16:P:333:PRO:HB2	1.65	0.62
22:W:104:THR:O	22:W:108:ARG:HG3	1.99	0.62
23:X:164:GLY:O	23:X:165:THR:C	2.41	0.62
38:m:17:THR:O	38:m:18:LEU:HB2	1.99	0.62
38:m:111:ARG:NE	55:m:202:3PE:H31	2.14	0.62
47:AC:145:VAL:CG2	49:Ae:222:CYS:SG	2.88	0.62
47:Ac:244:LEU:HD13	48:Ad:289:GLY:CA	2.23	0.62
52:Ah:41:CYS:O	52:Ah:45:ARG:N	2.33	0.62
4:D:80:MET:HB3	4:D:101:LEU:HB2	1.82	0.61
4:D:259:GLU:CB	25:Z:25:LEU:HD11	2.30	0.61
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.61
10:J:135:LEU:CD1	11:K:54:MET:CE	2.77	0.61
12:L:556:ILE:CG2	38:m:80:PHE:CZ	2.82	0.61
14:N:23:SER:HB2	30:e:15:ASP:OD2	1.99	0.61
19:S:22:HIS:O	19:S:58:CYS:SG	2.58	0.61
41:p:5:TRP:CH2	41:p:12:GLU:OE1	2.53	0.61
43:r:9:GLN:HA	43:r:12:ARG:HG2	1.80	0.61
46:AB:38:LEU:HD11	46:AB:396:ILE:HD13	1.81	0.61
48:AD:215:LEU:HD23	48:AD:244:MET:HE2	1.82	0.61
45:Aa:136:LEU:HD21	46:Ab:380:ALA:HA	1.81	0.61
45:Aa:182:VAL:CG1	45:Aa:186:TYR:CE2	2.83	0.61
45:Aa:399:LEU:HB3	45:Aa:426:LEU:CD2	2.30	0.61
46:Ab:108:GLY:HA2	46:Ab:124:GLU:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:Ad:402:3PH:H352	49:Ae:128:ALA:CB	2.30	0.61
49:Ae:159:ILE:HG21	49:Ae:178:HIS:HB2	1.81	0.61
2:B:171:TYR:CE1	4:D:135:TYR:CE1	2.88	0.61
4:D:217:VAL:CG1	4:D:240:LEU:CD2	2.74	0.61
5:E:71:GLU:OE1	44:s:96:SER:HB3	2.00	0.61
5:E:222:PHE:H	5:E:225:GLU:CD	2.08	0.61
12:L:10:LEU:HD23	12:L:46:ILE:HG21	1.82	0.61
13:M:98:MET:HE3	13:M:128:PRO:HA	1.81	0.61
15:O:117:PHE:HD1	15:O:128:SER:HA	1.64	0.61
15:O:249:MET:HE3	15:O:253:CYS:SG	2.40	0.61
18:R:98:GLU:CD	18:R:98:GLU:H	2.07	0.61
20:U:128:PHE:CZ	20:U:148:ILE:HG23	2.35	0.61
21:V:9:THR:HG21	21:V:78:GLU:HB2	1.81	0.61
34:i:19:ARG:HH11	39:n:173:ARG:HH21	1.48	0.61
40:o:69:CYS:C	40:o:80:CYS:SG	2.82	0.61
47:AC:254:ASP:HA	47:AC:257:MET:HE2	1.80	0.61
45:Aa:384:THR:O	45:Aa:387:GLU:HG2	2.00	0.61
46:Ab:163:ALA:HB1	49:Ai:43:LEU:HD23	1.79	0.61
49:Ae:152:ILE:HG13	49:Ae:154:ILE:HD11	1.82	0.61
52:Ah:39:GLU:HG2	52:Ah:40:LYS:H	1.65	0.61
3:C:120:THR:HG21	21:V:116:ILE:CG2	2.22	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.61
12:L:578:THR:CG2	14:N:168:GLY:HA2	2.30	0.61
13:M:73:LEU:CB	13:M:103:GLN:OE1	2.48	0.61
13:M:81:GLN:O	13:M:85:LYS:HB2	2.01	0.61
13:M:373:ILE:H	13:M:448:THR:HG22	1.65	0.61
14:N:17:PRO:HG2	14:N:133:TRP:CE2	2.35	0.61
15:O:76:GLU:HB3	15:O:266:PRO:HB3	1.82	0.61
15:O:99:GLY:O	28:c:30:TYR:HA	2.01	0.61
15:O:140:LEU:HD11	15:O:198:TYR:CZ	2.35	0.61
17:Q:69:GLU:HA	17:Q:72:ILE:HG22	1.82	0.61
32:g:106:TYR:CZ	33:h:86:ILE:HD12	2.35	0.61
38:m:100:PHE:O	38:m:104:VAL:HG23	2.00	0.61
47:AC:16:HIS:NE2	47:AC:201:HIS:NE2	2.49	0.61
45:Aa:91:TYR:CZ	45:Aa:95:HIS:HE1	2.17	0.61
47:Ac:45:ILE:HA	67:Ac:401:HEM:HAB	1.81	0.61
49:Ae:181:LYS:HA	49:Ae:184:ILE:HD12	1.81	0.61
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.83	0.61
3:C:63:TYR:CE2	3:C:67:ILE:CD1	2.83	0.61
4:D:84:PHE:HZ	4:D:90:ALA:HB3	1.65	0.61
7:G:473:MET:CE	7:G:514:ASN:HD21	2.12	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:288:LEU:HG	8:H:293:PHE:CE1	2.35	0.61
12:L:468:ILE:O	12:L:472:ILE:HG23	2.00	0.61
13:M:139:GLN:HB3	13:M:222:GLU:HG3	1.83	0.61
14:N:175:MET:HE1	14:N:227:ILE:HA	1.81	0.61
14:N:308:ASN:HB3	15:O:317:ILE:CG2	2.31	0.61
15:O:37:ARG:HB2	15:O:299:GLN:OE1	2.01	0.61
23:X:46:CYS:HB2	23:X:135:ARG:CZ	2.29	0.61
37:l:57:MET:HG2	37:l:104:PRO:HG2	1.82	0.61
48:AD:227:LEU:HD13	48:AD:231:LEU:O	2.00	0.61
49:AE:244:ASP:HB3	49:AE:250:ARG:HH11	1.65	0.61
46:Ab:412:VAL:O	46:Ab:415:GLN:HG2	2.00	0.61
52:Ah:51:CYS:SG	52:Ah:69:LEU:N	2.73	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.61
13:M:422:HIS:NE2	13:M:425:ASN:OD1	2.33	0.61
15:O:140:LEU:HD21	15:O:304:VAL:O	2.00	0.61
16:P:320:GLU:O	16:P:324:ILE:HG22	2.00	0.61
25:Z:82:ARG:HD2	26:a:53:ARG:NH1	2.16	0.61
25:Z:98:MET:HG2	30:e:92:TYR:CD1	2.36	0.61
35:j:102:ASP:OD1	40:o:111:ARG:HG3	1.99	0.61
46:AB:412:VAL:O	46:AB:415:GLN:HG2	2.00	0.61
48:AD:104:SER:HB2	48:AD:283:ASP:CG	2.25	0.61
45:Aa:97:ALA:O	45:Aa:98:PHE:HB2	2.00	0.61
45:Aa:463:GLU:OE2	51:Ag:6:GLY:N	2.34	0.61
50:Af:108:TRP:HA	50:Af:111:LYS:HZ2	1.64	0.61
52:Ah:32:ARG:HD3	52:Ah:76:ARG:HH11	1.59	0.61
53:Aj:23:LEU:HD22	54:Ak:23:MET:SD	2.40	0.61
1:A:66:ASP:CG	10:J:58:ILE:CD1	2.73	0.61
1:A:80:GLN:C	27:b:46:ASN:ND2	2.53	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.30	0.61
12:L:542:LEU:HD11	55:L:702:3PE:H261	1.83	0.61
12:L:559:GLU:HA	12:L:563:PRO:HG2	1.82	0.61
13:M:98:MET:HE1	13:M:128:PRO:HA	1.82	0.61
13:M:318:ALA:HB2	13:M:373:ILE:CG2	2.30	0.61
13:M:433:GLU:O	13:M:437:MET:HG2	2.01	0.61
16:P:321:ARG:O	16:P:325:SER:HB3	2.01	0.61
19:S:42:VAL:CG1	19:S:43:GLU:OE2	2.48	0.61
28:c:66:VAL:CG1	28:c:70:LYS:HE3	2.31	0.61
31:f:38:ARG:HH12	31:f:54:VAL:CG2	2.14	0.61
37:l:62:TYR:CZ	37:l:64:PRO:HG3	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:477:TRP:O	53:Aj:17:ARG:NH2	2.34	0.61
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.30	0.61
4:D:220:ALA:CB	9:I:98:ARG:HH21	2.14	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
12:L:180:ILE:HD11	13:M:400:ILE:HB	1.83	0.61
13:M:1:MET:CE	13:M:111:SER:HB2	2.29	0.61
14:N:218:ALA:HB1	14:N:240:MET:SD	2.40	0.61
20:U:72:PRO:CD	35:j:42:PRO:HG2	2.31	0.61
20:U:138:LEU:HB3	20:U:144:ILE:HG12	1.82	0.61
22:W:58:THR:HG23	22:W:61:GLN:H	1.65	0.61
25:Z:12:PRO:HD3	25:Z:16:TYR:CZ	2.35	0.61
48:AD:223:THR:CG2	52:AH:64:ASP:HA	2.31	0.61
52:AH:26:ASP:HB3	52:AH:29:THR:HG23	1.82	0.61
46:Ab:322:ASP:OD2	49:Ai:59:ALA:CB	2.47	0.61
47:Ac:16:HIS:NE2	47:Ac:201:HIS:NE2	2.49	0.61
47:Ac:137:GLN:HE21	47:Ac:264:THR:HA	1.66	0.61
48:Ad:274:LEU:HD11	69:Ad:401:HEC:HMB2	1.81	0.61
1:A:13:LEU:HD21	8:H:14:LEU:HD11	1.82	0.61
3:C:73:GLN:HG2	21:V:103:LEU:HD21	1.83	0.61
3:C:195:HIS:HE1	22:W:88:LYS:NZ	1.99	0.61
4:D:86:PRO:HA	4:D:95:LEU:O	2.00	0.61
4:D:360:ASP:OD1	4:D:360:ASP:C	2.37	0.61
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.61
7:G:614:GLY:O	22:W:129:HIS:CE1	2.54	0.61
8:H:90:PRO:HD2	8:H:240:ILE:HD13	1.81	0.61
12:L:70:THR:HG21	41:p:101:GLU:OE2	2.00	0.61
12:L:100:ILE:HG21	12:L:246:LEU:HD23	1.82	0.61
12:L:424:MET:HE2	12:L:502:LEU:CB	2.31	0.61
14:N:273:ASN:ND2	24:Y:143:VAL:HA	2.15	0.61
23:X:160:PRO:HG3	29:d:22:PRO:HD3	1.83	0.61
33:h:106:ILE:O	33:h:106:ILE:HG22	2.00	0.61
38:m:30:ARG:O	38:m:34:VAL:HG23	2.00	0.61
39:n:149:ILE:H	39:n:149:ILE:HD12	1.65	0.61
44:s:92:LEU:CB	44:s:93:PRO:HD2	2.23	0.61
48:AD:131:ALA:H	48:AD:134:HIS:HB2	1.64	0.61
48:AD:201:VAL:HG22	48:AD:278:SER:OG	2.01	0.61
2:B:97:LEU:CD1	4:D:94:VAL:HG13	2.25	0.61
3:C:223:VAL:HG23	3:C:225:LEU:CD1	2.26	0.61
5:E:243:GLY:O	6:F:257:ARG:HG3	2.00	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
8:H:138:GLN:NE2	8:H:191:ALA:O	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:190:LEU:HD13	8:H:270:PHE:CD1	2.36	0.61
12:L:174:TYR:HE1	55:L:702:3PE:H331	1.64	0.61
13:M:109:THR:HG22	13:M:121:LEU:HB3	1.82	0.61
13:M:423:MET:O	13:M:424:ILE:C	2.43	0.61
14:N:275:CYS:SG	24:Y:139:PRO:CG	2.89	0.61
32:g:109:ASP:HB3	32:g:114:GLU:HB3	1.83	0.61
38:m:25:VAL:HA	38:m:30:ARG:HD3	1.83	0.61
55:m:201:3PE:H2A1	55:m:201:3PE:H3C2	1.82	0.61
40:o:15:VAL:HG11	40:o:113:LYS:HD3	1.83	0.61
42:q:68:MET:HG3	42:q:71:LYS:HB2	1.83	0.61
47:AC:137:GLN:NE2	47:AC:264:THR:HA	2.16	0.61
47:AC:260:ASN:CG	47:AC:263:ASN:H	2.08	0.61
48:AD:89:LEU:HD13	52:AH:70:PHE:HB3	1.83	0.61
49:AE:115:TYR:HB3	53:AJ:21:PHE:CE1	2.36	0.61
45:Aa:373:GLN:O	45:Aa:377:MET:HG2	2.01	0.61
46:Ab:47:LEU:HD12	46:Ab:219:ALA:HA	1.83	0.61
3:C:84:GLU:HG2	3:C:141:ARG:HD2	1.83	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.61
12:L:538:PRO:HG2	37:l:117:VAL:HG22	1.83	0.61
13:M:209:LEU:HD23	13:M:210:TYR:N	2.16	0.61
16:P:235:THR:HG21	16:P:323:HIS:O	2.00	0.61
28:c:55:TRP:CZ2	29:d:66:THR:HG22	2.36	0.61
46:AB:100:THR:HG23	49:AI:70:LEU:HD13	1.81	0.61
48:AD:153:GLU:CG	48:AD:168:PRO:HB3	2.19	0.61
48:Ad:126:SER:HB3	48:Ad:178:PRO:HD3	1.83	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
13:M:178:ILE:HD12	33:h:143:GLU:HG3	1.83	0.60
16:P:209:ARG:O	16:P:210:GLU:HG2	2.00	0.60
28:c:66:VAL:HG12	28:c:70:LYS:HE3	1.83	0.60
37:l:108:ASP:HB3	37:l:111:MET:HE2	1.83	0.60
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.83	0.60
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.60
5:E:136:THR:HB	59:E:301:FES:S2	2.41	0.60
5:E:142:ARG:HG2	5:E:183:PRO:HD3	1.83	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
8:H:45:ILE:HD11	26:a:11:ILE:CD1	2.27	0.60
10:J:12:PHE:CZ	11:K:42:ILE:CD1	2.83	0.60
10:J:61:GLY:O	10:J:65:VAL:HB	2.02	0.60
12:L:40:ILE:HD12	12:L:101:MET:HG3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:182:PHE:CE2	12:L:186:MET:SD	2.94	0.60
12:L:482:MET:CE	12:L:486:LEU:HB3	2.31	0.60
14:N:59:TYR:CZ	14:N:63:GLN:HG3	2.36	0.60
16:P:97:MET:O	16:P:103:LEU:HD11	2.00	0.60
20:T:92:LYS:HE3	22:W:67:ARG:NH1	2.16	0.60
27:b:63:MET:HB2	27:b:66:VAL:HG12	1.83	0.60
48:Ad:201:VAL:HG22	48:Ad:278:SER:CB	2.31	0.60
48:Ad:315:LYS:C	50:Af:72:ARG:HH12	2.08	0.60
49:Ae:197:ASP:HB3	49:Ae:257:ASN:CG	2.25	0.60
4:D:35:ARG:HH22	32:g:56:ASP:C	2.09	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.82	0.60
12:L:42:PHE:O	12:L:46:ILE:HG12	2.01	0.60
16:P:228:LEU:HD13	16:P:232:GLY:HA3	1.82	0.60
24:Y:83:ARG:HH11	24:Y:90:LEU:HD22	1.66	0.60
30:e:95:PRO:HD2	30:e:98:HIS:HB2	1.82	0.60
62:h:201:CDL:H171	55:i:201:3PE:H352	1.81	0.60
46:AB:429:LYS:HA	46:AB:432:VAL:HG12	1.83	0.60
49:AE:93:ARG:CB	51:AG:25:ARG:HA	2.31	0.60
50:Af:92:GLU:HG2	50:Af:96:LYS:HE2	1.82	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
9:I:189:LYS:HG3	9:I:189:LYS:O	2.02	0.60
14:N:100:MET:HE3	14:N:111:PHE:HZ	1.66	0.60
23:X:159:LYS:O	23:X:160:PRO:C	2.43	0.60
25:Z:125:TYR:HA	25:Z:128:ARG:HD2	1.83	0.60
51:AG:43:ARG:O	51:AG:47:LEU:HG	2.02	0.60
45:Aa:104:ARG:HB3	45:Aa:108:ALA:CB	2.31	0.60
45:Aa:341:PHE:HE1	45:Aa:356:ALA:HB1	1.66	0.60
47:Ac:107:TYR:HB2	47:Ac:305:PRO:HG3	1.84	0.60
4:D:124:ILE:HG13	4:D:135:TYR:CD2	2.36	0.60
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.82	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
9:I:135:ARG:O	9:I:135:ARG:HG2	2.00	0.60
10:J:133:VAL:O	10:J:134:MET:HB2	1.99	0.60
12:L:511:LEU:CD1	39:n:36:LYS:HA	2.31	0.60
26:a:58:ASN:CB	26:a:60:TYR:CE1	2.84	0.60
37:l:162:PRO:HG3	40:o:39:MET:HE3	1.83	0.60
46:AB:45:ASN:HD21	46:AB:239:ASN:HA	1.63	0.60
47:AC:281:LEU:HD12	47:AC:290:GLY:HA3	1.82	0.60
48:AD:252:VAL:CG1	48:AD:253:LEU:N	2.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:138:LEU:HB3	46:Ab:237:PHE:HD2	1.66	0.60
51:Ag:46:ILE:HG21	55:Ag:103:3PE:H3H1	1.82	0.60
54:Ak:23:MET:O	54:Ak:27:VAL:HG23	2.02	0.60
1:A:52:SER:HB2	1:A:55:PHE:HD2	0.53	0.60
4:D:36:GLN:HA	13:M:138:ASN:HA	1.84	0.60
9:I:87:PRO:HG2	9:I:88:PHE:CD2	2.37	0.60
9:I:106:TYR:OH	18:R:88:HIS:HB3	2.01	0.60
12:L:141:PHE:CD2	13:M:370:PRO:HG3	2.35	0.60
12:L:446:ASN:HD21	35:j:51:THR:CG2	2.14	0.60
16:P:236:VAL:HG21	16:P:270:ARG:HG2	1.84	0.60
47:AC:302:ALA:O	47:AC:305:PRO:HD2	2.02	0.60
46:Ab:167:GLN:CG	49:Ai:43:LEU:HD13	2.32	0.60
48:Ad:126:SER:CB	48:Ad:177:LYS:HA	2.30	0.60
1:A:1:MET:O	1:A:4:TYR:N	2.35	0.60
7:G:382:ARG:O	7:G:383:SER:C	2.44	0.60
12:L:204:SER:HA	12:L:207:ASN:HD22	1.67	0.60
13:M:207:MET:HG3	13:M:239:GLY:HA3	1.84	0.60
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.84	0.60
14:N:224:SER:HB2	14:N:229:SER:CB	2.32	0.60
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.66	0.60
20:U:110:LEU:HD13	20:U:118:ILE:HD11	1.82	0.60
20:U:120:MET:HE1	39:n:24:LEU:HD12	1.83	0.60
21:V:75:GLY:HA3	21:V:79:GLU:OE1	2.01	0.60
45:AA:168:ILE:O	45:AA:171:GLU:HG2	2.02	0.60
45:Aa:168:ILE:O	45:Aa:171:GLU:HG2	2.01	0.60
46:Ab:225:VAL:HG11	46:Ab:230:LEU:HD21	1.83	0.60
48:Ad:158:PRO:HG2	48:Ad:166:MET:H	1.66	0.60
48:Ad:158:PRO:HA	48:Ad:167:ARG:CZ	2.31	0.60
49:Ae:207:LYS:NZ	49:Ae:268:ASP:HA	2.17	0.60
49:Ai:46:LYS:CG	49:Ai:47:ARG:H	2.15	0.60
4:D:36:GLN:HE22	13:M:135:ARG:HH11	1.45	0.60
7:G:145:MET:O	43:r:61:ARG:NH2	2.35	0.60
7:G:375:GLU:O	7:G:675:VAL:HG21	2.02	0.60
10:J:68:GLY:O	10:J:69:TYR:C	2.41	0.60
12:L:65:THR:HA	34:i:90:MET:HE2	1.83	0.60
13:M:77:LEU:HD23	13:M:99:LEU:HD12	1.83	0.60
15:O:209:VAL:HG23	15:O:214:VAL:CG1	2.31	0.60
19:S:18:GLU:CB	19:S:52:PRO:HB2	2.32	0.60
22:W:26:ARG:HB2	22:W:26:ARG:NH1	2.16	0.60
29:d:16:ASP:O	29:d:19:ARG:HG3	2.01	0.60
33:h:73:PHE:HD2	33:h:74:TYR:CD1	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:63:PHE:O	47:AC:67:THR:HG23	2.02	0.60
48:AD:119:GLN:HB2	48:AD:253:LEU:HD13	1.84	0.60
49:AE:119:ALA:HA	53:AJ:25:ILE:CG1	2.31	0.60
48:Ad:288:MET:SD	71:Ad:402:3PH:H2	2.42	0.60
58:B:304:PC1:H3B1	8:H:57:MET:CE	2.32	0.60
3:C:208:GLU:CG	3:C:221:GLU:HG3	2.31	0.60
4:D:149:GLN:HE21	4:D:171:ARG:HB3	1.65	0.60
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.82	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.31	0.60
12:L:222:GLY:CA	12:L:229:LEU:HD11	2.26	0.60
13:M:126:LEU:HD21	13:M:153:THR:HB	1.83	0.60
13:M:269:MET:HE3	13:M:399:ASN:CB	2.32	0.60
18:R:47:ARG:HB2	42:q:125:VAL:CG1	2.31	0.60
18:R:84:GLY:O	18:R:85:ALA:HB3	2.02	0.60
24:Y:137:LEU:CD2	24:Y:138:PHE:CD2	2.84	0.60
44:s:89:LYS:NZ	44:s:90:PHE:CE2	2.62	0.60
45:AA:283:PRO:HB2	49:AI:42:VAL:HG12	1.83	0.60
45:AA:341:PHE:HE1	45:AA:356:ALA:HB1	1.66	0.60
68:AC:403:UQ6:H101	68:AC:403:UQ6:C13	2.31	0.60
51:AG:31:PHE:CA	51:AG:35:ILE:HD12	2.24	0.60
52:AH:42:VAL:O	52:AH:46:GLU:HG3	2.01	0.60
54:AK:23:MET:O	54:AK:27:VAL:HG23	2.01	0.60
45:Aa:103:ASN:HD21	45:Aa:104:ARG:NH1	1.99	0.60
48:Ad:223:THR:HG23	52:Ah:55:VAL:HG21	1.83	0.60
55:Ag:103:3PE:H3D1	55:Ag:103:3PE:H391	1.82	0.60
4:D:137:ASP:OD2	4:D:223:HIS:CB	2.50	0.60
4:D:353:PRO:HA	25:Z:10:MET:HE1	1.84	0.60
5:E:223:CYS:SG	6:F:133:HIS:CE1	2.95	0.60
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.37	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
13:M:370:PRO:HA	13:M:375:LEU:HD22	1.83	0.60
33:h:73:PHE:CD2	33:h:74:TYR:CD1	2.90	0.60
33:h:102:PRO:HD2	33:h:105:TYR:CB	2.32	0.60
39:n:176:GLU:O	39:n:178:PRO:HD3	2.02	0.60
46:AB:113:THR:OG1	49:AI:65:VAL:HG11	2.02	0.60
48:AD:215:LEU:HD13	69:AD:401:HEC:HBB2	1.84	0.60
49:AE:127:TYR:O	53:AJ:33:GLU:OE1	2.20	0.60
51:AG:54:VAL:O	51:AG:58:LEU:HG	2.02	0.60
48:Ad:131:ALA:HB2	48:Ad:174:TYR:CD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Af:108:TRP:HA	50:Af:111:LYS:NZ	2.17	0.60
1:A:63:LEU:HD11	10:J:63:MET:HG2	1.84	0.59
2:B:171:TYR:CE1	4:D:135:TYR:HE1	2.20	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.31	0.59
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.67	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
9:I:93:LEU:HD11	9:I:173:PHE:CE2	2.37	0.59
10:J:120:LEU:CD2	10:J:124:LEU:HD22	2.32	0.59
12:L:173:LEU:CD2	55:L:702:3PE:H321	2.27	0.59
12:L:247:LEU:HD12	12:L:248:HIS:CG	2.36	0.59
14:N:258:THR:CG2	14:N:336:THR:HG22	2.32	0.59
14:N:276:LEU:C	14:N:276:LEU:HD12	2.27	0.59
15:O:54:HIS:HB2	15:O:56:TYR:CE1	2.37	0.59
27:b:69:HIS:CD2	27:b:70:PRO:HD2	2.36	0.59
28:c:65:ASP:OD2	29:d:73:TYR:OH	2.17	0.59
39:n:143:GLU:OE1	39:n:155:PRO:HB3	2.02	0.59
45:Aa:402:HIS:NE2	45:Aa:403:LEU:HD12	2.17	0.59
47:Ac:345:HIS:CE1	47:Ac:346:PRO:HB3	2.37	0.59
4:D:238:LEU:CB	43:r:36:GLN:HG3	2.23	0.59
4:D:241:LEU:CB	25:Z:16:TYR:OH	2.48	0.59
5:E:147:ILE:HD11	5:E:195:LEU:HB2	1.84	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
6:F:225:LEU:HD22	7:G:93:ALA:HB3	1.84	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
12:L:81:LYS:HB2	12:L:135:ASN:OD1	2.02	0.59
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.85	0.59
16:P:292:PRO:O	16:P:293:LEU:CG	2.47	0.59
20:U:90:TYR:CZ	20:U:92:LYS:HD2	2.35	0.59
29:d:113:LEU:HD22	32:g:148:PRO:HG3	1.84	0.59
45:AA:402:HIS:NE2	45:AA:403:LEU:HD12	2.17	0.59
47:AC:8:HIS:HE1	47:Ac:199:PHE:CZ	2.18	0.59
45:Aa:275:ILE:HD12	51:Ag:17:TYR:CE2	2.38	0.59
47:Ac:302:ALA:O	47:Ac:305:PRO:HD2	2.02	0.59
71:Ad:402:3PH:C38	49:Ae:128:ALA:HB1	2.32	0.59
71:Ad:402:3PH:H361	49:Ae:128:ALA:HB2	1.84	0.59
49:Ae:132:VAL:HA	49:Ae:135:GLN:NE2	2.17	0.59
1:A:79:ILE:CG1	1:A:87:MET:HE1	2.31	0.59
2:B:153:PRO:HG3	8:H:58:LYS:HE3	1.83	0.59
2:B:167:GLY:H	2:B:180:GLY:HA2	1.67	0.59
6:F:224:ARG:HD3	17:Q:164:PHE:CZ	2.37	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:123:LEU:HD22	12:L:150:MET:CG	2.32	0.59
12:L:313:MET:HE2	12:L:328:HIS:CE1	2.38	0.59
13:M:115:LEU:O	13:M:118:PHE:HB3	2.02	0.59
13:M:144:ASN:HA	13:M:147:ILE:HD12	1.82	0.59
15:O:164:TYR:CE2	15:O:195:LEU:HD21	2.36	0.59
16:P:238:GLN:HG2	16:P:270:ARG:HG3	1.83	0.59
17:Q:61:ILE:O	17:Q:65:THR:HG23	2.02	0.59
21:V:14:LEU:CD2	21:V:79:GLU:HG2	2.32	0.59
23:X:158:LEU:HB3	29:d:21:LEU:HD21	1.84	0.59
28:c:34:PRO:CG	28:c:37:ALA:HB2	2.32	0.59
33:h:69:ARG:O	33:h:73:PHE:HB2	2.02	0.59
38:m:18:LEU:HD11	39:n:72:TRP:CG	2.37	0.59
40:o:39:MET:HE1	40:o:58:TYR:HA	1.84	0.59
45:AA:402:HIS:CD2	45:AA:403:LEU:HD12	2.38	0.59
47:AC:211:LEU:HD21	50:AF:37:THR:HA	1.84	0.59
47:AC:345:HIS:CE1	47:AC:346:PRO:HB3	2.38	0.59
48:AD:110:ILE:O	48:AD:273:PHE:HB2	2.03	0.59
50:AF:52:PRO:HD3	46:Ab:148:ARG:NH2	2.18	0.59
51:AG:29:SER:CB	51:AG:32:SER:HB3	2.32	0.59
46:Ab:313:VAL:HG21	46:Ab:323:VAL:HG21	1.83	0.59
48:Ad:120:VAL:HG11	48:Ad:248:ILE:HD11	1.83	0.59
51:Ag:47:LEU:HB3	55:Ag:103:3PE:O22	2.02	0.59
1:A:106:TRP:CH2	27:b:19:LEU:HD21	2.38	0.59
5:E:162:THR:CG2	5:E:166:LYS:HA	2.33	0.59
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.59
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.65	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
10:J:55:VAL:HB	11:K:41:PHE:HE2	1.67	0.59
13:M:209:LEU:HD23	13:M:211:GLY:H	1.67	0.59
13:M:294:MET:HE3	13:M:319:HIS:CD2	2.37	0.59
35:j:94:ASP:HB3	35:j:99:ILE:HB	1.83	0.59
40:o:4:HIS:HA	40:o:7:ARG:HH11	1.67	0.59
45:AA:111:LYS:HA	46:AB:305:THR:HG21	1.84	0.59
46:AB:138:LEU:CD2	46:AB:238:LEU:HG	2.32	0.59
47:AC:51:LEU:HD12	67:AC:401:HEM:HBA1	1.83	0.59
48:AD:215:LEU:HD23	48:AD:244:MET:HE1	1.83	0.59
51:AG:51:PRO:HB2	51:AG:52:PRO:HD3	1.82	0.59
47:Ac:215:ALA:HA	51:Ag:11:ILE:HD11	1.84	0.59
47:Ac:276:PHE:HZ	47:Ac:298:ILE:HD11	1.67	0.59
4:D:81:THR:HG23	4:D:98:VAL:HG13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:217:PHE:CB	16:P:280:ILE:HD13	2.33	0.59
47:AC:198:LEU:HD21	47:Ac:9:PRO:O	2.02	0.59
48:AD:114:PHE:HD2	48:AD:140:TYR:CZ	2.20	0.59
51:AG:68:GLU:HA	51:AG:71:LYS:HE2	1.85	0.59
48:Ad:291:LYS:HB2	71:Ad:402:3PH:H32	1.83	0.59
4:D:35:ARG:HH21	32:g:59:PRO:HD3	1.68	0.59
4:D:222:MET:O	4:D:223:HIS:HB2	2.03	0.59
5:E:143:ASP:O	5:E:146:SER:HB3	2.02	0.59
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.59
7:G:310:GLU:OE1	7:G:313:LEU:HD21	2.01	0.59
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.37	0.59
9:I:105:ARG:NH2	9:I:191:LEU:HD22	2.17	0.59
12:L:149:ILE:HG21	13:M:364:LEU:HD21	1.84	0.59
15:O:249:MET:HB3	15:O:253:CYS:SG	2.42	0.59
16:P:192:ARG:HH12	16:P:260:GLY:HA2	1.67	0.59
18:R:33:HIS:CD2	18:R:34:THR:HG23	2.37	0.59
26:a:55:SER:HB3	26:a:61:TYR:CD2	2.38	0.59
45:AA:190:THR:HB	45:AA:275:ILE:CD1	2.31	0.59
45:AA:403:LEU:CD1	45:AA:403:LEU:H	2.16	0.59
46:AB:286:PHE:CE1	46:AB:427:ALA:HB1	2.38	0.59
47:AC:135:TRP:CG	47:AC:135:TRP:O	2.56	0.59
52:AH:54:ARG:HA	52:AH:57:SER:HB3	1.83	0.59
45:Aa:66:HIS:HE1	45:Aa:402:HIS:HB2	1.68	0.59
46:Ab:71:TYR:O	46:Ab:212:HIS:CE1	2.56	0.59
47:Ac:137:GLN:NE2	47:Ac:141:TRP:HE1	2.01	0.59
51:Ag:19:LEU:CD2	51:Ag:24:GLN:HB3	2.30	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.59
7:G:401:LEU:HD21	7:G:432:ILE:HD12	1.83	0.59
8:H:187:ILE:HG23	8:H:198:PHE:CZ	2.38	0.59
15:O:343:TYR:HE1	15:O:355:LYS:HB2	1.67	0.59
23:X:130:LYS:HB2	27:b:66:VAL:HG21	1.84	0.59
38:m:129:TYR:CZ	41:p:144:LEU:O	2.55	0.59
51:AG:49:VAL:O	51:AG:52:PRO:HD2	2.03	0.59
45:Aa:186:TYR:HB3	45:Aa:275:ILE:HG21	1.84	0.59
45:Aa:402:HIS:CD2	45:Aa:403:LEU:HD12	2.38	0.59
49:Ae:143:SER:HB2	49:Ae:146:VAL:HG22	1.84	0.59
52:Ah:72:PHE:HE2	52:Ah:76:ARG:HE	1.49	0.59
1:A:88:MET:HE1	8:H:309:ILE:HB	1.85	0.59
4:D:49:GLY:O	14:N:173:THR:HG21	2.03	0.59
6:F:261:TRP:HE3	6:F:262:PHE:CD1	2.21	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:32:ILE:HG12	7:G:45:PRO:HG3	1.85	0.59
12:L:227:PHE:CD2	12:L:283:LEU:CD2	2.86	0.59
12:L:312:LEU:CD2	12:L:395:ILE:HG21	2.33	0.59
12:L:605:ASN:O	12:L:606:LEU:C	2.46	0.59
14:N:223:ASN:HB3	15:O:306:ASN:HD21	1.67	0.59
15:O:114:LEU:HA	15:O:131:LEU:HD21	1.84	0.59
15:O:246:LEU:HD11	15:O:257:VAL:CG2	2.33	0.59
32:g:139:TYR:HD2	32:g:140:PHE:CD1	2.20	0.59
32:g:140:PHE:HB3	41:p:75:THR:HG21	1.84	0.59
37:l:109:LEU:O	37:l:113:ILE:HG23	2.03	0.59
45:AA:57:LEU:HD13	45:AA:229:MET:HB3	1.85	0.59
46:AB:100:THR:HG23	49:AI:70:LEU:HD11	1.84	0.59
53:AJ:33:GLU:HB2	54:AK:34:TRP:HE1	1.68	0.59
46:Ab:286:PHE:CE1	46:Ab:427:ALA:HB1	2.38	0.59
48:Ad:224:GLY:HA3	52:Ah:64:ASP:CB	2.32	0.59
2:B:93:MET:O	2:B:93:MET:HG3	2.02	0.59
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.85	0.59
8:H:196:ALA:C	8:H:198:PHE:H	2.10	0.59
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.38	0.59
12:L:358:LYS:HG3	39:n:80:TYR:CZ	2.38	0.59
12:L:390:TYR:CE2	35:j:68:TRP:HH2	2.21	0.59
13:M:275:ILE:HD11	13:M:288:TYR:CB	2.33	0.59
14:N:200:LEU:HD22	14:N:269:GLU:HG3	1.84	0.59
14:N:300:THR:HG23	14:N:301:SER:N	2.17	0.59
19:S:14:LEU:HB3	19:S:70:ALA:HB2	1.85	0.59
21:V:38:PHE:CE1	21:V:95:LEU:HB2	2.37	0.59
39:n:111:GLU:O	39:n:114:MET:HG2	2.03	0.59
47:AC:169:SER:HB3	49:Ae:172:LYS:CD	2.33	0.59
47:AC:198:LEU:HD21	47:Ac:10:LEU:CA	2.33	0.59
45:Aa:118:ALA:O	46:Ab:298:HIS:HB3	2.03	0.59
46:Ab:79:THR:HG23	46:Ab:205:LEU:HD23	1.83	0.59
48:Ad:158:PRO:HD2	48:Ad:164:MET:C	2.27	0.59
50:Af:106:GLU:O	50:Af:110:LYS:HG3	2.03	0.59
49:Ai:71:ASN:HB3	49:Ai:73:PRO:HD2	1.85	0.59
2:B:170:TYR:CE2	4:D:135:TYR:CE1	2.90	0.59
5:E:188:ASN:O	5:E:189:ASP:HB3	2.03	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59
7:G:126:LEU:CD2	7:G:157:LYS:HE3	2.33	0.59
7:G:182:CYS:HG	56:G:802:SF4:FE2	0.43	0.59
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.59
8:H:81:LEU:HD23	55:H:401:3PE:H391	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:38:TYR:CD2	9:I:41:LYS:HD3	2.38	0.59
12:L:466:PHE:CE1	12:L:470:TYR:HE2	2.21	0.59
12:L:570:HIS:O	12:L:571:THR:C	2.45	0.59
13:M:14:LEU:HD21	13:M:26:ASN:HB2	1.84	0.59
13:M:396:MET:HG3	13:M:396:MET:O	2.03	0.59
14:N:179:MET:CG	14:N:216:PHE:HE1	2.16	0.59
16:P:302:GLY:HA2	16:P:305:PHE:HD2	1.68	0.59
41:p:37:TYR:CZ	41:p:41:VAL:HG11	2.37	0.59
45:AA:64:SER:OG	45:AA:235:GLY:HA2	2.02	0.59
47:AC:48:GLY:HA3	67:AC:401:HEM:C2B	2.38	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.27	0.58
5:E:184:MET:HG3	5:E:192:TYR:O	2.03	0.58
7:G:136:GLU:HG2	17:Q:85:ASN:ND2	2.17	0.58
12:L:477:ILE:HG13	40:o:91:GLU:CD	2.28	0.58
14:N:342:GLN:NE2	29:d:30:ARG:HH11	2.01	0.58
15:O:351:TRP:CZ3	28:c:41:TRP:HH2	2.20	0.58
16:P:227:PRO:HB2	16:P:298:TYR:OH	2.01	0.58
30:e:87:MET:HE3	30:e:94:PRO:HD3	1.85	0.58
33:h:95:GLU:HB3	33:h:114:LYS:HG2	1.85	0.58
39:n:97:TYR:HB2	39:n:178:PRO:CB	2.32	0.58
40:o:50:GLN:OE1	41:p:120:ASN:ND2	2.36	0.58
46:AB:45:ASN:HD22	46:AB:239:ASN:HA	1.66	0.58
47:AC:137:GLN:NE2	47:AC:141:TRP:NE1	2.51	0.58
49:AE:163:LYS:O	49:AE:177:ARG:HG3	2.03	0.58
47:Ac:312:GLN:HE21	50:Af:37:THR:CB	2.16	0.58
48:Ad:92:PRO:HD3	48:Ad:236:TYR:CE1	2.38	0.58
71:Ad:402:3PH:C36	49:Ae:128:ALA:CB	2.80	0.58
49:Ae:93:ARG:NH2	51:Ag:24:GLN:O	2.36	0.58
1:A:23:TRP:CZ3	1:A:24:LEU:CD2	2.87	0.58
2:B:92:PRO:HG3	2:B:130:VAL:HG11	1.85	0.58
7:G:136:GLU:OE2	7:G:272:ARG:NH1	2.36	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
8:H:200:LEU:HD23	8:H:282:TYR:HD1	1.68	0.58
11:K:95:LEU:HG	14:N:54:GLU:CD	2.28	0.58
14:N:77:ASN:OD1	14:N:81:LEU:HD12	2.03	0.58
19:S:42:VAL:HG13	19:S:43:GLU:OE2	2.03	0.58
20:T:80:LYS:HG3	20:T:145:VAL:HG21	1.84	0.58
29:d:14:LEU:HD12	29:d:14:LEU:C	2.27	0.58
30:e:69:ARG:HD2	30:e:72:THR:HG21	1.85	0.58
38:m:49:LEU:HD22	39:n:140:LEU:HD23	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:65:SER:O	47:AC:69:ILE:HG13	2.03	0.58
47:AC:130:GLY:HA3	67:AC:401:HEM:C1D	2.39	0.58
47:AC:253:PRO:HB3	48:AD:202:ARG:O	2.03	0.58
51:AG:75:PRO:O	51:AG:79:GLU:HB2	2.03	0.58
48:Ad:112:ARG:HD3	48:Ad:257:ASP:OD2	2.04	0.58
2:B:92:PRO:HG3	2:B:130:VAL:HG12	1.85	0.58
2:B:194:CYS:O	56:B:301:SF4:S3	2.61	0.58
4:D:144:MET:SD	4:D:223:HIS:N	2.74	0.58
4:D:232:VAL:HG22	4:D:356:ILE:HB	1.85	0.58
9:I:51:LYS:HA	25:Z:33:TYR:HE2	1.68	0.58
9:I:90:LYS:H	42:q:90:LEU:HD21	1.67	0.58
12:L:230:HIS:N	12:L:231:PRO:CD	2.66	0.58
13:M:210:TYR:O	13:M:213:HIS:CD2	2.56	0.58
14:N:109:ALA:CB	14:N:110:PRO:CD	2.81	0.58
23:X:15:VAL:HG21	23:X:61:LYS:HG2	1.84	0.58
38:m:75:ASN:O	38:m:75:ASN:OD1	2.20	0.58
49:Ae:207:LYS:HD2	49:Ae:210:TRP:HD1	1.67	0.58
2:B:90:LEU:C	2:B:92:PRO:HD3	2.27	0.58
58:B:303:PC1:H112	42:q:75:TRP:HE3	1.68	0.58
4:D:253:LEU:HD22	43:r:23:LYS:HB2	1.85	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:379:CYS:SG	56:F:502:SF4:S1	3.02	0.58
12:L:407:TRP:CZ3	12:L:410:LEU:HD11	2.38	0.58
17:Q:161:GLY:HA2	17:Q:164:PHE:CD2	2.38	0.58
33:h:57:VAL:CG1	39:n:99:VAL:HG23	2.33	0.58
52:AH:67:GLU:HG3	52:AH:68:GLU:OE1	2.03	0.58
45:Aa:220:LEU:O	45:Aa:224:TYR:HB2	2.03	0.58
46:Ab:173:ILE:HG21	46:Ab:339:TYR:HE1	1.67	0.58
48:Ad:177:LYS:HD2	48:Ad:180:PRO:HA	1.85	0.58
4:D:37:TRP:CZ2	4:D:39:PRO:HA	2.38	0.58
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.63	0.58
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.10	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
8:H:157:ASN:C	8:H:157:ASN:OD1	2.47	0.58
8:H:196:ALA:CB	8:H:197:PRO:CD	2.81	0.58
8:H:287:HIS:HD2	8:H:291:LYS:HD2	1.67	0.58
12:L:404:THR:HG22	12:L:405:ASN:N	2.19	0.58
12:L:417:SER:HB3	12:L:493:ILE:CG1	2.31	0.58
14:N:307:THR:CG2	14:N:311:SER:OG	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:N:401:3PE:H261	55:d:201:3PE:H222	1.84	0.58
16:P:170:LEU:O	16:P:171:ASN:OD1	2.21	0.58
19:S:42:VAL:CG1	19:S:43:GLU:CD	2.76	0.58
21:V:114:TRP:CD2	21:V:114:TRP:O	2.56	0.58
25:Z:98:MET:SD	30:e:92:TYR:CZ	2.96	0.58
34:i:95:TYR:OH	41:p:11:PRO:O	2.20	0.58
46:Ab:195:TYR:CD1	46:Ab:262:ASN:HA	2.37	0.58
45:Aa:64:SER:OG	45:Aa:235:GLY:HA2	2.03	0.58
45:Aa:98:PHE:C	45:Aa:109:LEU:HD21	2.28	0.58
45:Aa:363:MET:HA	45:Aa:464:GLN:OE1	2.03	0.58
48:Ad:299:LEU:CD1	71:Ad:402:3PH:H371	2.33	0.58
2:B:157:TYR:HB3	2:B:188:ASP:OD2	2.03	0.58
6:F:133:HIS:O	6:F:134:ASP:C	2.46	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
9:I:68:ARG:HH12	25:Z:28:ARG:HG2	1.69	0.58
12:L:407:TRP:HE1	37:l:140:MET:CE	2.16	0.58
12:L:550:LEU:HB2	13:M:275:ILE:HG22	1.83	0.58
20:U:97:LYS:O	20:U:98:LEU:C	2.46	0.58
55:d:201:3PE:H111	55:d:201:3PE:H12	1.86	0.58
47:Ac:8:HIS:NE2	47:Ac:199:PHE:CE1	2.72	0.58
48:AD:136:VAL:HA	48:AD:140:TYR:O	2.03	0.58
49:AE:239:HIS:NE2	47:Ac:278:TYR:OH	2.33	0.58
46:Ab:208:PHE:CE1	46:Ab:212:HIS:HB2	2.39	0.58
47:Ac:18:PHE:CE1	68:Ac:405:UQ6:H71	2.34	0.58
52:Ah:69:LEU:CD2	52:Ah:73:LEU:CD1	2.81	0.58
1:A:104:TYR:HE2	10:J:167:ILE:HD12	1.68	0.58
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.69	0.58
5:E:230:LEU:HD21	6:F:48:ARG:NH2	2.19	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.16	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
15:O:326:ARG:HH21	32:g:56:ASP:CG	2.12	0.58
16:P:236:VAL:HG22	16:P:270:ARG:HG2	1.85	0.58
38:m:129:TYR:HE2	41:p:146:LEU:O	1.85	0.58
47:Ac:253:PRO:HG2	48:Ad:205:HIS:NE2	2.18	0.58
52:Ah:47:ARG:O	52:Ah:51:CYS:N	2.36	0.58
1:A:64:LEU:O	1:A:68:GLU:HG3	2.03	0.58
2:B:106:HIS:CE1	4:D:211:PHE:CE2	2.91	0.58
5:E:134:CYS:SG	5:E:175:CYS:HA	2.43	0.58
5:E:189:ASP:OD1	6:F:163:TYR:HB3	2.04	0.58
8:H:90:PRO:HB3	8:H:162:LEU:HB3	1.85	0.58
10:J:126:TYR:CD2	25:Z:120:LEU:HD11	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:261:VAL:C	12:L:264:HIS:HD2	2.12	0.58
12:L:390:TYR:CE2	35:j:68:TRP:CH2	2.92	0.58
13:M:123:GLU:CD	14:N:255:PRO:HG2	2.28	0.58
13:M:196:TRP:HZ3	13:M:261:PHE:CE2	2.21	0.58
14:N:314:MET:CB	15:O:305:LEU:HD11	2.33	0.58
16:P:209:ARG:CA	16:P:352:VAL:HG12	2.34	0.58
16:P:282:GLY:O	16:P:285:HIS:CE1	2.56	0.58
21:V:6:LYS:CG	21:V:16:VAL:HG23	2.34	0.58
26:a:18:ILE:N	26:a:19:PRO:HD3	2.19	0.58
29:d:113:LEU:O	29:d:113:LEU:HG	2.02	0.58
39:n:177:ARG:HG2	39:n:179:THR:OG1	2.04	0.58
45:AA:363:MET:HA	45:AA:464:GLN:OE1	2.03	0.58
46:AB:173:ILE:CG2	46:AB:339:TYR:HE1	2.16	0.58
46:AB:177:LEU:HD21	46:AB:272:VAL:CG1	2.34	0.58
48:AD:95:PRO:HA	48:AD:99:ARG:NH2	2.18	0.58
50:AF:75:ILE:HD12	50:AF:81:TRP:CZ2	2.39	0.58
45:Aa:403:LEU:CD1	45:Aa:403:LEU:H	2.16	0.58
46:Ab:126:ILE:O	46:Ab:130:ILE:HG23	2.04	0.58
47:Ac:137:GLN:HA	47:Ac:259:ALA:HA	1.85	0.58
48:Ad:294:LEU:HB2	53:Aj:36:PHE:HZ	1.69	0.58
49:Ae:144:ALA:HA	49:Ae:147:LEU:HG	1.86	0.58
4:D:202:TRP:CH2	4:D:261:MET:CE	2.86	0.58
6:F:184:LYS:HB3	44:s:92:LEU:CD2	2.33	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
11:K:59:ILE:HD12	14:N:27:MET:HG2	1.85	0.58
12:L:15:LEU:O	12:L:18:PRO:HD2	2.03	0.58
12:L:425:ARG:HG3	12:L:429:PHE:CE2	2.39	0.58
12:L:542:LEU:HB3	13:M:278:ARG:HD2	1.85	0.58
14:N:26:LEU:O	14:N:27:MET:C	2.46	0.58
14:N:149:LEU:HD11	14:N:195:PRO:HG3	1.84	0.58
15:O:351:TRP:CH2	28:c:41:TRP:HH2	2.22	0.58
23:X:9:THR:HB	23:X:12:GLU:HG3	1.86	0.58
32:g:121:GLU:HA	32:g:124:VAL:HG22	1.86	0.58
51:AG:65:GLN:O	51:AG:69:GLN:HG2	2.03	0.58
45:Aa:57:LEU:HD13	45:Aa:229:MET:HB3	1.85	0.58
2:B:81:LEU:HD21	8:H:53:MET:HE1	1.85	0.58
58:B:304:PC1:H3C1	8:H:53:MET:HG3	1.85	0.58
5:E:165:ASP:C	5:E:167:LEU:H	2.09	0.58
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.04	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:390:TYR:HE2	35:j:68:TRP:CH2	2.22	0.58
13:M:73:LEU:HB2	13:M:103:GLN:OE1	2.02	0.58
15:O:117:PHE:CD1	15:O:128:SER:CB	2.87	0.58
18:R:47:ARG:HG3	18:R:48:PHE:CD2	2.38	0.58
22:W:42:TRP:CZ2	66:W:201:EHZ:O1	2.57	0.58
23:X:168:PHE:O	23:X:170:TRP:CD1	2.57	0.58
29:d:93:TYR:CD2	33:h:156:VAL:HG13	2.39	0.58
30:e:20:PHE:CZ	33:h:178:PHE:HB2	2.39	0.58
34:i:70:PHE:O	34:i:73:SER:HB3	2.04	0.58
40:o:116:ALA:O	40:o:120:ALA:N	2.36	0.58
45:Aa:341:PHE:HB2	45:Aa:368:MET:HE1	1.84	0.58
47:Ac:71:ARG:NE	48:Ad:199:TYR:OH	2.36	0.58
2:B:126:ARG:HH21	8:H:63:PRO:HB3	1.69	0.57
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.67	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57
8:H:305:ILE:O	8:H:308:PRO:HD2	2.04	0.57
9:I:113:CYS:SG	56:I:303:SF4:FE3	1.80	0.57
12:L:232:TRP:CZ3	12:L:233:LEU:HD21	2.37	0.57
13:M:109:THR:HG22	13:M:121:LEU:CB	2.34	0.57
20:U:84:LEU:O	20:U:88:LYS:HG3	2.04	0.57
20:U:100:VAL:O	20:U:101:ASN:HB2	2.04	0.57
21:V:50:GLN:HE22	43:r:93:LYS:HA	1.69	0.57
30:e:14:LEU:HD12	30:e:15:ASP:CB	2.33	0.57
45:AA:66:HIS:HE1	45:AA:402:HIS:HB2	1.68	0.57
45:AA:70:THR:HG21	45:AA:407:THR:HA	1.85	0.57
45:AA:133:ILE:HG13	45:AA:147:LEU:HD21	1.86	0.57
46:AB:51:SER:HB2	46:AB:230:LEU:CD1	2.33	0.57
51:AG:19:LEU:HD23	51:AG:24:GLN:HB3	1.85	0.57
4:D:36:GLN:OE1	13:M:136:TRP:HA	2.03	0.57
8:H:158:GLY:HA3	8:H:315:PRO:HB2	1.86	0.57
12:L:592:LEU:O	12:L:596:ILE:HG12	2.04	0.57
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.85	0.57
13:M:423:MET:SD	38:m:59:HIS:NE2	2.78	0.57
14:N:33:LEU:HD11	14:N:141:ILE:HD12	1.86	0.57
17:Q:64:LEU:HD12	22:W:85:LEU:HD21	1.86	0.57
21:V:111:GLN:HG3	21:V:111:GLN:O	2.04	0.57
23:X:24:VAL:HG12	23:X:86:TRP:CG	2.39	0.57
39:n:26:HIS:CE1	39:n:79:PRO:HB3	2.39	0.57
40:o:5:LEU:HB3	40:o:9:TYR:CE2	2.38	0.57
42:q:88:ARG:HG2	42:q:94:THR:OG1	2.03	0.57
45:AA:402:HIS:ND1	45:AA:403:LEU:CD1	2.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:72:ASP:O	47:AC:73:VAL:C	2.45	0.57
47:AC:138:MET:HE1	47:AC:268:ILE:HG12	1.86	0.57
45:Aa:96:LEU:HD21	45:Aa:161:ILE:CA	2.31	0.57
47:Ac:253:PRO:CG	48:Ad:205:HIS:CD2	2.88	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:62:ARG:HD3	8:H:68:MET:SD	2.45	0.57
8:H:150:LEU:C	8:H:150:LEU:HD13	2.29	0.57
9:I:163:PRO:O	18:R:89:PRO:HD3	2.04	0.57
15:O:66:ILE:CD1	15:O:218:ILE:CD1	2.82	0.57
23:X:15:VAL:CG2	23:X:61:LYS:HG2	2.35	0.57
35:j:101:PRO:O	35:j:102:ASP:C	2.46	0.57
43:r:13:ASN:OD1	43:r:20:LEU:HB2	2.05	0.57
47:AC:198:LEU:HD11	47:Ac:9:PRO:HB2	1.85	0.57
50:AF:88:LYS:NZ	50:AF:90:TYR:HB3	2.20	0.57
47:Ac:147:THR:HG21	47:Ac:165:TRP:CD1	2.40	0.57
51:Ag:11:ILE:HG22	51:Ag:12:ARG:N	2.18	0.57
7:G:386:LEU:O	7:G:387:LEU:C	2.46	0.57
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.68	0.57
8:H:260:MET:CE	26:a:16:LEU:HB2	2.35	0.57
13:M:73:LEU:HD22	13:M:103:GLN:NE2	2.18	0.57
13:M:172:GLY:C	13:M:173:THR:HG23	2.28	0.57
13:M:297:VAL:O	13:M:301:ILE:HG12	2.03	0.57
14:N:253:GLY:N	14:N:290:LEU:HD11	2.19	0.57
14:N:307:THR:O	15:O:319:ILE:HG12	2.05	0.57
16:P:91:ILE:HD12	16:P:105:PHE:CD2	2.39	0.57
23:X:171:THR:O	23:X:172:VAL:C	2.48	0.57
46:AB:148:ARG:NH2	50:Af:52:PRO:HD3	2.19	0.57
48:AD:94:TYR:HB2	48:AD:96:TRP:NE1	2.19	0.57
48:AD:131:ALA:HB3	48:AD:133:ARG:HG2	1.87	0.57
4:D:267:ILE:CG2	8:H:278:PRO:O	2.48	0.57
5:E:183:PRO:HB2	5:E:195:LEU:H	1.68	0.57
12:L:145:GLU:HB3	13:M:370:PRO:CG	2.34	0.57
12:L:227:PHE:CD2	12:L:283:LEU:HD21	2.38	0.57
13:M:230:ILE:HG13	13:M:235:LEU:HG	1.87	0.57
13:M:444:LEU:O	13:M:448:THR:HG23	2.04	0.57
13:M:447:LEU:HD21	13:M:454:ILE:CD1	2.33	0.57
14:N:179:MET:HG3	14:N:216:PHE:CE1	2.39	0.57
16:P:128:ASN:ND2	16:P:149:PRO:HB3	2.20	0.57
20:T:90:TYR:CE2	20:T:93:ILE:HG12	2.38	0.57
62:a:101:CDL:HB61	42:q:6:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:60:ARG:HH12	42:q:95:ASP:CA	2.15	0.57
45:AA:310:ILE:HG22	45:AA:378:ARG:HH22	1.69	0.57
47:AC:8:HIS:HE1	47:Ac:199:PHE:HZ	1.51	0.57
47:AC:268:ILE:HD13	49:Ae:238:CYS:SG	2.42	0.57
49:AE:175:PHE:CZ	49:AE:224:PRO:HD2	2.38	0.57
51:AG:29:SER:HB3	51:AG:32:SER:HB3	1.84	0.57
46:Ab:300:LYS:HG2	46:Ab:301:ARG:HG3	1.86	0.57
51:Ag:35:ILE:HB	51:Ag:36:PRO:HD3	1.86	0.57
2:B:81:LEU:HD11	8:H:53:MET:SD	2.45	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.68	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
10:J:135:LEU:HA	11:K:54:MET:HE1	1.85	0.57
12:L:425:ARG:HG3	12:L:429:PHE:HE2	1.68	0.57
12:L:441:ILE:HG21	35:j:48:PRO:HD3	1.85	0.57
13:M:123:GLU:CG	14:N:255:PRO:HG2	2.35	0.57
13:M:255:LYS:HZ3	29:d:117:HIS:HB3	1.67	0.57
14:N:154:ILE:HG12	14:N:195:PRO:HG2	1.87	0.57
14:N:284:MET:O	14:N:287:LEU:HB2	2.04	0.57
20:T:104:PHE:HE2	20:T:144:ILE:HD11	1.69	0.57
32:g:147:LEU:HD11	41:p:163:MET:HB3	1.86	0.57
34:i:87:LYS:HG2	34:i:87:LYS:O	2.05	0.57
37:l:166:LEU:HB2	37:l:170:ARG:NH2	2.19	0.57
47:AC:18:PHE:CE1	68:AC:403:UQ6:H1M2	2.40	0.57
47:AC:168:PHE:HD2	49:Ae:170:ARG:HB3	1.70	0.57
48:AD:227:LEU:HD22	48:AD:231:LEU:HB2	1.86	0.57
67:Ac:402:HEM:O1A	67:Ac:402:HEM:HHA	2.04	0.57
48:Ad:126:SER:HB3	48:Ad:177:LYS:HA	1.85	0.57
49:Ae:207:LYS:HB3	49:Ae:209:GLU:OE1	2.05	0.57
51:Ag:27:PHE:HB3	51:Ag:30:TYR:HB2	1.87	0.57
2:B:199:GLU:HB2	9:I:173:PHE:CE1	2.40	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
14:N:273:ASN:O	14:N:274:ASN:HB2	2.05	0.57
16:P:293:LEU:HB2	16:P:298:TYR:OH	2.05	0.57
19:S:42:VAL:O	19:S:46:LYS:HG3	2.04	0.57
20:U:130:ILE:HG23	20:U:147:TYR:CE2	2.39	0.57
23:X:162:LYS:HB3	23:X:166:ARG:NH2	2.19	0.57
32:g:140:PHE:CZ	41:p:74:ILE:HG22	2.40	0.57
47:Ac:150:LEU:HD13	47:Ac:164:ILE:HD12	1.86	0.57
47:Ac:171:ASP:CG	47:Ac:172:LYS:H	2.13	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:441:ILE:HD12	35:j:46:GLU:O	2.05	0.57
13:M:14:LEU:HD11	13:M:26:ASN:HB3	1.87	0.57
13:M:421:ASN:HB2	38:m:51:TYR:OH	2.05	0.57
14:N:109:ALA:HB1	14:N:110:PRO:HD3	1.86	0.57
25:Z:101:VAL:HB	25:Z:102:PRO:CD	2.33	0.57
25:Z:104:TRP:CZ2	30:e:75:ARG:NH2	2.72	0.57
55:d:201:3PE:H232	55:d:201:3PE:H272	1.85	0.57
39:n:98:LYS:HG2	39:n:178:PRO:HG3	1.86	0.57
45:AA:87:ASN:OD1	45:AA:199:GLN:HB2	2.05	0.57
46:AB:113:THR:OG1	49:AI:65:VAL:HG12	2.04	0.57
48:AD:213:SER:HB3	48:AD:236:TYR:CD2	2.38	0.57
48:AD:311:TRP:HB3	48:AD:315:LYS:HE3	1.86	0.57
53:AJ:23:LEU:HA	54:AK:27:VAL:CG1	2.33	0.57
48:Ad:291:LYS:HE2	53:Aj:40:ALA:HB3	1.86	0.57
4:D:192:LEU:HD11	4:D:200:PHE:HB3	1.85	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.87	0.57
9:I:180:HIS:CD2	16:P:100:LEU:CD2	2.87	0.57
12:L:246:LEU:HD12	12:L:247:LEU:CA	2.34	0.57
13:M:12:LEU:HB2	13:M:13:PRO:HD3	1.86	0.57
13:M:424:ILE:HG13	38:m:57:VAL:O	2.05	0.57
15:O:135:LEU:HD13	63:O:401:ADP:C6	2.40	0.57
17:Q:163:ASN:OD1	17:Q:164:PHE:CD1	2.58	0.57
25:Z:98:MET:HE1	30:e:83:ARG:HB2	1.84	0.57
30:e:20:PHE:HZ	33:h:178:PHE:HB2	1.70	0.57
34:i:111:LEU:HD11	41:p:20:PRO:HD3	1.87	0.57
45:AA:74:TRP:CH2	45:AA:410:CYS:SG	2.97	0.57
45:AA:182:VAL:HG13	45:AA:186:TYR:CE2	2.40	0.57
45:AA:220:LEU:O	45:AA:224:TYR:HB2	2.03	0.57
48:AD:217:GLY:HA3	48:AD:236:TYR:HD2	1.69	0.57
48:AD:242:ILE:HG23	48:AD:243:GLY:N	2.18	0.57
52:AH:85:PHE:HA	52:AH:88:LEU:HD12	1.87	0.57
45:Aa:70:THR:HG21	45:Aa:407:THR:HA	1.85	0.57
45:Aa:402:HIS:CG	45:Aa:403:LEU:HD12	2.40	0.57
49:Ae:242:HIS:N	49:Ae:251:LYS:O	2.32	0.57
3:C:45:THR:HG22	4:D:358:VAL:HG23	1.87	0.57
4:D:267:ILE:HG22	8:H:278:PRO:CG	2.22	0.57
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.70	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.87	0.57
9:I:36:TYR:HD2	43:r:104:TRP:HB2	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:89:TYR:C	11:K:91:GLN:N	2.59	0.57
12:L:253:VAL:CG2	12:L:310:LEU:HD11	2.35	0.57
13:M:42:LEU:HD11	13:M:67:ILE:CD1	2.34	0.57
13:M:269:MET:HE3	13:M:399:ASN:HB2	1.86	0.57
13:M:310:MET:O	13:M:314:MET:HG3	2.04	0.57
15:O:80:GLN:CG	15:O:270:VAL:HG21	2.18	0.57
16:P:169:HIS:ND1	64:P:401:NDP:H5N	2.20	0.57
42:q:68:MET:O	42:q:71:LYS:HB2	2.05	0.57
45:Aa:74:TRP:CH2	45:Aa:410:CYS:SG	2.97	0.57
45:Aa:279:ASP:OD1	51:Ag:12:ARG:NE	2.37	0.57
51:Ag:42:THR:HA	62:Ag:101:CDL:HB61	1.86	0.57
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.56
2:B:81:LEU:HD21	8:H:53:MET:CE	2.35	0.56
4:D:356:ILE:HD11	4:D:357:LYS:HE3	1.87	0.56
7:G:330:LEU:HD13	7:G:546:PHE:CZ	2.39	0.56
9:I:64:THR:HG21	25:Z:35:MET:HE1	1.87	0.56
12:L:88:LEU:HD23	12:L:326:PHE:HE2	1.69	0.56
12:L:229:LEU:HD12	12:L:229:LEU:C	2.28	0.56
13:M:282:LEU:HD13	13:M:342:MET:HE2	1.87	0.56
16:P:249:ILE:O	16:P:253:THR:HG23	2.05	0.56
21:V:45:ARG:O	21:V:49:GLU:HB2	2.04	0.56
24:Y:110:TYR:HB2	55:m:203:3PE:H11	1.87	0.56
33:h:57:VAL:CG1	39:n:99:VAL:CG2	2.83	0.56
45:AA:87:ASN:HD22	45:AA:204:PRO:HD3	1.69	0.56
47:AC:171:ASP:CG	47:AC:172:LYS:H	2.13	0.56
48:Ad:159:ASN:H	48:Ad:164:MET:HB3	1.70	0.56
48:Ad:245:ALA:O	48:Ad:246:PRO:C	2.47	0.56
3:C:45:THR:OG1	43:r:57:ARG:HD2	2.04	0.56
3:C:184:ARG:NH2	4:D:110:ASP:OD2	2.38	0.56
4:D:137:ASP:OD1	4:D:137:ASP:C	2.48	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.84	0.56
9:I:79:ARG:HH21	43:r:20:LEU:HD13	1.69	0.56
10:J:33:ILE:HG23	10:J:60:LEU:HD22	1.85	0.56
10:J:133:VAL:HG12	26:a:41:VAL:HB	1.87	0.56
10:J:136:GLU:HG3	10:J:139:ILE:HG12	1.87	0.56
10:J:150:TRP:CD1	14:N:28:LEU:HD21	2.40	0.56
12:L:60:GLU:CG	12:L:83:ASP:HA	2.35	0.56
12:L:456:ARG:CG	55:L:701:3PE:H241	2.34	0.56
13:M:4:ILE:CG2	13:M:107:ILE:HD13	2.30	0.56
13:M:263:LEU:CD1	38:m:102:TYR:HD1	2.16	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:226:THR:HG22	14:N:228:ASN:H	1.70	0.56
14:N:254:LEU:CD1	14:N:255:PRO:HD2	2.35	0.56
15:O:173:MET:HE2	15:O:179:ILE:HG23	1.87	0.56
15:O:176:GLN:HG3	15:O:177:GLY:N	2.16	0.56
15:O:201:PRO:O	15:O:253:CYS:HB3	2.05	0.56
19:S:44:LEU:HD12	19:S:48:HIS:CD2	2.40	0.56
21:V:81:ILE:O	21:V:82:LEU:C	2.48	0.56
23:X:20:VAL:HG23	23:X:25:LEU:HD12	1.83	0.56
23:X:130:LYS:HD2	27:b:59:ASP:OD1	2.05	0.56
24:Y:92:TYR:CE1	24:Y:128:LYS:HD3	2.40	0.56
39:n:81:ILE:CD1	39:n:87:GLY:O	2.53	0.56
44:s:76:ASN:O	44:s:79:THR:HG22	2.05	0.56
45:AA:375:GLN:O	45:AA:378:ARG:HB3	2.05	0.56
53:AJ:23:LEU:HA	54:AK:27:VAL:HG22	1.87	0.56
45:Aa:402:HIS:ND1	45:Aa:403:LEU:HD12	2.20	0.56
48:Ad:117:TYR:OH	48:Ad:126:SER:HA	2.04	0.56
48:Ad:227:LEU:HB2	48:Ad:231:LEU:HB2	1.86	0.56
50:Af:22:TYR:CD2	50:Af:84:TYR:HB2	2.40	0.56
50:Af:107:GLU:OE2	50:Af:111:LYS:HD3	2.05	0.56
52:Ah:45:ARG:O	52:Ah:48:LEU:HB3	2.05	0.56
1:A:75:LEU:HD13	8:H:305:ILE:HD11	1.86	0.56
4:D:58:THR:HG23	4:D:61:TRP:CD2	2.40	0.56
4:D:90:ALA:HB2	8:H:205:SER:O	2.05	0.56
4:D:235:ASP:HA	4:D:356:ILE:HG21	1.86	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:330:LEU:HA	7:G:544:MET:HE1	1.86	0.56
7:G:667:GLN:NE2	19:S:38:VAL:HA	2.17	0.56
10:J:21:LEU:HA	55:K:101:3PE:H242	1.88	0.56
10:J:135:LEU:CD1	11:K:54:MET:HE3	2.35	0.56
11:K:89:TYR:C	11:K:91:GLN:H	2.13	0.56
12:L:9:LEU:CG	55:i:201:3PE:H2C1	2.35	0.56
15:O:125:ASP:OD1	15:O:126:GLY:N	2.39	0.56
15:O:295:ARG:HH12	15:O:299:GLN:HB2	1.67	0.56
18:R:38:TYR:HE1	18:R:44:ARG:HE	1.53	0.56
23:X:8:PRO:HG2	25:Z:84:LEU:HD21	1.88	0.56
26:a:37:ARG:HH11	26:a:59:ARG:HD2	1.70	0.56
34:i:14:GLN:HE22	39:n:157:ALA:HB3	1.71	0.56
40:o:25:PHE:HZ	40:o:109:LEU:HA	1.70	0.56
41:p:132:PHE:O	41:p:136:THR:OG1	2.17	0.56
45:AA:87:ASN:H	45:AA:207:ASN:HD22	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:95:PRO:HG2	52:AH:85:PHE:HB2	1.86	0.56
48:AD:247:PRO:HG3	69:AD:401:HEC:CHC	2.35	0.56
45:Aa:52:ILE:HG12	45:Aa:53:LEU:H	1.69	0.56
45:Aa:87:ASN:HD21	45:Aa:199:GLN:HB2	1.69	0.56
51:Ag:33:LYS:C	51:Ag:36:PRO:HD2	2.30	0.56
3:C:210:ARG:NH2	16:P:75:ARG:HD3	2.21	0.56
4:D:34:ALA:HB3	13:M:86:LYS:HZ3	1.71	0.56
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
8:H:114:TYR:CE1	10:J:33:ILE:HD13	2.40	0.56
11:K:1:MET:O	11:K:4:THR:HG22	2.04	0.56
13:M:57:SER:HB3	13:M:113:THR:HG22	1.87	0.56
13:M:78:MET:O	13:M:432:ARG:HD2	2.05	0.56
13:M:118:PHE:O	13:M:122:PHE:CB	2.54	0.56
14:N:196:TYR:HB3	14:N:273:ASN:OD1	2.05	0.56
16:P:258:ALA:O	16:P:261:LYS:HB2	2.05	0.56
16:P:271:TYR:HA	16:P:375:VAL:HG22	1.86	0.56
31:f:38:ARG:NH1	31:f:56:TRP:O	2.39	0.56
31:f:43:LEU:HD21	41:p:68:TYR:HD1	1.69	0.56
45:AA:87:ASN:ND2	45:AA:204:PRO:HD3	2.20	0.56
48:AD:120:VAL:HG23	48:AD:253:LEU:CD1	2.15	0.56
52:AH:43:LYS:HA	52:AH:46:GLU:CD	2.29	0.56
52:AH:86:LYS:HG3	52:AH:87:ASN:N	2.20	0.56
49:Ae:218:THR:OG1	49:Ae:254:ALA:HB1	2.05	0.56
4:D:158:LEU:HD12	4:D:411:LEU:HD23	1.87	0.56
4:D:375:MET:HE1	7:G:126:LEU:HA	1.86	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
11:K:45:SER:O	11:K:49:LEU:HG	2.06	0.56
14:N:120:GLN:O	14:N:176:ARG:CZ	2.54	0.56
15:O:66:ILE:CD1	15:O:218:ILE:CG1	2.84	0.56
16:P:88:VAL:HA	16:P:91:ILE:HG12	1.86	0.56
30:e:14:LEU:HD12	30:e:14:LEU:C	2.31	0.56
37:l:105:ILE:HG23	37:l:109:LEU:HD22	1.86	0.56
38:m:15:PRO:HG3	38:m:18:LEU:HD12	1.87	0.56
40:o:115:ARG:O	40:o:119:GLU:HB3	2.06	0.56
41:p:39:LEU:O	41:p:44:PRO:HD3	2.06	0.56
45:AA:402:HIS:CG	45:AA:403:LEU:HD12	2.40	0.56
48:AD:249:TYR:CE2	48:AD:252:VAL:HA	2.40	0.56
49:AE:123:VAL:HG13	53:AJ:29:ALA:CA	2.35	0.56
49:AE:218:THR:HG21	49:AE:256:LEU:C	2.30	0.56
46:Ab:146:PHE:CE1	46:Ab:206:HIS:ND1	2.73	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:155:LYS:HE2	49:Ae:157:SER:HB3	1.86	0.56
49:Ae:249:ILE:HG12	49:Ae:254:ALA:HB3	1.87	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
9:I:90:LYS:HE2	42:q:79:GLY:O	2.06	0.56
55:M:501:3PE:H342	14:N:280:THR:HG21	1.87	0.56
14:N:149:LEU:CD1	14:N:154:ILE:HG21	2.35	0.56
14:N:324:LEU:HD11	29:d:64:PHE:CZ	2.40	0.56
15:O:114:LEU:O	15:O:117:PHE:HB3	2.06	0.56
17:Q:62:THR:HB	17:Q:72:ILE:HD11	1.88	0.56
20:T:90:TYR:CE2	20:T:92:LYS:HB2	2.40	0.56
20:U:87:LEU:HD21	20:U:118:ILE:HG23	1.86	0.56
26:a:14:VAL:O	26:a:18:ILE:HG13	2.06	0.56
35:j:97:LEU:O	40:o:104:ARG:HG3	2.05	0.56
44:s:84:ASN:OD1	44:s:85:LEU:N	2.38	0.56
45:AA:402:HIS:ND1	45:AA:403:LEU:HD12	2.20	0.56
47:AC:97:HIS:CE1	47:AC:100:ARG:HH21	2.24	0.56
47:AC:137:GLN:HE21	47:AC:265:PRO:HD3	1.69	0.56
47:AC:375:LYS:NZ	50:AF:14:LEU:HD21	2.21	0.56
48:AD:111:ARG:HA	48:AD:140:TYR:CE1	2.40	0.56
48:AD:120:VAL:CG1	48:AD:247:PRO:HB2	2.35	0.56
48:AD:158:PRO:CB	48:AD:162:GLY:HA2	2.35	0.56
49:AE:123:VAL:HA	53:AJ:29:ALA:HB2	1.88	0.56
49:AE:219:HIS:HB2	49:AE:254:ALA:HA	1.88	0.56
48:Ad:89:LEU:HD11	52:Ah:74:HIS:HA	1.87	0.56
49:Ae:197:ASP:HB3	49:Ae:257:ASN:ND2	2.21	0.56
2:B:77:LYS:HE3	58:B:303:PC1:H271	1.88	0.56
2:B:168:GLY:HA3	2:B:172:HIS:HD2	1.71	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
12:L:385:PHE:CD1	35:j:72:ARG:CG	2.89	0.56
12:L:385:PHE:CE1	35:j:72:ARG:HG3	2.40	0.56
12:L:397:GLU:HB2	12:L:482:MET:SD	2.46	0.56
12:L:598:ILE:HD11	14:N:153:ILE:HG12	1.88	0.56
62:L:704:CDL:H1	13:M:357:THR:OG1	2.05	0.56
13:M:370:PRO:CA	13:M:375:LEU:CD2	2.83	0.56
14:N:193:ILE:HD11	14:N:269:GLU:HB2	1.88	0.56
14:N:314:MET:HB2	15:O:305:LEU:CD1	2.34	0.56
16:P:54:VAL:O	16:P:54:VAL:HG23	2.05	0.56
16:P:96:LEU:C	16:P:96:LEU:CD1	2.72	0.56
27:b:69:HIS:HB3	27:b:72:ASP:OD1	2.06	0.56
30:e:42:GLU:HG2	33:h:176:LYS:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:426:LYS:HA	46:AB:429:LYS:HZ3	1.70	0.56
47:AC:150:LEU:HD13	47:AC:164:ILE:HD12	1.86	0.56
48:Ad:114:PHE:CE1	48:Ad:175:PHE:HE2	2.18	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
7:G:652:ASN:OD1	7:G:652:ASN:O	2.23	0.56
12:L:14:LEU:HD21	34:i:74:HIS:O	2.06	0.56
55:L:701:3PE:H3B2	35:j:71:TRP:HH2	1.71	0.56
13:M:196:TRP:HE1	13:M:250:LEU:HD13	1.68	0.56
14:N:253:GLY:H	14:N:290:LEU:HD11	1.71	0.56
14:N:258:THR:OG1	14:N:336:THR:HG22	2.05	0.56
16:P:41:ILE:HB	16:P:43:HIS:CE1	2.41	0.56
16:P:192:ARG:HE	16:P:200:ILE:HD12	1.70	0.56
18:R:33:HIS:HD2	18:R:34:THR:HG23	1.70	0.56
18:R:77:ILE:HD11	18:R:111:PHE:CG	2.41	0.56
27:b:11:ASN:OD1	27:b:12:ALA:N	2.39	0.56
39:n:50:GLU:HG2	39:n:51:HIS:N	2.20	0.56
48:Ad:248:ILE:HG23	48:Ad:252:VAL:HG11	1.87	0.56
49:Ae:179:ARG:NH2	49:Ae:208:PRO:HA	2.21	0.56
53:Aj:30:LEU:HA	54:Ak:34:TRP:CG	2.40	0.56
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.35	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:87:VAL:HG23	8:H:96:ILE:HD11	1.88	0.56
12:L:589:MET:O	12:L:592:LEU:N	2.39	0.56
18:R:69:VAL:CG1	18:R:112:LYS:HB2	2.35	0.56
25:Z:129:THR:HG22	25:Z:131:GLU:H	1.70	0.56
39:n:57:MET:HE2	39:n:57:MET:HA	1.86	0.56
40:o:121:ARG:NH1	40:o:122:VAL:HB	2.21	0.56
50:AF:22:TYR:CE2	50:AF:28:ASN:HB3	2.41	0.56
47:Ac:311:LYS:O	50:Af:39:HIS:N	2.31	0.56
48:Ad:237:PHE:CG	48:Ad:238:PRO:HD2	2.41	0.56
2:B:224:ARG:HD3	16:P:85:ARG:HH12	1.70	0.56
3:C:67:ILE:HA	21:V:43:ALA:HB3	1.87	0.56
3:C:184:ARG:HH22	4:D:112:HIS:CD2	2.24	0.56
5:E:131:ILE:HD11	5:E:185:VAL:CB	2.24	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
12:L:538:PRO:O	12:L:542:LEU:HD13	2.06	0.56
12:L:598:ILE:HG21	14:N:100:MET:HE2	1.87	0.56
13:M:73:LEU:CD2	13:M:103:GLN:CD	2.79	0.56
13:M:158:ILE:HG21	14:N:283:ALA:HB1	1.88	0.56
18:R:69:VAL:HG12	18:R:112:LYS:N	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:160:PRO:HG3	29:d:22:PRO:CD	2.35	0.56
41:p:74:ILE:CD1	41:p:85:ILE:HG13	2.36	0.56
42:q:142:THR:HG1	42:q:143:PRO:HD2	1.68	0.56
46:AB:116:ARG:HH22	46:AB:175:GLU:CD	2.14	0.56
47:AC:98:VAL:HG22	67:AC:402:HEM:CBC	2.23	0.56
45:Aa:402:HIS:ND1	45:Aa:403:LEU:CD1	2.67	0.56
48:Ad:114:PHE:HD2	48:Ad:140:TYR:CZ	2.24	0.56
2:B:81:LEU:HA	58:B:303:PC1:H242	1.88	0.55
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.41	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
9:I:68:ARG:NH2	25:Z:26:PRO:O	2.39	0.55
13:M:309:PHE:O	13:M:313:THR:HG23	2.06	0.55
18:R:35:GLY:O	18:R:36:GLN:HB3	2.05	0.55
32:g:106:TYR:CE2	33:h:86:ILE:CD1	2.89	0.55
47:AC:147:THR:HG21	47:AC:165:TRP:CD1	2.40	0.55
47:AC:260:ASN:O	47:AC:261:PRO:C	2.43	0.55
45:Aa:403:LEU:CD1	45:Aa:403:LEU:N	2.69	0.55
46:Ab:366:LEU:HD21	46:Ab:425:VAL:HG22	1.87	0.55
47:Ac:119:LEU:HD22	67:Ac:402:HEM:CBB	2.32	0.55
47:Ac:294:LEU:HD21	70:Ac:404:U10:H1M3	1.88	0.55
49:Ae:132:VAL:O	49:Ae:135:GLN:HG2	2.06	0.55
6:F:42:PHE:HD2	6:F:275:LEU:HD11	1.70	0.55
8:H:102:ILE:CG2	8:H:150:LEU:HD11	2.35	0.55
14:N:325:MET:HE3	14:N:329:LEU:HD11	1.88	0.55
17:Q:126:LEU:HD13	17:Q:137:PHE:CE2	2.40	0.55
23:X:20:VAL:CG2	23:X:25:LEU:HD11	2.33	0.55
24:Y:76:THR:CG2	24:Y:95:GLY:HA3	2.34	0.55
38:m:49:LEU:CD2	39:n:140:LEU:HD23	2.35	0.55
40:o:69:CYS:O	40:o:69:CYS:SG	2.64	0.55
45:AA:118:ALA:HB2	45:AA:135:ALA:HB2	1.87	0.55
46:AB:236:GLN:HG3	46:AB:237:PHE:CD2	2.41	0.55
46:AB:366:LEU:HD21	46:AB:425:VAL:HG22	1.87	0.55
47:AC:129:MET:HB2	47:AC:182:HIS:HD1	1.71	0.55
47:AC:153:ILE:HB	47:AC:157:GLY:CA	2.36	0.55
45:Aa:120:LEU:HD23	46:Ab:299:ILE:HG12	1.88	0.55
48:Ad:224:GLY:HA3	52:Ah:64:ASP:HB3	1.87	0.55
49:Ae:159:ILE:CG2	49:Ae:163:LYS:HB2	2.35	0.55
52:Ah:42:VAL:HA	52:Ah:45:ARG:HB3	1.88	0.55
1:A:49:LEU:HD23	4:D:80:MET:SD	2.46	0.55
2:B:94:THR:N	57:B:302:UQ1:H113	2.16	0.55
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:545:LEU:HD21	7:G:547:LEU:HD21	1.88	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
8:H:114:TYR:OH	10:J:60:LEU:HD13	2.06	0.55
10:J:6:PHE:O	10:J:7:VAL:C	2.50	0.55
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.89	0.55
12:L:466:PHE:HB2	35:j:68:TRP:CH2	2.39	0.55
12:L:556:ILE:HG21	38:m:80:PHE:CZ	2.39	0.55
12:L:586:LEU:CD2	24:Y:47:PRO:HD3	2.35	0.55
13:M:4:ILE:H	13:M:4:ILE:HD12	1.70	0.55
14:N:3:PRO:HG2	15:O:289:TRP:CH2	2.42	0.55
15:O:224:PRO:HA	15:O:227:MET:CE	2.36	0.55
17:Q:163:ASN:OD1	17:Q:163:ASN:C	2.48	0.55
19:S:55:ILE:O	19:S:55:ILE:HG13	2.05	0.55
20:U:87:LEU:CB	20:U:98:LEU:HD22	2.36	0.55
23:X:158:LEU:HD13	29:d:17:GLU:HG3	1.88	0.55
24:Y:137:LEU:HD23	24:Y:138:PHE:CD2	2.41	0.55
26:a:40:ARG:HG2	26:a:41:VAL:HG13	1.87	0.55
45:AA:403:LEU:CD1	45:AA:403:LEU:N	2.69	0.55
45:AA:467:ASP:OD2	47:AC:223:TYR:HE2	1.88	0.55
46:AB:60:ARG:HG3	46:AB:124:GLU:HB3	1.89	0.55
52:AH:35:CYS:O	52:AH:38:LEU:HB2	2.07	0.55
45:Aa:113:VAL:CG2	45:Aa:118:ALA:HB3	2.36	0.55
54:Ak:10:TYR:HA	54:Ak:13:LEU:HD12	1.87	0.55
2:B:170:TYR:HE2	4:D:135:TYR:CE1	2.24	0.55
3:C:104:ASN:O	43:r:97:PRO:HD3	2.06	0.55
4:D:181:LEU:CD1	4:D:210:MET:CE	2.84	0.55
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.40	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
7:G:289:LYS:NZ	7:G:697:THR:OG1	2.36	0.55
7:G:400:VAL:HG22	7:G:473:MET:HG2	1.87	0.55
8:H:150:LEU:O	8:H:154:LEU:HG	2.07	0.55
8:H:161:SER:HB2	8:H:164:THR:HG23	1.87	0.55
11:K:93:LEU:HA	14:N:54:GLU:OE2	2.06	0.55
12:L:54:PHE:O	12:L:58:ASN:CA	2.55	0.55
12:L:94:LEU:CD2	12:L:125:LEU:HD21	2.35	0.55
12:L:145:GLU:HG2	13:M:370:PRO:HD3	1.88	0.55
13:M:162:ILE:CG2	14:N:271:MET:HE3	2.23	0.55
16:P:148:ILE:HB	16:P:149:PRO:HD3	1.87	0.55
20:T:134:ASP:HA	20:T:137:LYS:NZ	2.21	0.55
24:Y:71:MET:CG	24:Y:102:THR:HG21	2.37	0.55
25:Z:89:GLU:O	25:Z:93:GLU:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:97:ILE:HG13	25:Z:98:MET:H	1.71	0.55
45:AA:170:ARG:HG3	45:AA:171:GLU:N	2.22	0.55
48:AD:252:VAL:CG1	48:AD:253:LEU:H	2.20	0.55
52:AH:27:PRO:HB3	52:AH:87:ASN:ND2	2.22	0.55
52:AH:45:ARG:HG2	52:AH:49:GLU:HG2	1.88	0.55
45:Aa:74:TRP:CD2	45:Aa:414:GLY:HA3	2.42	0.55
46:Ab:177:LEU:HD21	46:Ab:272:VAL:CG1	2.37	0.55
71:Ad:402:3PH:C37	49:Ae:128:ALA:CB	2.84	0.55
55:A:201:3PE:H272	27:b:23:PHE:CD2	2.41	0.55
3:C:120:THR:CG2	3:C:121:ARG:N	2.68	0.55
4:D:380:HIS:O	4:D:384:LEU:HG	2.07	0.55
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.18	0.55
14:N:237:THR:O	14:N:237:THR:CG2	2.55	0.55
20:U:72:PRO:CG	35:j:42:PRO:HG2	2.35	0.55
27:b:69:HIS:CG	27:b:70:PRO:HD2	2.41	0.55
36:k:30:ILE:CD1	36:k:39:GLN:HB2	2.33	0.55
45:AA:68:THR:OG1	46:AB:387:GLU:OE1	2.24	0.55
48:AD:219:CYS:SG	48:AD:220:GLU:N	2.79	0.55
45:Aa:87:ASN:H	45:Aa:207:ASN:HD22	1.53	0.55
45:Aa:109:LEU:CG	45:Aa:110:GLU:N	2.70	0.55
71:Ad:402:3PH:C35	49:Ae:128:ALA:CB	2.85	0.55
49:Ae:169:TRP:CD1	49:Ae:170:ARG:HG3	2.40	0.55
49:Ai:72:VAL:HG23	49:Ai:73:PRO:HD3	1.88	0.55
1:A:6:VAL:HG11	8:H:87:VAL:CG1	2.36	0.55
4:D:123:LEU:HB3	4:D:135:TYR:OH	2.07	0.55
4:D:163:PRO:HG2	4:D:168:GLN:HE21	1.71	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.42	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.06	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
8:H:68:MET:O	8:H:72:ILE:HG12	2.06	0.55
12:L:230:HIS:N	12:L:231:PRO:HD3	2.22	0.55
13:M:453:LEU:HD12	13:M:454:ILE:CG2	2.34	0.55
14:N:224:SER:HB2	14:N:229:SER:HB3	1.89	0.55
15:O:230:THR:HG22	15:O:233:TYR:H	1.72	0.55
15:O:332:ARG:NH1	29:d:50:MET:HE1	2.21	0.55
21:V:22:GLU:O	21:V:23:ARG:C	2.50	0.55
21:V:33:ASP:O	21:V:36:LYS:N	2.34	0.55
22:W:42:TRP:CE2	22:W:93:LEU:HG	2.41	0.55
24:Y:115:MET:HG3	55:Y:201:3PE:H322	1.89	0.55
25:Z:115:ARG:NH2	30:e:39:GLU:OE1	2.39	0.55
31:f:43:LEU:HD21	41:p:68:TYR:CD1	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:49:ARG:HG3	31:f:52:GLU:HG2	1.89	0.55
35:j:99:ILE:HA	40:o:108:LEU:HD21	1.88	0.55
45:AA:182:VAL:CG1	45:AA:186:TYR:HE2	2.20	0.55
47:AC:198:LEU:CD1	47:Ac:9:PRO:HB2	2.37	0.55
52:AH:42:VAL:HG13	52:AH:45:ARG:NH2	2.20	0.55
52:AH:58:ARG:CZ	52:AH:60:GLN:HE21	2.20	0.55
45:Aa:109:LEU:HD12	45:Aa:110:GLU:HA	1.87	0.55
55:Aa:501:3PE:H112	55:Aa:501:3PE:H11	1.88	0.55
47:Ac:97:HIS:CE1	47:Ac:100:ARG:HH21	2.23	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:181:MET:HE3	8:H:300:LEU:HD13	1.89	0.55
9:I:180:HIS:NE2	16:P:100:LEU:HD21	2.21	0.55
12:L:358:LYS:NZ	39:n:34:ARG:HH12	2.05	0.55
12:L:561:THR:O	12:L:565:SER:HB2	2.07	0.55
15:O:170:LEU:HG	15:O:179:ILE:HD13	1.87	0.55
15:O:256:LEU:HD11	15:O:276:LEU:CD2	2.35	0.55
16:P:91:ILE:HD12	16:P:105:PHE:HD2	1.70	0.55
16:P:206:ILE:HG13	64:P:401:NDP:H42N	1.89	0.55
26:a:58:ASN:HB3	26:a:60:TYR:CE1	2.39	0.55
30:e:14:LEU:HD12	30:e:15:ASP:N	2.21	0.55
37:l:109:LEU:O	37:l:109:LEU:HG	2.06	0.55
47:AC:168:PHE:CD2	49:Ae:170:ARG:HB3	2.42	0.55
49:Ae:248:ARG:HA	49:Ae:257:ASN:CG	2.32	0.55
50:Af:15:ASP:OD2	50:Af:19:LYS:NZ	2.39	0.55
1:A:5:THR:O	1:A:9:ILE:HG12	2.07	0.55
1:A:52:SER:C	10:J:73:MET:HE3	2.32	0.55
4:D:171:ARG:HG2	4:D:227:ILE:HD12	1.88	0.55
5:E:130:HIS:NE2	5:E:132:GLN:HG2	2.21	0.55
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.55
7:G:304:GLU:HG3	7:G:305:PRO:HD2	1.89	0.55
8:H:157:ASN:OD1	8:H:158:GLY:N	2.40	0.55
12:L:69:VAL:HG11	12:L:71:MET:HE2	1.89	0.55
12:L:258:PHE:HE1	12:L:262:ARG:HH21	1.55	0.55
13:M:17:LEU:HD13	31:f:11:TRP:CH2	2.42	0.55
13:M:62:SER:C	13:M:64:PRO:HD2	2.32	0.55
14:N:230:ILE:O	14:N:233:LEU:HB2	2.07	0.55
15:O:76:GLU:O	15:O:80:GLN:HG2	2.07	0.55
16:P:232:GLY:HA2	16:P:273:LEU:HD23	1.88	0.55
31:f:46:ARG:HD2	33:h:106:ILE:HD13	1.87	0.55
49:AE:119:ALA:CA	53:AJ:25:ILE:HD11	2.29	0.55
51:AG:67:PHE:CE2	51:AG:71:LYS:HD3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AG:79:GLU:HG3	52:AH:58:ARG:CD	2.36	0.55
52:AH:35:CYS:SG	52:AH:80:VAL:HA	2.47	0.55
47:Ac:312:GLN:HE21	50:Af:37:THR:HB	1.72	0.55
49:Ae:244:ASP:HB3	49:Ae:250:ARG:HH11	1.71	0.55
52:Ah:73:LEU:O	52:Ah:74:HIS:C	2.50	0.55
2:B:97:LEU:CD2	2:B:141:MET:HG2	2.36	0.55
2:B:117:PHE:HZ	9:I:86:TYR:HB3	1.72	0.55
4:D:140:ASP:H	4:D:147:ASN:ND2	2.05	0.55
4:D:386:THR:CG2	9:I:118:LEU:CD1	2.85	0.55
6:F:48:ARG:HG2	6:F:48:ARG:O	2.06	0.55
7:G:377:ALA:HB3	7:G:384:ASN:ND2	2.19	0.55
12:L:162:THR:O	12:L:166:THR:HG23	2.06	0.55
12:L:386:LEU:HD11	35:j:69:ILE:HD11	1.89	0.55
15:O:238:GLU:HA	15:O:241:TYR:CD2	2.32	0.55
15:O:354:LEU:HG	28:c:44:VAL:HG22	1.89	0.55
16:P:272:LEU:HG	16:P:375:VAL:HG11	1.88	0.55
19:S:51:LEU:O	19:S:53:ILE:HG13	2.07	0.55
24:Y:115:MET:HE1	55:Y:201:3PE:H222	1.89	0.55
25:Z:97:ILE:HG13	30:e:92:TYR:HD1	1.70	0.55
25:Z:98:MET:CG	30:e:92:TYR:CD1	2.90	0.55
47:AC:256:TYR:CE1	48:AD:202:ARG:HD3	2.42	0.55
50:AF:39:HIS:HD2	50:AF:41:THR:HG22	1.71	0.55
53:AJ:30:LEU:HD12	54:AK:34:TRP:HB2	1.89	0.55
45:Aa:96:LEU:HD11	45:Aa:161:ILE:HG12	1.89	0.55
46:Ab:181:ALA:O	46:Ab:254:ARG:HG2	2.07	0.55
47:Ac:30:TRP:CE2	55:Ac:403:3PE:H232	2.42	0.55
49:Ae:207:LYS:CD	49:Ae:210:TRP:HD1	2.20	0.55
4:D:451:ILE:CG2	4:D:456:ILE:HD11	2.33	0.55
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:388:ASN:N	7:G:514:ASN:HB2	2.22	0.55
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.88	0.55
9:I:68:ARG:NH1	25:Z:28:ARG:HG2	2.22	0.55
9:I:211:TYR:CE1	43:r:39:PRO:HG3	2.41	0.55
11:K:1:MET:HA	11:K:4:THR:CG2	2.37	0.55
12:L:459:PHE:HD2	55:L:701:3PE:H242	1.71	0.55
12:L:566:THR:HG21	55:L:705:3PE:H361	1.87	0.55
13:M:231:LEU:CA	13:M:235:LEU:HD12	2.36	0.55
15:O:319:ILE:HG13	15:O:320:GLY:H	1.72	0.55
23:X:64:ASN:OD1	23:X:64:ASN:O	2.25	0.55
40:o:25:PHE:CZ	40:o:109:LEU:HA	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:74:TRP:CD2	45:AA:414:GLY:HA3	2.42	0.55
50:AF:77:PRO:HB2	50:AF:80:GLN:HG3	1.88	0.55
51:AG:74:ASN:HB3	51:AG:77:MET:CG	2.33	0.55
46:Ab:65:VAL:HG22	46:Ab:218:MET:CG	2.35	0.55
49:Ae:192:VAL:HA	49:Ae:195:LEU:CD1	2.37	0.55
49:Ae:228:ALA:HB3	49:Ae:235:TYR:HB3	1.88	0.55
49:Ae:241:SER:OG	49:Ae:253:PRO:HD2	2.07	0.55
52:Ah:45:ARG:HD2	52:Ah:48:LEU:HD23	1.89	0.55
1:A:52:SER:N	10:J:73:MET:HE3	2.22	0.54
4:D:80:MET:SD	4:D:101:LEU:HD12	2.46	0.54
4:D:174:PHE:CZ	4:D:240:LEU:HD21	2.43	0.54
4:D:202:TRP:CH2	4:D:261:MET:HE3	2.42	0.54
4:D:301:ASP:O	4:D:302:LEU:HB2	2.05	0.54
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.89	0.54
5:E:226:PRO:HD3	6:F:46:TYR:CE2	2.42	0.54
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.54
8:H:264:LEU:O	8:H:268:SER:N	2.37	0.54
10:J:132:GLY:O	26:a:42:GLN:HB2	2.06	0.54
11:K:66:PHE:CZ	14:N:35:PHE:CZ	2.95	0.54
12:L:25:ASN:HB2	33:h:72:LYS:HZ1	1.71	0.54
12:L:54:PHE:O	12:L:58:ASN:HA	2.07	0.54
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.43	0.54
13:M:6:LEU:HB3	13:M:7:PRO:HD3	1.88	0.54
18:R:44:ARG:HB3	18:R:47:ARG:NH1	2.22	0.54
30:e:101:ARG:O	30:e:104:PRO:HD3	2.06	0.54
34:i:83:HIS:HE1	34:i:87:LYS:HD2	1.71	0.54
38:m:129:TYR:CE2	41:p:146:LEU:O	2.60	0.54
40:o:103:GLU:OE2	40:o:106:ARG:HD2	2.07	0.54
46:AB:85:LEU:HD21	49:AI:68:VAL:HG11	1.88	0.54
47:AC:69:ILE:HA	47:AC:73:VAL:CB	2.36	0.54
51:AG:46:ILE:HD11	51:AG:50:ALA:HB2	1.88	0.54
45:Aa:296:TRP:HH2	45:Aa:415:ARG:HH11	1.55	0.54
48:Ad:231:LEU:HD22	48:Ad:241:ALA:HB1	1.88	0.54
2:B:175:TYR:OH	3:C:197:PHE:CE1	2.60	0.54
4:D:97:LEU:CD1	4:D:109:CYS:HB3	2.35	0.54
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.37	0.54
10:J:130:ASP:O	26:a:46:TYR:HB2	2.07	0.54
12:L:190:SER:HB2	12:L:196:TRP:NE1	2.22	0.54
13:M:415:GLN:O	13:M:416:ARG:HG3	2.08	0.54
14:N:246:LEU:HD11	55:N:401:3PE:H3A1	1.89	0.54
15:O:305:LEU:O	15:O:305:LEU:CD1	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:304:LEU:H	16:P:304:LEU:HD12	1.71	0.54
19:S:51:LEU:O	19:S:52:PRO:C	2.48	0.54
30:e:32:ARG:O	30:e:33:CYS:HB2	2.06	0.54
33:h:73:PHE:CD2	33:h:74:TYR:CE1	2.94	0.54
34:i:16:ARG:O	34:i:20:ARG:HG2	2.08	0.54
47:AC:8:HIS:NE2	47:Ac:199:PHE:HE1	2.05	0.54
45:Aa:139:ASP:O	45:Aa:143:VAL:HG23	2.07	0.54
46:Ab:297:PRO:CA	46:Ab:304:ASN:OD1	2.52	0.54
49:Ae:122:THR:HG21	53:Aj:25:ILE:HG21	1.89	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
8:H:90:PRO:CD	8:H:240:ILE:HD13	2.38	0.54
8:H:92:PRO:HG2	8:H:255:TYR:HB3	1.88	0.54
8:H:196:ALA:O	8:H:197:PRO:C	2.41	0.54
11:K:21:MET:O	55:K:101:3PE:H222	2.07	0.54
12:L:232:TRP:O	12:L:236:ALA:N	2.40	0.54
14:N:147:PRO:HB2	14:N:148:LEU:HD12	1.89	0.54
20:U:85:TYR:HA	20:U:88:LYS:HD3	1.89	0.54
23:X:158:LEU:HD13	29:d:17:GLU:CG	2.38	0.54
24:Y:17:GLY:O	24:Y:81:GLN:HG2	2.07	0.54
32:g:147:LEU:HD11	41:p:163:MET:HE2	1.89	0.54
40:o:24:SER:HB2	40:o:105:GLU:OE2	2.08	0.54
40:o:115:ARG:O	40:o:119:GLU:N	2.27	0.54
47:AC:184:ILE:HG12	47:AC:188:ILE:HG13	1.90	0.54
46:Ab:300:LYS:HG2	46:Ab:301:ARG:CG	2.37	0.54
49:Ae:190:VAL:HG11	49:Ae:195:LEU:HD21	1.90	0.54
51:Ag:39:LEU:O	51:Ag:42:THR:HG22	2.08	0.54
52:Ah:79:CYS:O	52:Ah:82:HIS:HB3	2.07	0.54
1:A:3:LEU:CD2	55:H:401:3PE:H31	2.35	0.54
2:B:84:TRP:CZ3	58:B:303:PC1:H371	2.42	0.54
2:B:107:MET:CE	2:B:114:MET:HE2	2.37	0.54
3:C:160:ILE:CD1	4:D:285:ASN:HD22	2.19	0.54
3:C:219:VAL:HG11	22:W:113:THR:CG2	2.37	0.54
4:D:411:LEU:HD11	4:D:419:PRO:HB3	1.90	0.54
6:F:167:SER:CB	44:s:75:TYR:CE2	2.91	0.54
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.54
7:G:246:ARG:NH2	17:Q:123:ASN:OD1	2.40	0.54
7:G:330:LEU:HD13	7:G:546:PHE:HZ	1.71	0.54
7:G:629:ILE:CD1	22:W:122:LEU:HD21	2.37	0.54
8:H:197:PRO:HD2	8:H:198:PHE:CD2	2.42	0.54
12:L:427:ILE:CD1	36:k:69:PHE:HE1	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:586:LEU:HD21	24:Y:47:PRO:HD3	1.89	0.54
14:N:307:THR:C	15:O:319:ILE:HG12	2.32	0.54
20:U:110:LEU:HD13	20:U:118:ILE:CD1	2.38	0.54
30:e:72:THR:O	30:e:73:MET:C	2.49	0.54
32:g:106:TYR:HE2	33:h:86:ILE:CD1	2.20	0.54
37:l:119:THR:HG23	38:m:11:LEU:HA	1.88	0.54
45:AA:74:TRP:HB3	45:AA:418:LEU:HD11	1.89	0.54
45:AA:311:ILE:HD11	45:AA:379:LEU:HD11	1.88	0.54
46:AB:60:ARG:CZ	46:AB:390:GLU:HB3	2.37	0.54
46:AB:313:VAL:HG13	46:AB:350:VAL:HG13	1.89	0.54
47:AC:45:ILE:CA	67:AC:401:HEM:HAB	2.31	0.54
47:AC:319:PRO:HD2	50:AF:21:TYR:CZ	2.42	0.54
46:Ab:237:PHE:O	46:Ab:240:MET:HG2	2.08	0.54
49:Ae:195:LEU:HD11	49:Ae:248:ARG:HH11	1.72	0.54
2:B:81:LEU:CG	8:H:53:MET:SD	2.95	0.54
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.89	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:197:PRO:HD3	8:H:273:ILE:CG2	2.36	0.54
10:J:63:MET:HE3	11:K:68:ALA:HA	1.90	0.54
11:K:1:MET:CA	11:K:4:THR:HG22	2.36	0.54
12:L:551:THR:HA	12:L:555:LEU:HD12	1.89	0.54
13:M:127:ILE:CD1	14:N:256:PRO:HG2	2.37	0.54
13:M:336:ARG:HH22	13:M:429:SER:HA	1.73	0.54
55:N:401:3PE:H2I2	62:X:201:CDL:H602	1.88	0.54
15:O:60:ILE:O	15:O:158:VAL:HA	2.08	0.54
19:S:16:LEU:HD21	19:S:19:ILE:HD11	1.89	0.54
19:S:26:ARG:HA	19:S:34:ARG:NH1	2.23	0.54
19:S:44:LEU:HD22	19:S:91:MET:HG2	1.89	0.54
20:U:131:PRO:HG2	20:U:134:ASP:HB2	1.90	0.54
23:X:41:LYS:CB	23:X:131:VAL:HG11	2.38	0.54
25:Z:58:ARG:HG2	27:b:45:ILE:CD1	2.38	0.54
28:c:72:ARG:NE	29:d:19:ARG:HB2	2.23	0.54
28:c:72:ARG:NH1	29:d:19:ARG:HD3	2.22	0.54
55:d:201:3PE:H221	55:d:201:3PE:H362	1.89	0.54
45:AA:186:TYR:HE1	49:AE:80:HIS:O	1.91	0.54
46:Ab:159:LYS:HB2	46:Ab:197:MET:SD	2.47	0.54
47:Ac:222:PRO:HG2	47:Ac:223:TYR:CD2	2.43	0.54
1:A:59:ALA:HB1	10:J:66:VAL:HG13	1.89	0.54
5:E:151:LEU:CD1	5:E:200:ILE:HD13	2.37	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.89	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
9:I:143:THR:HA	18:R:34:THR:HG21	1.89	0.54
10:J:60:LEU:HD13	10:J:61:GLY:N	2.21	0.54
10:J:120:LEU:HD21	10:J:124:LEU:HD22	1.89	0.54
12:L:362:ILE:HA	12:L:365:ILE:HG13	1.90	0.54
13:M:79:ALA:HB1	13:M:225:ILE:HD13	1.90	0.54
15:O:170:LEU:HG	15:O:179:ILE:CD1	2.37	0.54
22:W:27:ASP:HB2	22:W:30:GLU:HG3	1.89	0.54
23:X:9:THR:HG22	23:X:11:GLU:H	1.72	0.54
33:h:179:ILE:HG22	33:h:180:ASP:H	1.73	0.54
35:j:98:GLY:O	35:j:100:PRO:HD3	2.06	0.54
38:m:109:ARG:O	38:m:113:GLU:HG2	2.08	0.54
45:AA:407:THR:O	45:AA:408:PRO:C	2.49	0.54
46:AB:237:PHE:O	46:AB:238:LEU:HB2	2.07	0.54
47:AC:68:HIS:ND1	47:AC:73:VAL:HG23	2.22	0.54
47:AC:260:ASN:C	47:AC:262:LEU:N	2.62	0.54
45:Aa:74:TRP:HB3	45:Aa:418:LEU:HD11	1.89	0.54
45:Aa:96:LEU:CD1	45:Aa:161:ILE:HG12	2.37	0.54
47:Ac:153:ILE:HB	47:Ac:157:GLY:CA	2.37	0.54
49:Ae:152:ILE:HD13	49:Ae:169:TRP:CD1	2.42	0.54
1:A:52:SER:C	10:J:73:MET:CE	2.81	0.54
2:B:175:TYR:OH	4:D:117:HIS:CE1	2.61	0.54
4:D:159:LEU:HD21	4:D:391:VAL:HG12	1.90	0.54
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:557:ARG:HD3	42:q:144:TYR:CD2	2.43	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:100:LEU:HD23	10:J:53:LEU:HD12	1.89	0.54
8:H:157:ASN:ND2	8:H:165:LEU:CD1	2.71	0.54
10:J:133:VAL:HG12	26:a:41:VAL:CG2	2.38	0.54
10:J:168:GLU:OE2	14:N:1:MET:HE2	2.07	0.54
12:L:232:TRP:CH2	12:L:233:LEU:HD21	2.42	0.54
12:L:572:ASN:OD1	55:Y:201:3PE:H221	2.08	0.54
13:M:278:ARG:HG2	37:l:116:ARG:HH12	1.72	0.54
14:N:82:GLY:HA3	30:e:21:LEU:HG	1.89	0.54
17:Q:53:ILE:HG12	22:W:26:ARG:O	2.08	0.54
18:R:40:GLU:HA	18:R:45:ARG:HH11	1.72	0.54
46:AB:171:THR:HA	49:AI:64:LEU:HD21	1.88	0.54
46:AB:339:TYR:CD2	49:AI:59:ALA:HB1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:68:HIS:O	47:AC:72:ASP:N	2.34	0.54
47:AC:222:PRO:HG2	47:AC:223:TYR:CD2	2.43	0.54
48:AD:214:LEU:HD11	48:AD:237:PHE:HD1	1.72	0.54
49:AE:127:TYR:OH	53:AJ:36:PHE:CD1	2.51	0.54
53:AJ:33:GLU:CB	54:AK:34:TRP:HE1	2.20	0.54
45:Aa:170:ARG:HG3	45:Aa:171:GLU:N	2.22	0.54
47:Ac:77:TRP:HZ2	48:Ad:284:HIS:HD2	1.52	0.54
2:B:171:TYR:HE1	4:D:120:THR:HG1	1.54	0.54
2:B:194:CYS:HB3	2:B:195:PRO:CD	2.33	0.54
4:D:133:LEU:HB3	4:D:134:PRO:HD3	1.88	0.54
4:D:255:ILE:HG22	4:D:338:ARG:NH2	2.22	0.54
5:E:87:ARG:HD2	44:s:77:THR:HB	1.89	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
8:H:68:MET:O	8:H:69:SER:C	2.49	0.54
11:K:4:THR:CG2	11:K:5:PHE:N	2.71	0.54
12:L:131:LEU:CD1	12:L:140:LEU:CD1	2.78	0.54
13:M:160:LEU:HD23	13:M:164:LEU:HD13	1.89	0.54
13:M:276:CYS:HB3	13:M:285:LEU:HG	1.89	0.54
13:M:283:LYS:HG3	13:M:327:PHE:CE1	2.43	0.54
13:M:373:ILE:HD11	13:M:454:ILE:HD11	1.88	0.54
16:P:302:GLY:O	16:P:303:LYS:C	2.50	0.54
19:S:63:PRO:HB2	19:S:79:LEU:CD1	2.37	0.54
24:Y:114:ALA:HB2	55:m:203:3PE:H231	1.90	0.54
38:m:8:PRO:HB3	38:m:14:LEU:N	2.23	0.54
39:n:125:TRP:CE3	39:n:128:LEU:HD12	2.42	0.54
40:o:6:THR:HA	40:o:10:LEU:HD13	1.89	0.54
48:AD:183:GLU:HB3	48:Ad:161:ASP:HB3	1.89	0.54
48:AD:189:ASN:HB3	69:AD:401:HEC:CMD	2.29	0.54
48:AD:218:TYR:CE1	48:AD:242:ILE:HG21	2.39	0.54
48:AD:252:VAL:HG13	48:AD:253:LEU:HG	1.90	0.54
52:AH:45:ARG:O	52:AH:49:GLU:HG2	2.08	0.54
49:AI:43:LEU:O	49:AI:44:ASP:C	2.51	0.54
49:AI:72:VAL:HG23	49:AI:73:PRO:HD3	1.88	0.54
45:Aa:407:THR:O	45:Aa:408:PRO:C	2.49	0.54
48:Ad:178:PRO:HG2	48:Ad:179:TYR:H	1.72	0.54
4:D:311:TYR:HA	4:D:314:VAL:HG22	1.89	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
6:F:194:ASP:OD2	44:s:91:ARG:CB	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:179:CYS:HG	56:G:802:SF4:FE3	1.23	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
8:H:86:TRP:NE1	8:H:229:THR:HG22	2.20	0.54
8:H:317:TYR:O	8:H:318:MET:HB2	2.08	0.54
9:I:90:LYS:HD3	42:q:91:HIS:HE1	1.72	0.54
13:M:231:LEU:O	13:M:236:LEU:HG	2.06	0.54
14:N:307:THR:HB	15:O:319:ILE:HG12	1.89	0.54
17:Q:81:VAL:O	17:Q:81:VAL:HG13	2.07	0.54
17:Q:161:GLY:HA2	17:Q:164:PHE:HD2	1.72	0.54
22:W:69:MET:C	22:W:71:MET:N	2.62	0.54
22:W:120:ASP:HB3	22:W:123:SER:OG	2.08	0.54
23:X:108:ASP:O	23:X:112:LEU:N	2.41	0.54
27:b:80:TRP:CG	27:b:81:LEU:N	2.76	0.54
46:AB:313:VAL:HG11	46:AB:321:PHE:CG	2.42	0.54
48:AD:255:TYR:HB3	48:AD:257:ASP:OD1	2.08	0.54
50:AF:85:GLU:H	50:AF:85:GLU:CD	2.15	0.54
51:AG:45:ARG:HG2	51:AG:48:ARG:HH22	1.71	0.54
47:Ac:377:LEU:O	47:Ac:378:LYS:HB2	2.06	0.54
49:AI:62:ARG:HB2	49:AI:78:PHE:C	2.33	0.54
1:A:87:MET:HG3	1:A:88:MET:N	2.23	0.54
1:A:92:PHE:CE1	8:H:302:MET:HG3	2.42	0.54
55:A:201:3PE:H361	27:b:23:PHE:CE1	2.43	0.54
2:B:219:LYS:HD2	2:B:223:ARG:CZ	2.38	0.54
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.43	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
8:H:93:HIS:HB2	26:a:24:ALA:HB2	1.90	0.54
9:I:72:MET:O	9:I:75:SER:OG	2.23	0.54
12:L:141:PHE:CD2	13:M:370:PRO:CG	2.91	0.54
12:L:264:HIS:HA	12:L:267:THR:HG23	1.89	0.54
13:M:1:MET:HE2	13:M:52:PHE:CE2	2.42	0.54
13:M:17:LEU:HD22	31:f:11:TRP:HH2	1.73	0.54
13:M:31:SER:HA	13:M:34:ILE:HG12	1.90	0.54
20:U:95:PRO:HG2	20:U:96:GLU:HG3	1.88	0.54
20:U:99:SER:O	20:U:100:VAL:C	2.51	0.54
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.54
38:m:123:ARG:O	41:p:140:GLN:NE2	2.40	0.54
47:AC:129:MET:HB3	47:AC:182:HIS:CB	2.25	0.54
47:AC:253:PRO:HB2	48:AD:203:ALA:O	2.08	0.54
49:AI:62:ARG:HB2	49:AI:78:PHE:C	2.33	0.54
49:Ae:136:PHE:O	49:Ae:137:VAL:C	2.51	0.54
1:A:18:ILE:HD12	8:H:76:THR:HG21	1.86	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LYS:HE3	3:C:71:TYR:CZ	2.43	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.38	0.53
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53
12:L:66:TRP:CZ3	12:L:68:TRP:CD1	2.96	0.53
12:L:226:GLN:OE1	12:L:284:THR:HG21	2.07	0.53
12:L:247:LEU:HD11	12:L:248:HIS:CE1	2.43	0.53
12:L:477:ILE:HG13	40:o:91:GLU:OE1	2.07	0.53
32:g:151:ASP:C	41:p:171:ARG:HH22	2.16	0.53
40:o:93:LEU:O	40:o:97:LYS:HG2	2.07	0.53
45:AA:204:PRO:O	45:AA:205:SER:C	2.50	0.53
46:AB:50:ALA:HB3	46:AB:221:VAL:HG22	1.90	0.53
47:AC:148:ASN:HB2	49:Ae:220:LEU:CA	2.33	0.53
50:AF:92:GLU:O	50:AF:96:LYS:HG3	2.08	0.53
53:AJ:23:LEU:CB	54:AK:27:VAL:CG2	2.69	0.53
45:Aa:120:LEU:HD23	46:Ab:299:ILE:HG23	1.89	0.53
48:Ad:133:ARG:O	48:Ad:136:VAL:HG23	2.08	0.53
48:Ad:193:LEU:O	69:Ad:401:HEC:HAD1	2.09	0.53
49:Ae:206:LYS:HG3	49:Ae:206:LYS:O	2.07	0.53
2:B:126:ARG:NH2	8:H:61:MET:SD	2.81	0.53
5:E:230:LEU:HD11	6:F:48:ARG:HH21	1.72	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.07	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:206:GLU:HG3	8:H:207:LEU:N	2.24	0.53
10:J:126:TYR:HD2	25:Z:120:LEU:HD11	1.73	0.53
12:L:559:GLU:HG2	12:L:564:LYS:HD3	1.90	0.53
15:O:114:LEU:HA	15:O:131:LEU:HD22	1.91	0.53
20:T:79:ILE:HD13	20:T:148:ILE:HG22	1.91	0.53
22:W:93:LEU:HD22	22:W:97:ILE:HG13	1.89	0.53
30:e:41:ILE:HD13	33:h:174:PRO:HD2	1.89	0.53
40:o:57:ASP:CG	40:o:59:CYS:H	2.16	0.53
41:p:31:THR:O	41:p:35:LYS:HG3	2.07	0.53
48:AD:170:LYS:O	48:AD:173:ASP:HB3	2.07	0.53
71:Ad:402:3PH:H332	71:Ad:402:3PH:C26	2.38	0.53
49:Ae:172:LYS:HD3	49:Ae:216:VAL:HG21	1.89	0.53
49:Ae:191:GLU:H	49:Ae:191:GLU:CD	2.14	0.53
52:Ah:47:ARG:CZ	52:Ah:47:ARG:HB3	2.38	0.53
2:B:170:TYR:CE2	4:D:135:TYR:CE2	2.95	0.53
4:D:323:ARG:O	4:D:325:ASP:N	2.41	0.53
5:E:230:LEU:HD21	6:F:48:ARG:HH21	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
6:F:233:VAL:HG11	17:Q:164:PHE:HB2	1.90	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.53
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.39	0.53
8:H:90:PRO:CB	8:H:162:LEU:HB3	2.37	0.53
8:H:181:MET:HE3	8:H:300:LEU:CD1	2.39	0.53
10:J:59:TYR:HD1	10:J:63:MET:SD	2.31	0.53
12:L:400:ASN:HD21	12:L:413:LEU:HD11	1.73	0.53
13:M:269:MET:CE	13:M:396:MET:HA	2.36	0.53
13:M:395:LEU:HD21	38:m:101:TRP:CZ2	2.43	0.53
14:N:179:MET:HE2	14:N:216:PHE:CE1	2.43	0.53
18:R:94:ASN:OD1	18:R:96:ASP:HB2	2.08	0.53
40:o:25:PHE:HB3	40:o:26:PRO:CD	2.37	0.53
41:p:103:MET:CE	41:p:135:VAL:HG12	2.38	0.53
45:AA:296:TRP:HH2	45:AA:415:ARG:HH11	1.55	0.53
49:AE:222:CYS:SG	47:Ac:268:ILE:HD12	2.47	0.53
46:Ab:91:THR:HG23	46:Ab:99:ILE:HD11	1.90	0.53
49:Ae:179:ARG:HH21	49:Ae:208:PRO:HA	1.74	0.53
53:Aj:23:LEU:HA	54:Ak:27:VAL:HG13	1.90	0.53
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.53
6:F:362:ASP:O	6:F:363:ILE:C	2.51	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
8:H:245:PRO:HG2	8:H:255:TYR:CE2	2.44	0.53
10:J:130:ASP:HB2	25:Z:79:LYS:HE3	1.90	0.53
12:L:387:THR:HG22	12:L:465:GLY:N	2.23	0.53
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.90	0.53
15:O:319:ILE:HG13	15:O:320:GLY:N	2.23	0.53
16:P:122:HIS:CD2	18:R:45:ARG:HB2	2.43	0.53
16:P:366:ILE:O	16:P:369:THR:HG22	2.08	0.53
21:V:44:TYR:CE2	21:V:94:MET:HG3	2.44	0.53
27:b:27:GLY:O	27:b:28:LEU:C	2.51	0.53
28:c:68:GLU:HG3	29:d:19:ARG:NH2	2.22	0.53
30:e:101:ARG:NE	30:e:104:PRO:HD2	2.24	0.53
45:AA:148:ALA:O	45:AA:152:GLN:HG2	2.09	0.53
50:AF:29:LYS:HA	50:AF:81:TRP:CG	2.44	0.53
45:Aa:98:PHE:O	45:Aa:109:LEU:HD11	2.08	0.53
4:D:390:GLN:HG3	4:D:415:GLY:O	2.09	0.53
6:F:166:ALA:HB1	44:s:80:PHE:CE1	2.44	0.53
6:F:382:CYS:SG	56:F:502:SF4:S4	3.06	0.53
8:H:261:MET:O	8:H:265:LEU:HD23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:362:ILE:HD12	12:L:430:VAL:HG13	1.87	0.53
12:L:362:ILE:CD1	12:L:430:VAL:CG1	2.82	0.53
15:O:140:LEU:HD11	15:O:198:TYR:OH	2.09	0.53
20:T:86:VAL:HG11	20:T:122:MET:SD	2.48	0.53
20:T:90:TYR:HD2	20:T:93:ILE:HB	1.73	0.53
30:e:101:ARG:CZ	30:e:104:PRO:HD2	2.38	0.53
37:l:184:TYR:CA	40:o:36:GLU:HA	2.30	0.53
47:AC:135:TRP:O	47:AC:135:TRP:CD1	2.60	0.53
48:AD:252:VAL:HG13	48:AD:253:LEU:H	1.72	0.53
46:Ab:52:LEU:HD22	46:Ab:392:PHE:HE2	1.72	0.53
7:G:161:GLU:OE1	18:R:97:LYS:HE2	2.09	0.53
7:G:243:TRP:NE1	9:I:121:ALA:HB2	2.23	0.53
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.53
9:I:54:THR:HA	27:b:13:TRP:NE1	2.24	0.53
9:I:57:ALA:HB2	27:b:13:TRP:O	2.09	0.53
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.90	0.53
12:L:20:LEU:C	12:L:20:LEU:CD1	2.81	0.53
12:L:361:ASN:HA	12:L:431:THR:O	2.09	0.53
13:M:55:MET:HG3	13:M:56:PHE:CD2	2.44	0.53
13:M:453:LEU:HD12	13:M:453:LEU:C	2.33	0.53
16:P:143:ASP:O	16:P:148:ILE:HG12	2.09	0.53
24:Y:50:SER:HB3	24:Y:53:GLU:HG2	1.91	0.53
32:g:147:LEU:HD21	41:p:163:MET:HB2	1.90	0.53
38:m:17:THR:HB	39:n:68:GLU:OE1	2.09	0.53
46:AB:70:ARG:NH2	46:AB:332:ASP:OD2	2.42	0.53
47:AC:122:ALA:HB1	47:AC:189:ILE:HG12	1.89	0.53
48:AD:217:GLY:O	48:AD:235:PRO:HD2	2.09	0.53
45:Aa:187:LEU:HD22	45:Aa:288:ALA:HB1	1.89	0.53
47:Ac:164:ILE:O	47:Ac:177:ARG:HD2	2.08	0.53
48:Ad:124:CYS:O	48:Ad:194:PRO:HB2	2.08	0.53
48:Ad:182:PRO:C	48:Ad:186:ARG:HH21	2.15	0.53
48:Ad:288:MET:SD	71:Ad:402:3PH:H11	2.48	0.53
53:Aj:33:GLU:O	53:Aj:34:ARG:C	2.50	0.53
2:B:170:TYR:CE2	4:D:135:TYR:CZ	2.97	0.53
57:B:302:UQ1:HM31	4:D:192:LEU:HB3	1.91	0.53
8:H:114:TYR:CZ	10:J:33:ILE:HD13	2.43	0.53
12:L:124:PHE:HZ	12:L:252:MET:HB2	1.74	0.53
13:M:57:SER:CB	13:M:113:THR:HG22	2.39	0.53
13:M:73:LEU:HD23	13:M:103:GLN:NE2	2.23	0.53
14:N:120:GLN:HE22	14:N:174:GLN:CB	2.21	0.53
16:P:130:ILE:HD13	16:P:148:ILE:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:301:ILE:HG22	16:P:305:PHE:CE2	2.43	0.53
18:R:44:ARG:O	18:R:47:ARG:HG2	2.09	0.53
30:e:41:ILE:HG23	33:h:179:ILE:HD11	1.91	0.53
32:g:139:TYR:CD2	32:g:140:PHE:CD1	2.96	0.53
40:o:29:LEU:O	40:o:104:ARG:NH2	2.41	0.53
48:AD:213:SER:HB3	48:AD:236:TYR:CD1	2.43	0.53
46:Ab:145:GLU:C	46:Ab:146:PHE:CD1	2.87	0.53
48:Ad:147:ALA:O	48:Ad:150:GLU:HB3	2.08	0.53
48:Ad:185:ALA:HB1	48:Ad:194:PRO:HD3	1.90	0.53
49:Ae:162:GLY:H	49:Ae:178:HIS:HD2	1.52	0.53
4:D:136:PHE:HZ	4:D:422:CYS:SG	2.31	0.53
5:E:165:ASP:C	5:E:167:LEU:N	2.64	0.53
7:G:382:ARG:HB3	7:G:386:LEU:HD12	1.89	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.09	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
10:J:103:ILE:HG22	10:J:107:ASN:OD1	2.08	0.53
12:L:79:SER:CB	12:L:135:ASN:HB2	2.36	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.53
12:L:128:MET:CG	12:L:251:THR:HB	2.36	0.53
13:M:15:THR:HG21	13:M:100:ILE:HD12	1.90	0.53
13:M:17:LEU:HD13	31:f:11:TRP:CZ3	2.43	0.53
15:O:170:LEU:HD13	15:O:187:TYR:CD2	2.44	0.53
16:P:48:ARG:NH2	16:P:98:GLY:O	2.42	0.53
16:P:76:MET:HE3	16:P:78:SER:OG	2.08	0.53
18:R:33:HIS:HB3	18:R:59:PHE:CD1	2.44	0.53
20:T:133:ILE:HG13	20:T:137:LYS:HZ2	1.73	0.53
20:U:78:GLY:O	20:U:79:ILE:C	2.51	0.53
21:V:35:LEU:CD1	21:V:48:THR:HG23	2.37	0.53
23:X:41:LYS:HB2	23:X:131:VAL:HG11	1.91	0.53
25:Z:24:ASN:O	25:Z:25:LEU:C	2.52	0.53
26:a:6:LEU:O	26:a:7:PRO:C	2.51	0.53
27:b:74:LEU:H	27:b:74:LEU:HD12	1.73	0.53
29:d:109:TYR:O	29:d:110:ALA:C	2.51	0.53
30:e:40:TRP:CG	30:e:40:TRP:O	2.61	0.53
33:h:156:VAL:CG1	33:h:160:MET:HE3	2.39	0.53
37:l:55:TYR:O	37:l:104:PRO:HG3	2.09	0.53
44:s:87:LEU:HB3	44:s:91:ARG:NH1	2.23	0.53
47:AC:131:TYR:O	47:AC:134:PRO:HD2	2.09	0.53
47:AC:145:VAL:HA	49:Ae:220:LEU:HB3	1.90	0.53
47:AC:170:VAL:HG23	47:AC:174:THR:CB	2.39	0.53
48:AD:127:MET:HE1	48:AD:197:LEU:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:170:VAL:HG23	47:Ac:174:THR:CB	2.39	0.53
48:Ad:111:ARG:HG3	48:Ad:140:TYR:CZ	2.43	0.53
48:Ad:202:ARG:CG	48:Ad:278:SER:HB3	2.35	0.53
48:Ad:227:LEU:HD13	48:Ad:231:LEU:O	2.08	0.53
54:Ak:6:LEU:HD12	54:Ak:11:ARG:HH12	1.72	0.53
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.44	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
9:I:210:LEU:HD12	43:r:39:PRO:CD	2.39	0.53
12:L:501:ALA:HA	12:L:504:LEU:HD12	1.90	0.53
13:M:188:ALA:H	13:M:253:LEU:HD11	1.74	0.53
13:M:313:THR:HA	13:M:316:MET:HE3	1.89	0.53
13:M:314:MET:HE1	13:M:380:PHE:CD2	2.44	0.53
13:M:354:LEU:O	13:M:357:THR:N	2.41	0.53
17:Q:79:ILE:H	17:Q:79:ILE:HD12	1.73	0.53
18:R:98:GLU:HA	18:R:113:GLN:CD	2.34	0.53
19:S:44:LEU:HD12	19:S:48:HIS:HD2	1.72	0.53
20:U:105:MET:CG	20:U:139:MET:HE1	2.39	0.53
23:X:17:GLU:HA	23:X:64:ASN:HD21	1.74	0.53
23:X:57:LEU:HD11	25:Z:84:LEU:HD21	1.90	0.53
34:i:108:ASP:OD2	41:p:18:PRO:CB	2.57	0.53
38:m:49:LEU:HD23	39:n:140:LEU:CD2	2.38	0.53
40:o:8:ARG:CB	40:o:16:GLU:HG2	2.30	0.53
43:r:6:ARG:C	43:r:9:GLN:HG2	2.34	0.53
45:AA:136:LEU:HD21	46:AB:380:ALA:HA	1.90	0.53
47:AC:164:ILE:O	47:AC:177:ARG:HD2	2.08	0.53
49:Ae:181:LYS:O	49:Ae:185:ASP:N	2.41	0.53
1:A:101:GLY:HA3	10:J:163:ILE:CD1	2.39	0.53
2:B:194:CYS:O	2:B:196:PRO:HD3	2.09	0.53
4:D:216:ARG:O	4:D:237:PRO:HG3	2.09	0.53
5:E:244:VAL:HG11	6:F:64:LYS:NZ	2.23	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
8:H:197:PRO:HB3	8:H:277:TYR:HB2	1.91	0.53
9:I:65:GLU:HG3	9:I:65:GLU:O	2.08	0.53
10:J:2:ASN:HB3	10:J:120:LEU:O	2.09	0.53
13:M:73:LEU:HD21	13:M:100:ILE:HG12	1.90	0.53
13:M:213:HIS:O	13:M:217:PRO:HD3	2.09	0.53
13:M:348:LEU:HD12	13:M:415:GLN:NE2	2.24	0.53
18:R:95:LEU:HD21	18:R:111:PHE:CB	2.37	0.53
19:S:22:HIS:HB3	19:S:58:CYS:SG	2.48	0.53
22:W:130:ASP:O	22:W:130:ASP:OD1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:13:LEU:O	23:X:15:VAL:HG23	2.08	0.53
23:X:18:VAL:HA	23:X:68:LEU:CD2	2.39	0.53
27:b:19:LEU:HB3	27:b:23:PHE:CE2	2.44	0.53
30:e:41:ILE:CD1	33:h:174:PRO:HD2	2.39	0.53
34:i:106:PRO:HD2	40:o:64:ILE:CG2	2.38	0.53
38:m:85:LYS:O	38:m:85:LYS:HG2	2.09	0.53
39:n:39:TYR:CZ	39:n:43:LEU:HD11	2.44	0.53
39:n:136:GLU:OE2	39:n:167:TRP:NE1	2.42	0.53
43:r:12:ARG:NH2	43:r:21:GLN:NE2	2.46	0.53
45:AA:158:ASP:O	45:AA:162:GLU:HG2	2.09	0.53
45:AA:207:ASN:O	45:AA:211:LEU:HG	2.10	0.53
47:AC:181:PHE:HA	47:AC:184:ILE:CG2	2.38	0.53
52:AH:35:CYS:O	52:AH:41:CYS:HB2	2.09	0.53
47:Ac:253:PRO:HG3	48:Ad:205:HIS:CD2	2.44	0.53
48:Ad:118:LYS:HZ2	48:Ad:148:LEU:HD22	1.73	0.53
48:Ad:295:MET:HB3	71:Ad:402:3PH:H361	1.91	0.53
52:Ah:32:ARG:NE	52:Ah:76:ARG:HH12	2.06	0.53
1:A:24:LEU:HD11	58:B:304:PC1:H3B2	1.91	0.52
4:D:52:MET:O	4:D:54:PRO:HD3	2.09	0.52
4:D:154:ALA:HB2	4:D:398:THR:HG21	1.90	0.52
4:D:386:THR:HG23	9:I:118:LEU:CD1	2.39	0.52
5:E:143:ASP:HB3	5:E:146:SER:HB2	1.91	0.52
5:E:223:CYS:SG	6:F:133:HIS:NE2	2.81	0.52
5:E:230:LEU:HD21	6:F:48:ARG:CZ	2.40	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:364:ASP:C	7:G:364:ASP:OD1	2.51	0.52
8:H:288:LEU:HD21	55:I:301:3PE:H222	1.90	0.52
11:K:24:SER:O	11:K:90:VAL:HG13	2.10	0.52
12:L:108:MET:HB2	12:L:114:ILE:HD13	1.90	0.52
12:L:332:HIS:CD2	12:L:336:LYS:HG3	2.44	0.52
12:L:450:LEU:HG	12:L:454:ILE:HD12	1.91	0.52
13:M:310:MET:HG3	13:M:455:THR:CA	2.39	0.52
13:M:447:LEU:HD11	13:M:454:ILE:HG23	1.90	0.52
14:N:227:ILE:HA	14:N:230:ILE:CG2	2.39	0.52
15:O:66:ILE:O	63:O:401:ADP:H5'1	2.09	0.52
19:S:18:GLU:HB2	19:S:52:PRO:HB2	1.90	0.52
24:Y:65:ALA:O	24:Y:68:ILE:HG12	2.09	0.52
39:n:56:ASP:O	39:n:57:MET:C	2.50	0.52
47:AC:59:THR:HG23	47:AC:172:LYS:HG2	1.91	0.52
47:AC:128:PHE:HZ	47:AC:143:ALA:HA	1.74	0.52
48:AD:124:CYS:HA	48:AD:179:TYR:CE2	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:92:PRO:HD3	48:Ad:236:TYR:CZ	2.44	0.52
49:Ae:171:GLY:O	49:Ae:172:LYS:HE3	2.09	0.52
49:Ae:239:HIS:CG	49:Ae:239:HIS:O	2.61	0.52
1:A:55:PHE:HD1	10:J:69:TYR:OH	1.91	0.52
2:B:137:LEU:CD2	2:B:145:LEU:CD2	2.86	0.52
3:C:125:PHE:HZ	3:C:198:ARG:HE	1.56	0.52
4:D:259:GLU:CG	25:Z:25:LEU:CD1	2.87	0.52
4:D:266:ARG:NH1	9:I:66:LEU:HG	2.24	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.92	0.52
12:L:228:GLY:O	12:L:229:LEU:CG	2.47	0.52
12:L:247:LEU:O	12:L:252:MET:HB3	2.09	0.52
12:L:385:PHE:HE2	35:j:73:PHE:HD1	1.56	0.52
12:L:536:ILE:HG23	12:L:537:THR:N	2.25	0.52
12:L:556:ILE:HD11	38:m:76:ILE:CG2	2.39	0.52
13:M:160:LEU:CD2	13:M:164:LEU:HD13	2.39	0.52
20:T:80:LYS:O	20:T:84:LEU:HG	2.08	0.52
20:U:103:HIS:NE2	20:U:140:CYS:SG	2.82	0.52
22:W:31:ALA:O	22:W:34:ARG:N	2.40	0.52
23:X:54:ARG:HD3	25:Z:116:TRP:CZ3	2.44	0.52
30:e:101:ARG:HH21	30:e:104:PRO:HD2	1.74	0.52
31:f:49:ARG:CG	31:f:52:GLU:HG3	2.39	0.52
39:n:163:LEU:O	39:n:164:PRO:C	2.51	0.52
43:r:6:ARG:HA	43:r:9:GLN:CD	2.34	0.52
50:AF:92:GLU:O	50:AF:93:PRO:C	2.48	0.52
45:Aa:207:ASN:O	45:Aa:211:LEU:HG	2.09	0.52
46:Ab:168:ASN:OD1	46:Ab:168:ASN:N	2.42	0.52
47:Ac:30:TRP:HB3	47:Ac:100:ARG:HD3	1.90	0.52
48:Ad:114:PHE:CZ	48:Ad:118:LYS:HE3	2.45	0.52
49:Ae:207:LYS:HD2	49:Ae:210:TRP:CD1	2.44	0.52
50:Af:102:ARG:HH21	50:Af:103:LYS:HE3	1.73	0.52
54:Ak:14:ALA:O	54:Ak:18:ILE:HG12	2.08	0.52
1:A:79:ILE:HG12	1:A:87:MET:HE1	1.92	0.52
5:E:179:CYS:HA	59:E:301:FES:S1	2.49	0.52
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.52
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.74	0.52
6:F:167:SER:HB3	44:s:75:TYR:CE2	2.43	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
7:G:67:GLU:HB3	17:Q:156:LYS:HD2	1.91	0.52
10:J:71:THR:O	10:J:76:GLU:HB2	2.08	0.52
10:J:130:ASP:HB2	25:Z:79:LYS:HE2	1.90	0.52
12:L:586:LEU:HA	12:L:589:MET:CE	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:59:ASP:O	13:M:60:PRO:C	2.49	0.52
15:O:121:PRO:C	15:O:122:LYS:HG2	2.33	0.52
16:P:203:PRO:HG2	64:P:401:NDP:C5N	2.39	0.52
18:R:113:GLN:CD	18:R:113:GLN:N	2.66	0.52
21:V:97:TRP:O	21:V:98:LYS:C	2.52	0.52
28:c:55:TRP:HE1	29:d:66:THR:HG21	1.75	0.52
46:AB:171:THR:HG23	49:AI:64:LEU:CD2	2.39	0.52
47:AC:343:VAL:HG21	49:Ae:239:HIS:CD2	2.44	0.52
49:AE:172:LYS:HE2	49:AE:172:LYS:HA	1.90	0.52
50:AF:34:ARG:HH22	50:AF:92:GLU:CD	2.16	0.52
50:AF:101:GLU:HB3	50:AF:105:ARG:HH12	1.75	0.52
50:AF:110:LYS:HA	54:Ak:10:TYR:CE1	2.45	0.52
51:AG:69:GLN:HB3	51:AG:72:ARG:NH1	2.25	0.52
48:Ad:270:VAL:O	48:Ad:274:LEU:HG	2.09	0.52
4:D:113:ILE:CG2	4:D:432:LEU:CD2	2.87	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
10:J:162:GLY:O	10:J:166:ILE:HG12	2.10	0.52
11:K:14:LEU:HD22	55:K:101:3PE:H292	1.90	0.52
11:K:38:LEU:HG	11:K:42:ILE:CD1	2.39	0.52
12:L:123:LEU:HD22	12:L:150:MET:HG3	1.91	0.52
12:L:197:GLU:HB2	41:p:111:LYS:HE3	1.90	0.52
13:M:196:TRP:HE1	13:M:254:THR:HB	1.75	0.52
13:M:422:HIS:HB3	38:m:51:TYR:CE2	2.45	0.52
14:N:335:MET:CB	62:X:201:CDL:H642	2.40	0.52
15:O:168:VAL:CG2	15:O:241:TYR:OH	2.56	0.52
15:O:180:ARG:NH1	32:g:50:THR:HG21	2.25	0.52
15:O:220:LYS:HG3	15:O:221:LYS:N	2.24	0.52
15:O:310:ILE:HG13	15:O:311:PRO:HD2	1.91	0.52
15:O:336:GLY:N	15:O:344:ASN:ND2	2.56	0.52
16:P:59:PHE:CD1	16:P:83:PRO:HG2	2.44	0.52
16:P:236:VAL:HG23	16:P:271:TYR:C	2.35	0.52
17:Q:111:LEU:HD12	18:R:47:ARG:HH21	1.75	0.52
20:U:114:ASP:O	20:U:115:GLN:C	2.53	0.52
23:X:133:THR:HG22	23:X:134:ASP:N	2.24	0.52
25:Z:50:MET:SD	25:Z:54:ASN:ND2	2.82	0.52
29:d:1:MET:HG3	29:d:2:MET:N	2.24	0.52
30:e:34:HIS:O	30:e:38:LYS:HG3	2.08	0.52
34:i:31:ARG:O	34:i:32:GLU:C	2.51	0.52
37:l:169:GLU:C	37:l:171:GLY:N	2.55	0.52
42:q:21:ARG:O	42:q:25:ARG:HG3	2.09	0.52
46:AB:167:GLN:HE21	49:AI:43:LEU:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:376:MET:HE3	50:AF:18:ARG:HA	1.91	0.52
48:AD:112:ARG:HD3	48:AD:257:ASP:OD2	2.09	0.52
48:AD:124:CYS:HA	48:AD:179:TYR:HE2	1.74	0.52
49:AE:107:SER:HA	49:AE:110:ARG:NE	2.25	0.52
46:Ab:234:ALA:HB1	46:Ab:238:LEU:HD12	1.91	0.52
48:Ad:321:TYR:CD2	48:Ad:323:PRO:HD3	2.44	0.52
49:Ae:263:TYR:CA	49:Ae:273:VAL:HA	2.09	0.52
2:B:79:ASP:HA	2:B:82:ILE:HB	1.92	0.52
3:C:149:LEU:O	22:W:23:ILE:HD11	2.10	0.52
4:D:376:GLU:HG3	7:G:121:LEU:HD13	1.85	0.52
5:E:226:PRO:HG2	5:E:229:GLY:O	2.10	0.52
6:F:225:LEU:CD2	7:G:93:ALA:HB3	2.39	0.52
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
12:L:522:PHE:HA	12:L:528:PHE:CZ	2.44	0.52
13:M:403:THR:HA	13:M:406:TYR:CE2	2.44	0.52
14:N:10:TYR:O	14:N:13:ILE:HG22	2.09	0.52
14:N:175:MET:HG2	14:N:219:LEU:HD22	1.91	0.52
15:O:170:LEU:HD13	15:O:187:TYR:CG	2.44	0.52
20:U:133:ILE:CD1	39:n:7:PRO:HD3	2.39	0.52
62:h:201:CDL:H721	34:i:84:TYR:CD2	2.45	0.52
34:i:22:TRP:CE3	39:n:172:THR:HG22	2.45	0.52
38:m:125:PHE:HA	41:p:136:THR:HG21	1.91	0.52
43:r:6:ARG:HA	43:r:9:GLN:CG	2.40	0.52
45:AA:165:ARG:HD3	45:AA:209:ARG:HA	1.91	0.52
45:AA:378:ARG:HG2	45:AA:382:SER:HB2	1.90	0.52
48:AD:145:ALA:O	48:AD:149:ALA:N	2.40	0.52
48:AD:251:GLU:N	48:AD:261:ALA:O	2.37	0.52
45:Aa:74:TRP:HH2	45:Aa:410:CYS:SG	2.31	0.52
46:Ab:60:ARG:O	46:Ab:223:LEU:N	2.42	0.52
46:Ab:348:GLY:HA2	46:Ab:448:PRO:HD3	1.91	0.52
47:Ac:233:LEU:HD23	48:Ad:300:LEU:HD23	1.92	0.52
48:Ad:288:MET:SD	71:Ad:402:3PH:C2	2.98	0.52
49:Ae:164:ASN:HD21	49:Ae:175:PHE:HB3	1.74	0.52
3:C:186:ILE:HG13	4:D:113:ILE:HD11	1.92	0.52
3:C:186:ILE:CG2	3:C:187:LEU:HG	2.23	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.50	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:313:LEU:O	7:G:313:LEU:HD12	2.10	0.52
7:G:557:ARG:CG	7:G:579:MET:HE3	2.38	0.52
10:J:92:LEU:O	10:J:96:VAL:HG23	2.10	0.52
10:J:99:GLU:O	10:J:103:ILE:HG13	2.10	0.52
11:K:36:MET:HE3	14:N:68:MET:HG3	1.92	0.52
11:K:57:MET:N	11:K:58:PRO:HD2	2.24	0.52
14:N:175:MET:HG2	14:N:219:LEU:CD2	2.40	0.52
24:Y:14:VAL:HA	52:Ah:82:HIS:HE1	1.74	0.52
29:d:94:ILE:HD13	33:h:152:LYS:HE3	1.92	0.52
35:j:99:ILE:HD12	40:o:107:ARG:HB2	1.91	0.52
40:o:31:PHE:HB3	40:o:34:ARG:HB3	1.90	0.52
45:AA:170:ARG:HA	45:AA:173:GLN:CD	2.34	0.52
46:AB:117:GLU:OE2	46:AB:330:TYR:HB3	2.09	0.52
46:AB:312:SER:O	46:AB:315:LYS:HG2	2.10	0.52
46:AB:348:GLY:HA2	46:AB:448:PRO:HD3	1.91	0.52
47:AC:137:GLN:NE2	47:AC:263:ASN:O	2.39	0.52
47:AC:138:MET:CE	47:AC:268:ILE:HG23	2.40	0.52
47:AC:221:HIS:O	47:AC:225:THR:HB	2.10	0.52
48:AD:154:VAL:HG23	48:AD:176:PRO:HB3	1.92	0.52
48:AD:232:TYR:O	48:AD:242:ILE:HG22	2.09	0.52
48:AD:248:ILE:HD12	48:AD:252:VAL:HG11	1.92	0.52
48:AD:321:TYR:CD2	48:AD:323:PRO:HD3	2.44	0.52
49:AE:242:HIS:CD2	49:AE:251:LYS:HB3	2.45	0.52
46:Ab:138:LEU:HB3	46:Ab:237:PHE:CD2	2.45	0.52
46:Ab:425:VAL:HG12	46:Ab:429:LYS:HZ1	1.75	0.52
48:Ad:300:LEU:HB2	48:Ad:301:PRO:HD3	1.91	0.52
1:A:57:LEU:O	1:A:58:VAL:C	2.52	0.52
1:A:106:TRP:NE1	55:A:201:3PE:H32	2.24	0.52
3:C:136:PHE:CE1	43:r:96:THR:HB	2.44	0.52
4:D:222:MET:HG2	4:D:223:HIS:CD2	2.44	0.52
4:D:358:VAL:O	4:D:364:SER:OG	2.25	0.52
5:E:198:LYS:O	5:E:201:GLU:HB3	2.10	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
8:H:200:LEU:HD22	8:H:285:LEU:HD23	1.90	0.52
8:H:253:GLU:O	8:H:254:LEU:C	2.52	0.52
12:L:108:MET:HB2	12:L:114:ILE:CD1	2.39	0.52
12:L:145:GLU:HB3	13:M:370:PRO:HG2	1.90	0.52
12:L:297:ASP:HB3	12:L:300:LYS:CG	2.39	0.52
12:L:483:PRO:HG2	12:L:486:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:496:LEU:C	12:L:496:LEU:CD1	2.79	0.52
13:M:84:LEU:HD21	13:M:95:TYR:HB3	1.90	0.52
14:N:335:MET:HB2	62:X:201:CDL:H642	1.90	0.52
19:S:90:ALA:O	19:S:94:VAL:HG23	2.09	0.52
20:T:110:LEU:HD21	20:T:118:ILE:HD12	1.91	0.52
23:X:7:LEU:CD2	25:Z:87:LEU:HD11	2.38	0.52
33:h:87:THR:HG22	62:h:201:CDL:H512	1.91	0.52
34:i:128:HIS:O	40:o:85:HIS:NE2	2.41	0.52
42:q:4:VAL:HG23	42:q:5:GLU:OE2	2.10	0.52
46:AB:226:SER:O	46:AB:229:VAL:HG22	2.09	0.52
48:AD:189:ASN:OD1	48:AD:194:PRO:HG3	2.09	0.52
48:AD:232:TYR:CG	48:AD:246:PRO:HD3	2.45	0.52
50:AF:41:THR:O	50:AF:42:GLU:C	2.50	0.52
47:Ac:320:ILE:HD12	47:Ac:373:GLU:HG2	1.92	0.52
54:Ak:6:LEU:HD12	54:Ak:11:ARG:NH1	2.25	0.52
1:A:55:PHE:HB3	10:J:69:TYR:CE2	2.45	0.52
2:B:92:PRO:CG	2:B:130:VAL:CG1	2.87	0.52
3:C:209:LEU:HD21	22:W:108:ARG:NH1	2.25	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.24	0.52
9:I:79:ARG:NH2	43:r:20:LEU:HD13	2.24	0.52
10:J:168:GLU:OE2	14:N:1:MET:HG2	2.10	0.52
13:M:68:LEU:HG	13:M:234:ILE:HD11	1.92	0.52
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.91	0.52
13:M:115:LEU:HD21	13:M:176:LEU:CD2	2.37	0.52
13:M:346:ARG:O	13:M:419:LEU:HA	2.09	0.52
14:N:29:MET:HE2	14:N:141:ILE:HG12	1.92	0.52
20:U:128:PHE:CE1	20:U:148:ILE:HG23	2.45	0.52
20:U:133:ILE:HG23	20:U:134:ASP:N	2.25	0.52
21:V:95:LEU:HA	21:V:100:TRP:HH2	1.75	0.52
23:X:45:LEU:HD23	27:b:56:PRO:O	2.09	0.52
23:X:142:TYR:O	23:X:143:HIS:C	2.52	0.52
32:g:123:LEU:HD12	41:p:98:VAL:CG1	2.40	0.52
43:r:27:ARG:HD2	43:r:31:ILE:CG2	2.40	0.52
45:AA:74:TRP:HH2	45:AA:410:CYS:SG	2.31	0.52
47:AC:119:LEU:HD21	47:AC:192:LEU:HB2	1.92	0.52
47:AC:120:LEU:HD23	47:AC:298:ILE:HG23	1.92	0.52
47:AC:346:PRO:O	47:AC:349:ILE:HG22	2.10	0.52
48:AD:114:PHE:CE2	48:AD:148:LEU:HD13	2.45	0.52
48:AD:242:ILE:HG12	48:AD:244:MET:HB3	1.92	0.52
48:AD:308:ARG:HD3	51:AG:27:PHE:CZ	2.44	0.52
50:AF:26:GLY:HA2	50:AF:28:ASN:OD1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AG:74:ASN:ND2	51:AG:76:ALA:HB3	2.25	0.52
46:Ab:235:GLU:OE1	46:Ab:235:GLU:N	2.42	0.52
49:Ae:161:GLU:O	49:Ae:163:LYS:HG2	2.10	0.52
49:Ae:249:ILE:HG12	49:Ae:254:ALA:O	2.10	0.52
2:B:122:ARG:NH1	2:B:132:ILE:HD12	2.25	0.52
3:C:170:TRP:CD1	3:C:183:LEU:HD21	2.44	0.52
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.92	0.52
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.45	0.52
5:E:143:ASP:HB3	5:E:146:SER:CB	2.40	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:402:LEU:O	7:G:431:LEU:HA	2.09	0.52
12:L:202:MET:CE	12:L:265:PRO:HG3	2.33	0.52
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.90	0.52
12:L:513:MET:HE1	39:n:30:TRP:HB3	1.89	0.52
13:M:171:VAL:HG11	13:M:179:LEU:CD2	2.35	0.52
13:M:263:LEU:HD11	38:m:102:TYR:CD1	2.41	0.52
18:R:69:VAL:HG11	18:R:112:LYS:HB2	1.92	0.52
35:j:87:PRO:HG3	40:o:96:VAL:HG23	1.92	0.52
41:p:50:GLU:HG3	41:p:54:ARG:HH21	1.75	0.52
45:AA:339:GLN:HB2	45:AA:359:VAL:O	2.10	0.52
45:AA:453:CYS:SG	45:AA:472:ARG:NH1	2.82	0.52
45:AA:468:TYR:O	45:AA:469:ASN:C	2.52	0.52
47:AC:107:TYR:HB2	47:AC:305:PRO:HG3	1.92	0.52
49:AE:241:SER:OG	49:AE:253:PRO:HD2	2.09	0.52
52:AH:79:CYS:O	52:AH:83:LYS:HG2	2.10	0.52
46:Ab:159:LYS:O	46:Ab:162:LYS:HG2	2.09	0.52
48:Ad:298:LEU:O	48:Ad:301:PRO:HD2	2.10	0.52
2:B:98:ALA:HB1	2:B:100:CYS:H	1.74	0.52
2:B:124:SER:HB3	2:B:125:PRO:CD	2.39	0.52
3:C:230:ARG:NH1	9:I:128:ILE:O	2.43	0.52
4:D:254:ARG:HE	43:r:25:GLN:HB3	1.74	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.92	0.52
7:G:524:ALA:HB2	7:G:597:VAL:HG22	1.91	0.52
12:L:286:LEU:HG	12:L:290:ILE:CD1	2.40	0.52
12:L:533:ILE:HG23	12:L:534:HIS:HD2	1.74	0.52
13:M:139:GLN:HB3	13:M:222:GLU:CG	2.39	0.52
15:O:121:PRO:HB3	15:O:178:TYR:CE1	2.45	0.52
15:O:132:GLN:NE2	63:O:401:ADP:HN62	2.08	0.52
15:O:351:TRP:CZ3	28:c:41:TRP:CH2	2.97	0.52
16:P:279:TYR:CD1	16:P:372:ALA:HB2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:55:VAL:HB	17:Q:57:GLU:OE2	2.10	0.52
20:T:102:SER:HB2	20:T:107:ASP:HB2	1.90	0.52
21:V:42:ALA:O	21:V:43:ALA:C	2.53	0.52
22:W:110:PHE:O	22:W:111:HIS:C	2.53	0.52
26:a:52:ARG:HH21	26:a:57:VAL:HG23	1.75	0.52
34:i:108:ASP:OD2	41:p:18:PRO:HB2	2.10	0.52
39:n:143:GLU:O	39:n:143:GLU:HG2	2.10	0.52
45:AA:180:GLN:HG3	45:AA:181:ASN:N	2.25	0.52
47:AC:126:THR:HB	67:AC:401:HEM:HBC2	1.92	0.52
47:AC:259:ALA:O	47:AC:261:PRO:HD3	2.09	0.52
48:AD:136:VAL:HG21	48:AD:142:GLU:HG2	1.92	0.52
48:AD:152:VAL:HG23	48:AD:156:ASP:OD2	2.09	0.52
48:AD:321:TYR:HB2	50:AF:61:PHE:CD1	2.45	0.52
49:AE:127:TYR:CZ	53:AJ:36:PHE:CD1	2.97	0.52
45:Aa:160:GLN:HA	45:Aa:163:LYS:HZ3	1.75	0.52
45:Aa:338:CYS:CB	45:Aa:368:MET:SD	2.97	0.52
46:Ab:36:GLN:NE2	46:Ab:55:TYR:HE2	2.08	0.52
47:Ac:346:PRO:O	47:Ac:349:ILE:HG22	2.10	0.52
48:Ad:157:GLY:H	48:Ad:158:PRO:HD3	1.75	0.52
1:A:55:PHE:HD1	10:J:69:TYR:HH	1.57	0.51
4:D:451:ILE:HG23	4:D:456:ILE:CD1	2.35	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
13:M:103:GLN:O	13:M:107:ILE:HB	2.10	0.51
13:M:168:GLN:O	13:M:172:GLY:N	2.43	0.51
14:N:168:GLY:O	14:N:172:GLN:HG2	2.10	0.51
29:d:62:LEU:O	29:d:66:THR:OG1	2.22	0.51
29:d:87:ASP:O	29:d:88:HIS:C	2.51	0.51
30:e:44:ALA:HA	30:e:47:ILE:HG12	1.92	0.51
35:j:81:LEU:O	35:j:82:GLY:C	2.51	0.51
41:p:164:LEU:O	41:p:168:LYS:N	2.42	0.51
46:AB:173:ILE:HD11	46:AB:439:ALA:O	2.09	0.51
46:AB:227:HIS:HD2	46:AB:231:LYS:HE2	1.75	0.51
47:AC:51:LEU:HD21	47:AC:80:ARG:HA	1.92	0.51
47:AC:198:LEU:HD21	47:Ac:10:LEU:HA	1.93	0.51
52:AH:33:GLU:O	52:AH:37:GLN:HG2	2.11	0.51
3:C:63:TYR:OH	3:C:102:HIS:HE1	1.93	0.51
4:D:270:ASN:HB3	8:H:284:GLN:NE2	2.25	0.51
4:D:321:GLY:HA3	4:D:328:ASP:OD1	2.09	0.51
6:F:64:LYS:H	6:F:256:ARG:HE	1.58	0.51
6:F:119:GLU:CD	60:F:501:FMN:HN3	2.18	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.75	0.51
7:G:473:MET:HE3	7:G:514:ASN:ND2	2.22	0.51
7:G:617:ARG:NH1	22:W:129:HIS:HA	2.24	0.51
10:J:60:LEU:CD1	10:J:61:GLY:N	2.72	0.51
10:J:77:GLU:O	10:J:78:TYR:C	2.51	0.51
11:K:59:ILE:O	11:K:60:PRO:C	2.49	0.51
12:L:49:LEU:HB3	12:L:50:PRO:HD3	1.91	0.51
20:T:104:PHE:CB	20:T:110:LEU:HD22	2.39	0.51
25:Z:87:LEU:O	25:Z:91:LEU:HB2	2.10	0.51
30:e:96:PRO:HB2	30:e:102:GLU:CD	2.36	0.51
34:i:77:ILE:HD13	34:i:80:TRP:CZ3	2.46	0.51
37:l:88:PRO:HB2	39:n:86:PRO:CB	2.40	0.51
47:AC:145:VAL:CG1	49:Ae:220:LEU:CD1	2.77	0.51
49:AE:126:ALA:HB1	54:AK:34:TRP:CH2	2.45	0.51
45:Aa:98:PHE:CZ	45:Aa:122:ALA:HB2	2.46	0.51
45:Aa:170:ARG:HA	45:Aa:173:GLN:CD	2.34	0.51
45:Aa:280:ASP:OD2	51:Ag:10:ARG:HA	2.10	0.51
45:Aa:467:ASP:OD2	47:Ac:223:TYR:CE2	2.63	0.51
2:B:92:PRO:CB	2:B:122:ARG:NH1	2.57	0.51
2:B:200:ALA:O	2:B:201:LEU:C	2.53	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
4:D:385:TYR:HB2	9:I:118:LEU:HD11	1.93	0.51
5:E:178:ALA:HB2	5:E:191:TYR:CE2	2.45	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:338:VAL:HG13	7:G:546:PHE:CE1	2.37	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.53	0.51
7:G:670:GLU:HB2	19:S:42:VAL:CG2	2.40	0.51
12:L:569:LEU:O	12:L:573:MET:HG2	2.11	0.51
13:M:151:PHE:CE2	14:N:291:PHE:HB2	2.44	0.51
15:O:66:ILE:CD1	15:O:218:ILE:HG12	2.40	0.51
16:P:137:ARG:HG3	16:P:138:ASN:OD1	2.10	0.51
16:P:206:ILE:H	64:P:401:NDP:H71N	1.58	0.51
16:P:316:LYS:O	16:P:320:GLU:HG3	2.10	0.51
55:Y:201:3PE:H122	55:Y:201:3PE:H231	1.91	0.51
25:Z:97:ILE:HG13	25:Z:98:MET:N	2.25	0.51
34:i:106:PRO:HD2	40:o:64:ILE:HG21	1.93	0.51
45:AA:172:MET:HE1	45:AA:205:SER:HA	1.92	0.51
45:AA:392:LYS:HE3	45:AA:433:ILE:O	2.11	0.51
46:AB:303:ASN:O	46:AB:304:ASN:C	2.52	0.51
47:AC:65:SER:O	47:AC:68:HIS:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:70:CYS:SG	47:AC:80:ARG:NH1	2.83	0.51
48:AD:112:ARG:HE	48:AD:269:ASP:CG	2.18	0.51
48:AD:115:GLN:HG2	48:AD:140:TYR:OH	2.10	0.51
48:AD:117:TYR:CZ	48:AD:127:MET:HG2	2.46	0.51
45:Aa:339:GLN:HB2	45:Aa:359:VAL:O	2.10	0.51
47:Ac:147:THR:HG21	47:Ac:165:TRP:NE1	2.26	0.51
71:Ad:402:3PH:C36	49:Ae:128:ALA:HB2	2.39	0.51
4:D:97:LEU:HA	4:D:111:PRO:HA	1.92	0.51
6:F:194:ASP:OD1	44:s:91:ARG:HG2	2.10	0.51
8:H:148:ILE:HB	8:H:297:THR:CG2	2.41	0.51
9:I:105:ARG:NH2	18:R:56:ASN:ND2	2.58	0.51
11:K:22:PHE:HZ	14:N:61:VAL:HG11	1.75	0.51
12:L:295:GLN:OE1	39:n:78:GLN:NE2	2.41	0.51
12:L:427:ILE:HD11	36:k:69:PHE:CE1	2.46	0.51
12:L:578:THR:HG21	14:N:168:GLY:HA2	1.91	0.51
13:M:458:THR:HG21	41:p:148:ALA:HB1	1.92	0.51
31:f:37:PHE:HA	31:f:40:LYS:HB2	1.92	0.51
36:k:39:GLN:HE22	36:k:49:ASP:HB3	1.75	0.51
39:n:168:TRP:HD1	39:n:169:HIS:CE1	2.27	0.51
40:o:89:TYR:O	40:o:90:CYS:C	2.52	0.51
42:q:26:VAL:HG11	42:q:32:ASP:O	2.10	0.51
46:AB:319:GLN:HB3	46:AB:320:PRO:HD2	1.93	0.51
47:AC:117:VAL:HG11	47:AC:302:ALA:CA	2.41	0.51
47:AC:150:LEU:HB2	47:AC:161:VAL:HG22	1.93	0.51
48:AD:318:LYS:CD	49:AE:86:PRO:HB2	2.40	0.51
45:Aa:91:TYR:CZ	45:Aa:95:HIS:CE1	2.98	0.51
48:Ad:158:PRO:HD2	48:Ad:164:MET:O	2.10	0.51
49:Ae:93:ARG:HD2	49:Ae:110:ARG:CD	2.38	0.51
51:Ag:74:ASN:HD21	51:Ag:76:ALA:HB3	1.74	0.51
2:B:94:THR:N	57:B:302:UQ1:C11	2.73	0.51
2:B:182:ASP:HA	2:B:187:VAL:HG23	1.93	0.51
3:C:186:ILE:CG2	3:C:187:LEU:N	2.73	0.51
6:F:167:SER:OG	44:s:75:TYR:CE2	2.63	0.51
6:F:382:CYS:HA	7:G:74:ASN:O	2.11	0.51
7:G:238:PHE:CE1	9:I:140:ARG:HD2	2.46	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:136:VAL:O	8:H:137:ALA:C	2.54	0.51
13:M:11:LEU:O	13:M:15:THR:HG23	2.09	0.51
13:M:20:PRO:HB3	13:M:89:ASN:ND2	2.25	0.51
13:M:129:THR:CG2	13:M:235:LEU:HD11	2.40	0.51
23:X:52:ASP:OD1	23:X:53:PRO:HD2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:47:SER:HB2	29:d:59:HIS:HD2	1.76	0.51
34:i:83:HIS:CE1	34:i:87:LYS:HD2	2.46	0.51
34:i:85:TYR:CE2	34:i:90:MET:HE3	2.46	0.51
55:m:201:3PE:H332	55:m:202:3PE:H341	1.93	0.51
40:o:39:MET:HE1	40:o:57:ASP:O	2.11	0.51
42:q:19:GLY:O	42:q:23:LEU:N	2.41	0.51
47:AC:8:HIS:CE1	47:Ac:199:PHE:CE1	2.98	0.51
47:AC:121:PHE:HZ	47:AC:299:LEU:HG	1.75	0.51
48:AD:242:ILE:CG1	48:AD:244:MET:HB3	2.39	0.51
45:Aa:92:PHE:HD1	45:Aa:168:ILE:HD12	1.75	0.51
46:Ab:69:SER:O	46:Ab:70:ARG:C	2.51	0.51
48:Ad:133:ARG:NH1	49:Ae:145:ASP:HA	2.26	0.51
55:A:201:3PE:H361	27:b:23:PHE:CZ	2.46	0.51
2:B:189:ILE:HD12	2:B:207:GLN:HB3	1.93	0.51
3:C:92:VAL:O	3:C:96:LEU:HD13	2.11	0.51
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.51
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.08	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:611:THR:HG21	17:Q:105:GLU:N	2.25	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:39:ILE:HG12	42:q:31:ASN:OD1	2.11	0.51
8:H:98:LEU:CD2	55:H:401:3PE:H2	2.41	0.51
12:L:161:ARG:NE	12:L:163:ASP:HB2	2.26	0.51
12:L:249:SER:HB2	12:L:340:PHE:CE2	2.46	0.51
12:L:536:ILE:HD11	12:L:540:LYS:HD2	1.93	0.51
12:L:595:ILE:O	12:L:599:ILE:HG13	2.11	0.51
13:M:251:ASP:N	13:M:252:PRO:HD2	2.26	0.51
13:M:388:TRP:NE1	38:m:109:ARG:HD2	2.26	0.51
17:Q:135:ILE:HD11	17:Q:147:VAL:HG21	1.91	0.51
17:Q:154:LYS:CB	17:Q:155:PRO:HD2	2.39	0.51
21:V:31:THR:HG22	21:V:88:LEU:HB2	1.92	0.51
22:W:95:GLU:HB3	22:W:101:LYS:HG3	1.93	0.51
23:X:53:PRO:HD2	25:Z:116:TRP:CG	2.46	0.51
29:d:28:ASP:O	29:d:29:PRO:C	2.52	0.51
33:h:159:LEU:HD23	33:h:163:ARG:HH12	1.75	0.51
36:k:34:PRO:HD2	36:k:59:TYR:CG	2.46	0.51
46:AB:232:GLN:O	46:AB:235:GLU:HG3	2.11	0.51
47:AC:215:ALA:HB2	50:AF:60:MET:CE	2.39	0.51
48:AD:109:SER:OG	48:AD:269:ASP:HA	2.10	0.51
48:AD:215:LEU:CD1	69:AD:401:HEC:HBB2	2.39	0.51
50:AF:28:ASN:OD1	50:AF:29:LYS:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:113:VAL:HG23	45:Aa:118:ALA:HB3	1.92	0.51
45:Aa:392:LYS:HE3	45:Aa:433:ILE:O	2.11	0.51
46:Ab:126:ILE:HG22	46:Ab:128:SER:H	1.76	0.51
47:Ac:137:GLN:NE2	47:Ac:264:THR:HA	2.26	0.51
47:Ac:278:TYR:CZ	47:Ac:282:ARG:HD2	2.46	0.51
49:Ae:196:ARG:HD2	49:Ae:249:ILE:CG2	2.41	0.51
52:Ah:45:ARG:O	52:Ah:49:GLU:HG2	2.11	0.51
52:Ah:51:CYS:SG	52:Ah:68:GLU:HB2	2.51	0.51
4:D:181:LEU:HD11	4:D:210:MET:CG	2.41	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
9:I:64:THR:CG2	25:Z:35:MET:HE1	2.41	0.51
10:J:22:LYS:HE2	11:K:18:GLY:O	2.10	0.51
12:L:13:ILE:CD1	55:i:201:3PE:H2C2	2.32	0.51
12:L:60:GLU:HG3	12:L:83:ASP:HA	1.93	0.51
12:L:530:PRO:O	12:L:534:HIS:HB2	2.11	0.51
12:L:590:SER:HB2	24:Y:45:LEU:HD11	1.91	0.51
13:M:31:SER:HA	13:M:34:ILE:CG1	2.41	0.51
13:M:304:GLN:HA	13:M:309:PHE:CE1	2.45	0.51
14:N:240:MET:HE2	14:N:326:PHE:CZ	2.45	0.51
16:P:215:ASN:O	16:P:216:HIS:C	2.54	0.51
17:Q:112:MET:SD	42:q:126:PRO:HB3	2.51	0.51
17:Q:131:LYS:HG2	17:Q:135:ILE:HD11	1.89	0.51
19:S:24:CYS:HB2	19:S:30:SER:HB3	1.92	0.51
23:X:151:ASN:ND2	30:e:51:ARG:HH11	2.08	0.51
34:i:10:LEU:HA	34:i:13:GLN:HB3	1.91	0.51
37:l:158:PRO:HD3	40:o:22:ILE:CB	2.40	0.51
46:AB:323:VAL:HA	46:AB:339:TYR:O	2.11	0.51
48:AD:235:PRO:HA	48:AD:240:GLN:HE21	1.74	0.51
49:AE:89:SER:HA	49:AE:92:ARG:CB	2.30	0.51
49:AE:130:LYS:HB2	54:AK:34:TRP:CZ2	2.45	0.51
45:Aa:148:ALA:HA	45:Aa:250:LEU:HD21	1.92	0.51
46:Ab:38:LEU:HA	46:Ab:51:SER:O	2.11	0.51
46:Ab:116:ARG:HG2	46:Ab:190:LEU:HD21	1.91	0.51
46:Ab:432:VAL:O	46:Ab:432:VAL:HG22	2.10	0.51
48:Ad:281:GLU:CD	48:Ad:281:GLU:H	2.18	0.51
52:Ah:77:ASP:O	52:Ah:78:HIS:C	2.50	0.51
3:C:70:LYS:O	21:V:103:LEU:HD12	2.10	0.51
4:D:58:THR:HG23	4:D:61:TRP:CE2	2.46	0.51
4:D:179:ARG:NH2	4:D:401:GLU:O	2.43	0.51
4:D:256:ASP:O	4:D:260:GLU:N	2.33	0.51
4:D:259:GLU:HG2	25:Z:25:LEU:CD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:304:GLU:HG3	7:G:615:LEU:HD12	1.93	0.51
7:G:382:ARG:NH2	7:G:386:LEU:HD11	2.25	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:14:LEU:HB3	61:H:400:UQ9:H23	1.92	0.51
8:H:43:TYR:CE1	26:a:4:GLU:HG2	2.45	0.51
10:J:3:ASN:OD1	10:J:3:ASN:N	2.43	0.51
13:M:127:ILE:HG12	14:N:254:LEU:HD21	1.93	0.51
14:N:246:LEU:HD11	55:N:401:3PE:H3A2	1.91	0.51
14:N:313:MET:HG2	15:O:305:LEU:HD22	1.93	0.51
15:O:246:LEU:HD11	15:O:257:VAL:HG22	1.93	0.51
29:d:40:CYS:SG	55:d:201:3PE:H252	2.51	0.51
45:AA:377:MET:HE2	45:AA:377:MET:HA	1.93	0.51
47:AC:107:TYR:HE1	47:AC:308:HIS:HB2	1.76	0.51
45:Aa:52:ILE:HG12	45:Aa:53:LEU:N	2.26	0.51
45:Aa:169:LEU:O	45:Aa:173:GLN:HG3	2.11	0.51
46:Ab:164:VAL:O	46:Ab:167:GLN:HG3	2.10	0.51
47:Ac:150:LEU:HB2	47:Ac:161:VAL:HG22	1.93	0.51
47:Ac:211:LEU:HD21	50:Af:37:THR:HA	1.93	0.51
47:Ac:221:HIS:O	47:Ac:225:THR:HB	2.10	0.51
3:C:190:TYR:HB3	22:W:101:LYS:HG2	1.92	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HE3	1.93	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
10:J:169:ILE:HD11	14:N:41:ILE:HG22	1.92	0.51
12:L:404:THR:HG22	12:L:405:ASN:H	1.75	0.51
13:M:178:ILE:HG12	41:p:82:VAL:HG11	1.93	0.51
13:M:354:LEU:O	13:M:355:MET:C	2.52	0.51
15:O:289:TRP:HA	15:O:289:TRP:CE3	2.46	0.51
16:P:154:GLN:O	16:P:158:GLU:HG3	2.10	0.51
18:R:72:VAL:HG12	18:R:73:GLU:N	2.26	0.51
23:X:46:CYS:HB2	23:X:135:ARG:NE	2.26	0.51
25:Z:134:SER:O	25:Z:138:PHE:N	2.40	0.51
29:d:108:THR:HG23	29:d:110:ALA:HB3	1.93	0.51
30:e:70:TYR:OH	30:e:74:ARG:HD3	2.11	0.51
31:f:49:ARG:CG	31:f:52:GLU:CG	2.88	0.51
32:g:115:TRP:HA	32:g:118:ARG:HH11	1.75	0.51
38:m:45:ARG:CZ	39:n:140:LEU:HD11	2.41	0.51
55:m:201:3PE:H261	55:m:201:3PE:H3B1	1.93	0.51
45:AA:226:ALA:HB2	45:AA:253:VAL:HB	1.93	0.51
45:AA:378:ARG:CG	45:AA:382:SER:HB2	2.41	0.51
49:AE:91:TYR:O	51:AG:25:ARG:N	2.40	0.51
47:Ac:140:PHE:CE1	47:Ac:170:VAL:HG13	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:145:ALA:HA	48:Ad:148:LEU:HD12	1.92	0.51
49:Ae:243:TYR:OH	49:Ae:254:ALA:HB1	2.11	0.51
4:D:137:ASP:CB	4:D:223:HIS:HA	2.41	0.51
4:D:140:ASP:H	4:D:147:ASN:HD21	1.59	0.51
5:E:62:ILE:HG21	5:E:103:VAL:HG11	1.93	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
5:E:176:LEU:HB2	5:E:184:MET:CE	2.41	0.51
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.25	0.51
7:G:130:ILE:CA	9:I:140:ARG:HH11	2.10	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:376:GLY:C	7:G:378:GLY:N	2.64	0.51
8:H:107:ALA:HB1	10:J:56:PHE:HD2	1.76	0.51
10:J:98:MET:O	10:J:101:PHE:HB3	2.11	0.51
12:L:477:ILE:HG13	40:o:91:GLU:OE2	2.11	0.51
14:N:45:ILE:HA	14:N:52:SER:OG	2.11	0.51
17:Q:58:LYS:O	17:Q:59:LEU:HB2	2.10	0.51
20:U:119:ILE:CD1	20:U:138:LEU:HB2	2.40	0.51
26:a:45:TRP:O	26:a:46:TYR:C	2.54	0.51
33:h:73:PHE:CE2	33:h:74:TYR:CE1	2.98	0.51
45:AA:109:LEU:O	45:AA:113:VAL:HG12	2.11	0.51
45:AA:169:LEU:O	45:AA:173:GLN:HG3	2.11	0.51
49:AE:119:ALA:HA	53:AJ:25:ILE:HG12	1.93	0.51
51:AG:9:ALA:O	51:AG:11:ILE:HD12	2.10	0.51
45:Aa:338:CYS:SG	45:Aa:339:GLN:N	2.84	0.51
47:Ac:140:PHE:HE1	47:Ac:170:VAL:HG13	1.76	0.51
48:Ad:157:GLY:N	48:Ad:158:PRO:HD3	2.26	0.51
48:Ad:220:GLU:O	48:Ad:221:PRO:C	2.52	0.51
49:Ae:195:LEU:HD11	49:Ae:248:ARG:NH1	2.26	0.51
49:Ai:46:LYS:HG2	49:Ai:47:ARG:H	1.71	0.51
1:A:104:TYR:HE2	10:J:167:ILE:CD1	2.23	0.50
58:B:304:PC1:H3B1	8:H:57:MET:HE2	1.92	0.50
3:C:123:ASN:ND2	21:V:108:PRO:HG2	2.25	0.50
4:D:271:ARG:NH1	8:H:279:ARG:O	2.43	0.50
4:D:323:ARG:O	4:D:324:GLY:C	2.52	0.50
4:D:348:LEU:O	25:Z:11:PRO:CG	2.44	0.50
5:E:140:MET:HE1	6:F:366:ALA:HA	1.92	0.50
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
8:H:90:PRO:HB3	8:H:162:LEU:CB	2.41	0.50
9:I:63:TRP:CZ3	55:I:301:3PE:H322	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:105:ARG:NH2	18:R:56:ASN:HD21	2.09	0.50
12:L:362:ILE:CD1	12:L:430:VAL:HG13	2.41	0.50
12:L:383:MET:CB	12:L:386:LEU:HD12	2.30	0.50
12:L:516:ALA:HB1	12:L:520:SER:CB	2.41	0.50
12:L:525:LEU:HD21	39:n:77:PRO:CB	2.39	0.50
15:O:62:VAL:HG21	15:O:73:LEU:HD23	1.93	0.50
15:O:182:GLN:O	15:O:183:CYS:C	2.54	0.50
16:P:153:ALA:HB2	16:P:164:PHE:CE2	2.46	0.50
16:P:157:LYS:HD3	16:P:195:PHE:CE1	2.46	0.50
17:Q:53:ILE:HG23	22:W:20:VAL:HG23	1.94	0.50
20:U:86:VAL:HG13	36:k:54:ASN:ND2	2.26	0.50
24:Y:90:LEU:O	24:Y:94:ILE:HG12	2.11	0.50
27:b:41:TYR:CD1	27:b:84:LEU:HD11	2.46	0.50
30:e:101:ARG:NH2	30:e:103:GLU:HA	2.26	0.50
37:l:117:VAL:HG12	37:l:118:ASP:N	2.25	0.50
41:p:49:ARG:O	41:p:52:ILE:HB	2.11	0.50
47:AC:237:LEU:HD22	48:AD:300:LEU:HD11	1.93	0.50
45:Aa:113:VAL:O	45:Aa:116:ILE:HG12	2.11	0.50
45:Aa:285:ALA:O	45:Aa:359:VAL:HA	2.11	0.50
45:Aa:397:ASN:HD21	46:Ab:126:ILE:HD11	1.76	0.50
46:Ab:38:LEU:HD11	46:Ab:396:ILE:HD13	1.92	0.50
48:Ad:248:ILE:HD12	48:Ad:252:VAL:HG11	1.93	0.50
4:D:105:MET:HA	4:D:443:MET:HA	1.92	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.69	0.50
8:H:91:MET:O	8:H:92:PRO:C	2.50	0.50
9:I:111:GLU:OE2	9:I:187:LYS:HE3	2.11	0.50
10:J:77:GLU:OE1	11:K:87:THR:C	2.54	0.50
12:L:451:MET:O	12:L:452:ASN:C	2.53	0.50
12:L:483:PRO:HB2	12:L:485:PHE:CE1	2.46	0.50
13:M:4:ILE:HD11	13:M:41:LEU:HD21	1.92	0.50
13:M:249:ILE:HG22	13:M:250:LEU:N	2.26	0.50
16:P:270:ARG:HB3	16:P:375:VAL:O	2.11	0.50
19:S:23:LEU:HD12	19:S:23:LEU:O	2.12	0.50
22:W:67:ARG:O	22:W:71:MET:HB2	2.11	0.50
23:X:32:TYR:HE1	23:X:67:ALA:HA	1.76	0.50
25:Z:119:PRO:HA	25:Z:123:GLU:OE2	2.12	0.50
34:i:22:TRP:CZ2	39:n:172:THR:HG22	2.46	0.50
34:i:103:ARG:NH1	40:o:67:LEU:HD22	2.26	0.50
37:l:87:ASP:OD1	37:l:88:PRO:HD2	2.11	0.50
41:p:5:TRP:HZ3	41:p:10:TYR:O	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:113:CYS:O	41:p:113:CYS:SG	2.69	0.50
44:s:84:ASN:OD1	44:s:84:ASN:C	2.53	0.50
45:AA:338:CYS:SG	45:AA:339:GLN:N	2.84	0.50
47:AC:138:MET:HE1	47:AC:268:ILE:HA	1.92	0.50
51:AG:68:GLU:HA	51:AG:71:LYS:CE	2.41	0.50
48:Ad:174:TYR:O	48:Ad:175:PHE:C	2.53	0.50
52:Ah:43:LYS:HA	52:Ah:46:GLU:CD	2.36	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
6:F:391:TRP:HH2	7:G:118:GLU:OE2	1.93	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:382:ARG:HB3	7:G:386:LEU:CD1	2.41	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
10:J:12:PHE:CZ	11:K:42:ILE:HD12	2.45	0.50
12:L:349:SER:HB2	12:L:443:ILE:HG23	1.93	0.50
13:M:118:PHE:O	13:M:122:PHE:HB2	2.11	0.50
14:N:36:SER:HB2	14:N:134:GLN:HE22	1.76	0.50
14:N:175:MET:O	14:N:179:MET:HG2	2.12	0.50
14:N:248:LEU:CD1	14:N:296:LEU:HD23	2.41	0.50
15:O:326:ARG:NH2	32:g:56:ASP:OD1	2.45	0.50
16:P:45:LYS:O	16:P:50:SER:HB3	2.11	0.50
20:U:122:MET:HA	20:U:122:MET:HE2	1.91	0.50
20:U:124:ASP:OD1	39:n:25:ARG:NH2	2.41	0.50
21:V:67:LYS:O	21:V:68:LEU:C	2.52	0.50
28:c:46:LEU:O	28:c:50:ALA:HB2	2.12	0.50
32:g:74:TYR:CE2	32:g:85:MET:HB3	2.47	0.50
62:h:201:CDL:H132	62:h:201:CDL:H172	1.92	0.50
38:m:45:ARG:NE	39:n:140:LEU:HD11	2.27	0.50
47:AC:147:THR:HG21	47:AC:165:TRP:NE1	2.25	0.50
48:AD:140:TYR:HA	48:AD:144:GLU:CD	2.35	0.50
48:AD:218:TYR:CZ	48:AD:246:PRO:HG3	2.46	0.50
45:Aa:73:VAL:HG23	45:Aa:147:LEU:HD13	1.93	0.50
46:Ab:212:HIS:HE1	46:Ab:246:LEU:CD2	1.95	0.50
46:Ab:297:PRO:HB3	46:Ab:304:ASN:OD1	2.12	0.50
48:Ad:249:TYR:O	48:Ad:250:THR:C	2.54	0.50
54:Ak:9:ARG:NH1	54:Ak:13:LEU:HD11	2.26	0.50
1:A:49:LEU:N	1:A:49:LEU:HD12	2.26	0.50
4:D:55:SER:HB2	12:L:575:THR:HG23	1.93	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:382:ARG:NH1	7:G:527:ASP:CG	2.69	0.50
8:H:181:MET:CE	8:H:300:LEU:HD12	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:200:GLU:HG2	42:q:88:ARG:HB2	1.93	0.50
10:J:55:VAL:HB	11:K:41:PHE:CE2	2.47	0.50
12:L:21:ILE:HG12	12:L:27:ILE:HG23	1.93	0.50
13:M:127:ILE:CG1	14:N:254:LEU:HD21	2.41	0.50
13:M:275:ILE:CD1	13:M:288:TYR:CG	2.84	0.50
13:M:309:PHE:HB2	13:M:458:THR:HG21	1.93	0.50
13:M:370:PRO:CA	13:M:375:LEU:HD22	2.40	0.50
14:N:25:ASN:HB3	30:e:15:ASP:CG	2.37	0.50
14:N:189:TRP:HB2	14:N:204:ASN:HD21	1.77	0.50
15:O:135:LEU:HD13	63:O:401:ADP:C5	2.46	0.50
20:T:104:PHE:CG	20:T:110:LEU:HD22	2.46	0.50
20:T:144:ILE:O	20:T:148:ILE:HG12	2.12	0.50
20:U:125:GLU:OE2	35:j:44:TYR:HE1	1.95	0.50
55:m:201:3PE:H3G2	55:m:201:3PE:H2D2	1.93	0.50
45:AA:162:GLU:HA	45:AA:165:ARG:NH1	2.26	0.50
48:AD:193:LEU:O	69:AD:401:HEC:HAD2	2.11	0.50
48:AD:249:TYR:CD1	48:AD:252:VAL:HG23	2.46	0.50
48:AD:255:TYR:OH	48:AD:269:ASP:HB2	2.12	0.50
51:AG:35:ILE:HA	51:AG:38:VAL:HB	1.94	0.50
52:AH:60:GLN:H	52:AH:60:GLN:CD	2.19	0.50
46:Ab:138:LEU:HD13	46:Ab:233:VAL:O	2.11	0.50
46:Ab:218:MET:HE1	46:Ab:238:LEU:HD22	1.92	0.50
48:Ad:133:ARG:NH2	48:Ad:174:TYR:OH	2.45	0.50
49:Ae:142:ALA:C	49:Ae:147:LEU:HD23	2.36	0.50
1:A:2:ASN:HB2	25:Z:143:TYR:CE1	2.44	0.50
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.38	0.50
2:B:170:TYR:HE2	4:D:135:TYR:CE2	2.30	0.50
5:E:178:ALA:HB2	5:E:191:TYR:HE2	1.76	0.50
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.50
12:L:117:PHE:HE1	12:L:243:VAL:CG2	2.23	0.50
12:L:365:ILE:CD1	12:L:366:MET:HE2	2.42	0.50
12:L:395:ILE:O	12:L:399:ILE:HG13	2.11	0.50
12:L:424:MET:HE2	12:L:502:LEU:HA	1.93	0.50
13:M:248:ILE:HG13	13:M:249:ILE:N	2.25	0.50
13:M:294:MET:HE3	13:M:319:HIS:HD2	1.76	0.50
17:Q:62:THR:HB	17:Q:72:ILE:CD1	2.42	0.50
20:U:90:TYR:HD2	20:U:93:ILE:H	1.59	0.50
34:i:10:LEU:HD12	34:i:13:GLN:HB3	1.94	0.50
37:l:49:ALA:HA	37:l:59:VAL:HG13	1.93	0.50
40:o:39:MET:CE	40:o:58:TYR:HA	2.42	0.50
43:r:6:ARG:O	43:r:9:GLN:CG	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:171:GLU:O	45:AA:175:ASN:N	2.45	0.50
45:AA:397:ASN:HA	46:AB:58:LEU:HD11	1.93	0.50
46:AB:101:ARG:HB3	50:Af:108:TRP:CZ2	2.46	0.50
47:AC:117:VAL:HG11	47:AC:302:ALA:HA	1.93	0.50
47:AC:313:ARG:HB2	50:AF:39:HIS:ND1	2.27	0.50
48:AD:126:SER:HB3	48:AD:178:PRO:HD3	1.93	0.50
49:AE:165:MET:O	49:AE:176:VAL:N	2.44	0.50
50:AF:97:GLU:HA	50:AF:100:ARG:NH1	2.26	0.50
53:AJ:17:ARG:HG2	53:AJ:20:THR:H	1.77	0.50
45:Aa:180:GLN:HG3	45:Aa:181:ASN:N	2.25	0.50
47:Ac:107:TYR:HE1	47:Ac:308:HIS:HB2	1.75	0.50
48:Ad:321:TYR:HB2	50:Af:61:PHE:CE2	2.47	0.50
71:Ad:402:3PH:O31	49:Ae:131:ASN:ND2	2.43	0.50
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.50
5:E:233:LEU:HD23	6:F:43:THR:O	2.10	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:403:VAL:HG13	7:G:403:VAL:O	2.12	0.50
7:G:406:ASN:O	7:G:407:PRO:C	2.53	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
8:H:86:TRP:CZ2	8:H:233:LEU:HG	2.47	0.50
8:H:181:MET:CE	8:H:300:LEU:CD1	2.90	0.50
8:H:224:PHE:CE2	61:H:400:UQ9:H11	2.46	0.50
11:K:73:VAL:HG21	14:N:38:LEU:HD22	1.93	0.50
12:L:539:MET:SD	38:m:11:LEU:HD21	2.52	0.50
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.52	0.50
13:M:371:PRO:HG2	55:M:502:3PE:H2F1	1.93	0.50
16:P:301:ILE:CG2	16:P:305:PHE:HE2	2.22	0.50
20:T:79:ILE:HG23	20:T:126:PHE:CE1	2.47	0.50
20:U:74:LEU:HB3	20:U:79:ILE:HG13	1.93	0.50
20:U:125:GLU:OE2	35:j:44:TYR:CE1	2.65	0.50
20:U:142:GLN:O	20:U:145:VAL:N	2.43	0.50
21:V:8:THR:O	21:V:8:THR:CG2	2.59	0.50
21:V:9:THR:HG21	21:V:78:GLU:CB	2.41	0.50
27:b:67:PRO:HB3	27:b:74:LEU:HB2	1.93	0.50
43:r:7:VAL:O	43:r:11:LEU:HG	2.11	0.50
45:AA:96:LEU:HD11	45:AA:161:ILE:HG12	1.93	0.50
45:AA:118:ALA:CB	45:AA:135:ALA:HB2	2.42	0.50
45:AA:393:ASN:HB3	46:AB:106:VAL:O	2.12	0.50
46:AB:64:PHE:HZ	46:AB:394:SER:HA	1.77	0.50
47:AC:141:TRP:CH2	49:Ae:223:VAL:CG2	2.93	0.50
47:AC:274:PHE:O	47:AC:275:LEU:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:234:ASN:OD1	48:AD:236:TYR:HB2	2.11	0.50
49:AE:127:TYR:HB2	53:AJ:32:PHE:HD1	1.76	0.50
46:Ab:209:VAL:HA	46:Ab:213:PHE:HB2	1.94	0.50
48:Ad:186:ARG:O	48:Ad:191:GLY:N	2.45	0.50
48:Ad:291:LYS:HA	48:Ad:294:LEU:HD12	1.92	0.50
49:Ae:146:VAL:HA	49:Ae:149:MET:HE3	1.94	0.50
50:Af:97:GLU:HA	50:Af:100:ARG:HH11	1.75	0.50
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.46	0.50
4:D:333:ARG:HH12	4:D:453:THR:HA	1.77	0.50
4:D:371:MET:CE	9:I:163:PRO:HB3	2.41	0.50
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.76	0.50
6:F:225:LEU:HB3	6:F:227:PRO:CD	2.37	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
8:H:231:ILE:O	8:H:235:ASN:ND2	2.45	0.50
9:I:78:PHE:CD1	43:r:8:ILE:HG23	2.47	0.50
10:J:16:CYS:SG	11:K:11:ALA:HB1	2.52	0.50
12:L:60:GLU:O	12:L:61:TYR:CD1	2.65	0.50
12:L:109:HIS:O	12:L:110:SER:HB2	2.11	0.50
13:M:4:ILE:HG22	13:M:107:ILE:CD1	2.32	0.50
14:N:25:ASN:HB3	30:e:15:ASP:OD2	2.10	0.50
14:N:258:THR:HG23	14:N:336:THR:HG22	1.93	0.50
15:O:211:VAL:HB	15:O:212:PRO:HD3	1.92	0.50
16:P:68:TYR:CD2	16:P:242:VAL:HG11	2.46	0.50
16:P:165:ILE:HG21	16:P:249:ILE:HG23	1.93	0.50
17:Q:85:ASN:O	17:Q:86:ASN:C	2.52	0.50
18:R:70:ASN:HD22	18:R:111:PHE:HE1	1.60	0.50
20:T:92:LYS:NZ	20:T:92:LYS:HB3	2.27	0.50
20:U:93:ILE:HD11	20:U:118:ILE:HD11	1.92	0.50
23:X:166:ARG:HB3	33:h:150:ARG:HE	1.77	0.50
24:Y:12:HIS:NE2	24:Y:127:PHE:HZ	2.09	0.50
25:Z:86:ILE:HG21	25:Z:124:MET:O	2.11	0.50
25:Z:92:GLU:O	25:Z:95:ALA:N	2.45	0.50
26:a:52:ARG:HD2	26:a:57:VAL:HG22	1.94	0.50
30:e:93:THR:O	30:e:94:PRO:C	2.55	0.50
32:g:53:TRP:H	32:g:53:TRP:HD1	1.56	0.50
36:k:34:PRO:CG	36:k:59:TYR:CD1	2.94	0.50
46:AB:162:LYS:HE3	46:AB:166:PHE:HE2	1.76	0.50
47:AC:50:PHE:CZ	49:AE:136:PHE:CZ	2.99	0.50
47:AC:138:MET:HE1	47:AC:268:ILE:HG23	1.93	0.50
47:AC:291:VAL:O	47:AC:295:ILE:HG12	2.11	0.50
48:Ad:227:LEU:HB2	48:Ad:231:LEU:CB	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:248:ILE:HG23	48:Ad:252:VAL:CG1	2.42	0.50
48:Ad:260:PRO:HB3	52:Ah:24:LEU:CD2	2.42	0.50
3:C:96:LEU:HD22	3:C:155:ILE:HG21	1.94	0.50
4:D:462:ASP:O	4:D:463:ARG:C	2.54	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.11	0.50
9:I:203:ALA:HB2	42:q:88:ARG:HH11	1.76	0.50
11:K:38:LEU:HG	11:K:42:ILE:HD11	1.93	0.50
12:L:149:ILE:HG21	13:M:364:LEU:CD2	2.42	0.50
13:M:63:THR:N	13:M:64:PRO:HD2	2.27	0.50
14:N:175:MET:HE1	14:N:227:ILE:HG22	1.94	0.50
14:N:190:MET:HB3	14:N:201:THR:HG23	1.94	0.50
16:P:209:ARG:HG2	16:P:352:VAL:HG12	1.93	0.50
16:P:228:LEU:HD22	16:P:273:LEU:HD21	1.93	0.50
20:T:130:ILE:HG23	20:T:134:ASP:OD2	2.12	0.50
30:e:42:GLU:HG2	33:h:176:LYS:HE2	1.94	0.50
55:m:201:3PE:H241	55:m:201:3PE:C2	2.42	0.50
39:n:114:MET:O	39:n:115:TYR:C	2.52	0.50
44:s:87:LEU:HB2	44:s:91:ARG:HH12	1.76	0.50
45:AA:296:TRP:NE1	45:AA:347:SER:O	2.45	0.50
46:AB:177:LEU:HD21	46:AB:272:VAL:HG13	1.92	0.50
46:AB:304:ASN:CB	46:AB:307:SER:HB2	2.40	0.50
50:AF:36:ASP:OD1	50:AF:90:TYR:OH	2.23	0.50
52:AH:54:ARG:NE	52:AH:63:GLU:HB3	2.26	0.50
45:Aa:442:ARG:CZ	54:Ak:16:ASN:ND2	2.75	0.50
48:Ad:232:TYR:CG	48:Ad:245:ALA:HA	2.47	0.50
4:D:123:LEU:CB	4:D:135:TYR:OH	2.60	0.50
4:D:399:ALA:HB1	4:D:406:GLU:HG3	1.93	0.50
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.93	0.50
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.47	0.50
12:L:141:PHE:CD2	13:M:370:PRO:CB	2.94	0.50
12:L:354:GLN:O	12:L:354:GLN:HG2	2.12	0.50
13:M:231:LEU:CD1	13:M:235:LEU:CD1	2.85	0.50
13:M:432:ARG:HA	13:M:435:THR:HG22	1.94	0.50
14:N:133:TRP:CG	14:N:133:TRP:O	2.63	0.50
16:P:140:ASP:C	16:P:142:GLU:N	2.68	0.50
20:U:105:MET:HG3	20:U:139:MET:HE1	1.94	0.50
23:X:76:SER:OG	23:X:77:HIS:N	2.45	0.50
23:X:151:ASN:CG	30:e:51:ARG:HH11	2.20	0.50
26:a:50:ARG:CZ	26:a:54:ILE:HD11	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:124:LYS:HE2	38:m:125:PHE:CE2	2.47	0.50
47:AC:128:PHE:HE2	47:AC:178:PHE:CE2	2.30	0.50
47:AC:182:HIS:HE1	67:AC:401:HEM:C4C	2.29	0.50
48:AD:95:PRO:HG2	52:AH:85:PHE:CB	2.42	0.50
48:Ad:309:HIS:CE1	51:Ag:21:PRO:HB2	2.46	0.50
49:Ae:142:ALA:O	49:Ae:147:LEU:HD23	2.12	0.50
1:A:52:SER:HG	1:A:55:PHE:HB2	1.74	0.49
2:B:97:LEU:O	2:B:135:GLY:HA3	2.10	0.49
4:D:256:ASP:CG	43:r:18:GLN:HE22	2.20	0.49
5:E:229:GLY:O	5:E:231:THR:HG23	2.12	0.49
6:F:227:PRO:HB3	7:G:95:PRO:HD3	1.94	0.49
8:H:85:LEU:HD21	8:H:108:THR:HB	1.94	0.49
12:L:123:LEU:CD2	12:L:150:MET:HG3	2.42	0.49
13:M:122:PHE:CE1	13:M:238:LEU:HG	2.46	0.49
13:M:207:MET:SD	13:M:240:SER:HA	2.52	0.49
13:M:441:MET:HG3	13:M:445:ILE:HD12	1.94	0.49
15:O:341:PRO:HB2	28:c:34:PRO:HB3	1.94	0.49
21:V:95:LEU:O	21:V:95:LEU:HD23	2.12	0.49
23:X:49:GLU:CG	23:X:50:GLU:HG3	2.40	0.49
24:Y:115:MET:HE1	55:Y:201:3PE:C21	2.42	0.49
40:o:22:ILE:O	40:o:105:GLU:HG2	2.12	0.49
41:p:74:ILE:O	41:p:75:THR:C	2.54	0.49
51:AG:57:TYR:CE2	51:AG:61:THR:HG21	2.47	0.49
45:Aa:272:GLY:O	51:Ag:19:LEU:HD12	2.12	0.49
48:Ad:114:PHE:HD2	48:Ad:140:TYR:CE2	2.29	0.49
48:Ad:157:GLY:O	48:Ad:158:PRO:C	2.55	0.49
49:Ae:242:HIS:CD2	49:Ae:251:LYS:HB3	2.47	0.49
2:B:194:CYS:CB	2:B:195:PRO:HD3	2.36	0.49
2:B:222:TYR:HA	16:P:137:ARG:HH12	1.77	0.49
4:D:112:HIS:HE1	22:W:100:TRP:CD1	2.30	0.49
5:E:193:GLU:OE1	5:E:217:PRO:HG3	2.13	0.49
5:E:240:PRO:HB3	6:F:60:GLY:CA	2.41	0.49
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.37	0.49
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.11	0.49
8:H:102:ILE:HG21	8:H:150:LEU:HD11	1.93	0.49
13:M:88:ASN:O	13:M:89:ASN:HB3	2.12	0.49
13:M:184:HIS:CD2	13:M:249:ILE:HG23	2.47	0.49
15:O:48:LYS:H	15:O:51:LYS:HE3	1.75	0.49
15:O:136:TYR:OH	15:O:191:LYS:HA	2.11	0.49
15:O:319:ILE:HD12	15:O:324:GLY:HA3	1.94	0.49
16:P:150:ARG:HE	16:P:190:GLU:HB3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:223:PHE:CG	16:P:223:PHE:O	2.64	0.49
23:X:45:LEU:HG	23:X:131:VAL:HG23	1.94	0.49
39:n:20:TYR:CE2	39:n:24:LEU:CD1	2.91	0.49
39:n:96:CYS:SG	39:n:97:TYR:CZ	3.05	0.49
42:q:66:THR:HG23	42:q:74:PHE:CD1	2.47	0.49
45:AA:373:GLN:NE2	45:AA:471:ILE:O	2.44	0.49
47:AC:145:VAL:CA	49:Ae:220:LEU:HB3	2.41	0.49
45:Aa:113:VAL:CG1	46:Ab:299:ILE:HD11	2.43	0.49
45:Aa:171:GLU:O	45:Aa:175:ASN:N	2.45	0.49
46:Ab:45:ASN:HD22	46:Ab:239:ASN:CA	2.23	0.49
46:Ab:67:ALA:HB1	46:Ab:208:PHE:HE1	1.76	0.49
46:Ab:297:PRO:CA	46:Ab:304:ASN:CG	2.83	0.49
48:Ad:114:PHE:CD2	48:Ad:140:TYR:CE2	3.00	0.49
48:Ad:156:ASP:CB	48:Ad:167:ARG:HB3	2.38	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
5:E:200:ILE:HG22	5:E:204:ILE:HG13	1.92	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
7:G:70:SER:O	7:G:184:ARG:NH1	2.45	0.49
7:G:181:ARG:HA	7:G:184:ARG:HH21	1.77	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:372:PHE:CZ	7:G:385:TYR:HB3	2.47	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
12:L:217:LEU:HD13	12:L:273:ILE:HG23	1.94	0.49
12:L:316:THR:CG2	12:L:325:ALA:CB	2.89	0.49
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.47	0.49
15:O:170:LEU:HD21	15:O:184:VAL:HG22	1.95	0.49
15:O:276:LEU:HD11	15:O:278:TYR:CE2	2.47	0.49
16:P:91:ILE:HG13	16:P:95:ARG:NH1	2.23	0.49
16:P:209:ARG:CG	16:P:352:VAL:HG12	2.43	0.49
20:T:84:LEU:HD22	20:T:98:LEU:CD2	2.42	0.49
22:W:49:THR:O	22:W:50:VAL:C	2.56	0.49
23:X:5:VAL:HG11	25:Z:109:SER:HB3	1.95	0.49
45:AA:205:SER:O	45:AA:206:GLU:C	2.55	0.49
48:AD:129:TYR:HD2	48:AD:198:SER:CB	2.25	0.49
48:AD:158:PRO:C	48:AD:166:MET:HB2	2.37	0.49
48:AD:295:MET:HG2	53:AJ:36:PHE:CE1	2.46	0.49
48:AD:318:LYS:HD2	49:AE:86:PRO:HB2	1.94	0.49
49:AE:242:HIS:HD2	49:AE:251:LYS:HB3	1.76	0.49
53:AJ:30:LEU:HD12	54:AK:34:TRP:CB	2.42	0.49
55:Aa:501:3PE:H341	47:Ac:225:THR:HG21	1.93	0.49
46:Ab:375:LYS:NZ	46:Ab:419:VAL:O	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:131:ALA:HA	48:Ad:174:TYR:HA	1.94	0.49
48:Ad:224:GLY:HA3	52:Ah:64:ASP:CG	2.36	0.49
48:Ad:288:MET:SD	71:Ad:402:3PH:C1	3.01	0.49
49:Ae:227:ASN:N	49:Ae:233:GLY:O	2.45	0.49
49:Ae:231:PHE:CD1	49:Ae:250:ARG:HB2	2.47	0.49
1:A:2:ASN:HB3	8:H:2:PHE:CZ	2.48	0.49
2:B:137:LEU:CD2	2:B:145:LEU:HD22	2.42	0.49
2:B:170:TYR:OH	4:D:135:TYR:CD2	2.64	0.49
6:F:42:PHE:HE1	6:F:137:LYS:HG2	1.76	0.49
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.95	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
12:L:9:LEU:HD21	55:i:201:3PE:C2A	2.41	0.49
12:L:173:LEU:HD23	55:L:702:3PE:C32	2.30	0.49
12:L:393:ASP:OD1	12:L:393:ASP:C	2.56	0.49
13:M:139:GLN:HG3	13:M:140:THR:N	2.27	0.49
13:M:348:LEU:HD12	13:M:415:GLN:HE22	1.77	0.49
14:N:230:ILE:HG21	14:N:296:LEU:HD11	1.94	0.49
15:O:132:GLN:CD	63:O:401:ADP:HN62	2.20	0.49
15:O:237:ILE:CG2	15:O:241:TYR:CE2	2.95	0.49
20:T:90:TYR:HE2	20:T:93:ILE:HG12	1.77	0.49
20:T:115:GLN:O	20:T:119:ILE:HG12	2.12	0.49
20:T:134:ASP:HA	20:T:137:LYS:HZ3	1.76	0.49
25:Z:10:MET:HG3	25:Z:11:PRO:HD2	1.93	0.49
26:a:49:GLU:O	26:a:53:ARG:HG3	2.13	0.49
33:h:129:PRO:HG3	41:p:66:ARG:CZ	2.42	0.49
34:i:83:HIS:CD2	41:p:37:TYR:CE2	3.01	0.49
37:l:81:ARG:HD3	37:l:85:GLU:OE2	2.13	0.49
37:l:122:THR:O	38:m:6:TYR:CE1	2.65	0.49
49:AE:172:LYS:HE2	49:AE:173:PRO:HD3	1.93	0.49
46:Ab:145:GLU:O	46:Ab:146:PHE:C	2.55	0.49
47:Ac:361:ILE:HA	47:Ac:365:LEU:HB2	1.95	0.49
48:Ad:189:ASN:O	48:Ad:190:ASN:HB2	2.13	0.49
49:Ae:142:ALA:HB3	49:Ae:147:LEU:HD22	1.92	0.49
49:Ae:207:LYS:HZ3	49:Ae:268:ASP:HA	1.75	0.49
2:B:109:ALA:HB1	2:B:110:PRO:CD	2.41	0.49
4:D:35:ARG:HE	32:g:59:PRO:CD	2.24	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
5:E:73:HIS:ND1	6:F:236:PHE:CD1	2.81	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:151:LEU:O	8:H:152:SER:C	2.54	0.49
12:L:264:HIS:HA	12:L:267:THR:OG1	2.12	0.49
12:L:399:ILE:HG22	12:L:409:LEU:HD13	1.93	0.49
13:M:278:ARG:HH22	37:l:108:ASP:CG	2.21	0.49
13:M:285:LEU:HD22	13:M:410:MET:SD	2.53	0.49
15:O:49:THR:HG21	15:O:151:LEU:HG	1.93	0.49
20:T:120:MET:HE1	22:W:43:TYR:CG	2.47	0.49
23:X:142:TYR:OH	33:h:189:ASN:ND2	2.45	0.49
30:e:34:HIS:CE1	30:e:38:LYS:HD2	2.47	0.49
34:i:90:MET:O	34:i:91:ALA:C	2.53	0.49
36:k:47:LEU:CD1	39:n:43:LEU:HD23	2.42	0.49
37:l:101:TRP:HE1	38:m:62:ASP:HA	1.76	0.49
39:n:145:SER:HB2	39:n:146:PRO:HD2	1.94	0.49
48:AD:189:ASN:HD22	69:AD:401:HEC:HMD2	1.78	0.49
50:AF:44:VAL:O	50:AF:48:ILE:HG13	2.12	0.49
50:AF:75:ILE:HD12	50:AF:81:TRP:HZ2	1.76	0.49
45:Aa:226:ALA:HB2	45:Aa:253:VAL:HB	1.94	0.49
45:Aa:341:PHE:HE1	45:Aa:356:ALA:CB	2.26	0.49
46:Ab:84:ARG:CG	49:Ai:68:VAL:HG22	2.33	0.49
46:Ab:226:SER:O	46:Ab:227:HIS:C	2.56	0.49
47:Ac:218:ILE:HB	47:Ac:219:PRO:HD2	1.94	0.49
47:Ac:291:VAL:O	47:Ac:295:ILE:HG12	2.11	0.49
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HD2	1.94	0.49
48:Ad:227:LEU:HD12	48:Ad:227:LEU:O	2.11	0.49
1:A:66:ASP:OD2	10:J:58:ILE:HD12	2.05	0.49
2:B:99:CYS:SG	56:B:301:SF4:S4	3.03	0.49
3:C:148:GLU:OE2	17:Q:140:LYS:NZ	2.30	0.49
3:C:234:LEU:O	3:C:234:LEU:CG	2.60	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:45:LEU:O	6:F:46:TYR:HB2	2.12	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
12:L:23:MET:HE1	62:L:704:CDL:C19	2.43	0.49
12:L:445:GLU:CB	12:L:450:LEU:HD23	2.37	0.49
12:L:496:LEU:HA	12:L:499:LEU:HB2	1.94	0.49
15:O:352:ILE:HG21	29:d:52:PRO:HG2	1.94	0.49
16:P:156:SER:HB2	16:P:161:VAL:HG21	1.95	0.49
16:P:163:ARG:HH22	16:P:256:PRO:HA	1.76	0.49
23:X:24:VAL:HG23	23:X:25:LEU:HD12	1.95	0.49
38:m:127:ILE:HG22	41:p:136:THR:HG23	1.95	0.49
45:AA:389:THR:O	45:AA:390:ARG:C	2.55	0.49
46:AB:40:PHE:CZ	46:AB:406:TYR:HB2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:90:THR:HG23	46:AB:95:SER:HA	1.95	0.49
47:AC:199:PHE:HE1	47:Ac:8:HIS:HE2	1.42	0.49
47:Ac:136:GLY:O	47:Ac:259:ALA:HB2	2.12	0.49
47:Ac:185:LEU:HD23	47:Ac:188:ILE:HD12	1.95	0.49
47:Ac:253:PRO:HG3	48:Ad:205:HIS:CG	2.48	0.49
52:Ah:44:ALA:O	52:Ah:48:LEU:HB2	2.13	0.49
1:A:104:TYR:CE2	10:J:167:ILE:HD12	2.48	0.49
3:C:80:LEU:O	3:C:81:ASP:HB2	2.12	0.49
4:D:163:PRO:HG2	4:D:168:GLN:HG2	1.94	0.49
7:G:382:ARG:CZ	7:G:652:ASN:ND2	2.74	0.49
13:M:193:ASN:HA	13:M:253:LEU:HD23	1.94	0.49
13:M:420:THR:HG21	13:M:423:MET:HG2	1.93	0.49
14:N:231:SER:HA	14:N:300:THR:HA	1.93	0.49
15:O:72:LYS:O	15:O:73:LEU:C	2.56	0.49
15:O:146:ALA:HB2	15:O:159:LEU:HD21	1.95	0.49
15:O:260:SER:O	15:O:263:ALA:HB3	2.13	0.49
16:P:132:ARG:HD2	16:P:134:TRP:CZ2	2.47	0.49
16:P:157:LYS:CB	16:P:195:PHE:HD1	2.24	0.49
18:R:88:HIS:O	18:R:89:PRO:C	2.56	0.49
23:X:153:VAL:O	23:X:155:GLU:HG3	2.12	0.49
23:X:170:TRP:CZ3	62:X:201:CDL:H552	2.47	0.49
25:Z:128:ARG:HB3	25:Z:132:GLU:OE1	2.13	0.49
30:e:36:PHE:O	30:e:39:GLU:N	2.45	0.49
35:j:45:ARG:HD3	36:k:57:TRP:CD1	2.47	0.49
47:AC:137:GLN:HE22	47:AC:263:ASN:C	2.18	0.49
47:AC:297:SER:O	47:AC:300:ILE:HG22	2.13	0.49
48:AD:107:HIS:HA	48:AD:110:ILE:HD12	1.95	0.49
45:Aa:108:ALA:O	45:Aa:112:GLU:HG3	2.12	0.49
45:Aa:296:TRP:NE1	45:Aa:347:SER:O	2.45	0.49
47:Ac:244:LEU:HD12	48:Ad:292:MET:HE2	1.94	0.49
48:Ad:300:LEU:O	48:Ad:301:PRO:C	2.54	0.49
52:Ah:39:GLU:O	52:Ah:42:VAL:HG12	2.12	0.49
4:D:51:VAL:HG21	4:D:58:THR:HG22	1.95	0.49
4:D:260:GLU:OE1	9:I:72:MET:SD	2.71	0.49
4:D:304:LYS:HD3	4:D:318:VAL:HG23	1.95	0.49
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
7:G:617:ARG:HH22	22:W:128:GLY:N	2.11	0.49
8:H:183:MET:SD	55:I:301:3PE:H331	2.53	0.49
12:L:67:HIS:HE2	12:L:69:VAL:C	2.21	0.49
12:L:590:SER:HB2	24:Y:45:LEU:CD1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:5:ILE:HG13	13:M:6:LEU:N	2.28	0.49
13:M:248:ILE:CG1	13:M:249:ILE:HD12	2.39	0.49
18:R:48:PHE:HD1	18:R:52:GLN:O	1.95	0.49
19:S:30:SER:O	19:S:31:GLN:C	2.56	0.49
20:U:94:ASP:OD1	20:U:95:PRO:HD2	2.12	0.49
28:c:62:HIS:O	28:c:66:VAL:HG23	2.12	0.49
31:f:25:TYR:OH	31:f:29:LYS:HE3	2.13	0.49
45:AA:341:PHE:HE1	45:AA:356:ALA:CB	2.26	0.49
47:AC:181:PHE:CA	47:AC:184:ILE:HG22	2.43	0.49
49:AE:92:ARG:HA	51:AG:24:GLN:HA	1.94	0.49
51:AG:67:PHE:CZ	51:AG:71:LYS:HD3	2.47	0.49
46:Ab:178:HIS:CD2	46:Ab:335:LEU:HD12	2.47	0.49
47:Ac:297:SER:O	47:Ac:300:ILE:HG22	2.13	0.49
48:Ad:175:PHE:H	48:Ad:175:PHE:HD1	1.61	0.49
48:Ad:232:TYR:CZ	48:Ad:245:ALA:HB2	2.48	0.49
48:Ad:250:THR:HA	48:Ad:263:MET:HB2	1.94	0.49
48:Ad:309:HIS:HD2	48:Ad:310:LYS:HD3	1.78	0.49
2:B:126:ARG:HH12	2:B:151:GLN:HG2	1.78	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
7:G:648:GLU:O	19:S:22:HIS:HE1	1.95	0.49
9:I:76:TYR:CE1	9:I:79:ARG:CZ	2.95	0.49
12:L:68:TRP:CE3	12:L:76:LEU:HD21	2.47	0.49
12:L:427:ILE:HD11	36:k:69:PHE:HE1	1.78	0.49
16:P:113:LYS:C	16:P:115:SER:H	2.21	0.49
16:P:157:LYS:HD3	16:P:195:PHE:CD1	2.48	0.49
17:Q:154:LYS:HB2	17:Q:155:PRO:CD	2.39	0.49
22:W:102:GLN:H	22:W:105:HIS:CD2	2.30	0.49
22:W:107:MET:HE3	22:W:112:GLU:OE2	2.11	0.49
27:b:60:ASP:HB2	27:b:62:ASN:OD1	2.12	0.49
45:AA:197:LEU:HD21	45:AA:348:TYR:CD2	2.48	0.49
47:AC:361:ILE:HA	47:AC:365:LEU:HB2	1.94	0.49
49:AE:218:THR:OG1	49:AE:254:ALA:HB1	2.13	0.49
49:AE:239:HIS:CD2	47:Ac:278:TYR:OH	2.65	0.49
50:AF:83:LYS:HB2	50:AF:86:GLU:HG3	1.95	0.49
51:AG:11:ILE:HD12	51:AG:11:ILE:N	2.27	0.49
45:Aa:186:TYR:CZ	49:Ae:80:HIS:HB2	2.47	0.49
46:Ab:38:LEU:HD22	46:Ab:38:LEU:H	1.78	0.49
46:Ab:225:VAL:HG22	46:Ab:226:SER:H	1.78	0.49
48:Ad:249:TYR:CE2	48:Ad:252:VAL:HG23	2.48	0.49
49:Ae:159:ILE:HD11	49:Ae:165:MET:SD	2.52	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
7:G:617:ARG:NH1	22:W:129:HIS:CA	2.76	0.49
9:I:144:ARG:NE	9:I:146:ASP:OD2	2.46	0.49
12:L:41:LYS:HG3	12:L:98:TRP:CH2	2.45	0.49
13:M:1:MET:HB2	13:M:52:PHE:CE2	2.47	0.49
13:M:227:GLY:HA2	13:M:230:ILE:HG22	1.95	0.49
15:O:256:LEU:HB3	15:O:258:TYR:CE1	2.48	0.49
19:S:18:GLU:HB3	19:S:52:PRO:HB2	1.94	0.49
23:X:93:ASN:HB2	26:a:38:VAL:HG23	1.93	0.49
24:Y:143:VAL:HG23	33:h:157:ARG:O	2.13	0.49
32:g:109:ASP:HB2	32:g:114:GLU:HB3	1.94	0.49
38:m:75:ASN:OD1	38:m:79:ASN:ND2	2.46	0.49
39:n:20:TYR:OH	39:n:45:ARG:HB2	2.12	0.49
39:n:81:ILE:HD12	39:n:87:GLY:O	2.12	0.49
39:n:114:MET:HG3	39:n:115:TYR:HD2	1.78	0.49
42:q:65:THR:HG22	42:q:81:MET:HE1	1.95	0.49
47:AC:218:ILE:HB	47:AC:219:PRO:HD2	1.94	0.49
48:AD:227:LEU:HD11	48:AD:233:PHE:N	2.28	0.49
48:AD:262:THR:CB	52:AH:26:ASP:HA	2.40	0.49
49:AE:172:LYS:HD2	47:Ac:169:SER:HB3	1.94	0.49
48:Ad:132:TYR:O	48:Ad:135:LEU:HB2	2.13	0.49
49:Ae:152:ILE:HG13	49:Ae:154:ILE:CD1	2.42	0.49
49:Ae:155:LYS:CE	49:Ae:157:SER:HB3	2.42	0.49
49:Ae:163:LYS:N	49:Ae:178:HIS:HB3	2.19	0.49
49:Ae:172:LYS:HA	49:Ae:172:LYS:CE	2.43	0.49
49:Ae:179:ARG:NH1	49:Ae:184:ILE:HA	2.28	0.49
1:A:52:SER:HG	1:A:55:PHE:CB	2.26	0.48
2:B:98:ALA:HB1	2:B:100:CYS:N	2.28	0.48
6:F:67:GLU:O	6:F:71:LYS:HG2	2.13	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
8:H:229:THR:O	8:H:229:THR:CG2	2.52	0.48
8:H:277:TYR:CE2	55:I:301:3PE:H272	2.48	0.48
10:J:22:LYS:CD	11:K:23:ARG:HG2	2.40	0.48
12:L:101:MET:HE1	12:L:121:LEU:CB	2.43	0.48
12:L:227:PHE:CD2	12:L:283:LEU:HD23	2.48	0.48
12:L:361:ASN:O	12:L:361:ASN:CG	2.54	0.48
13:M:134:THR:O	13:M:142:ARG:CD	2.59	0.48
13:M:348:LEU:HB2	13:M:415:GLN:OE1	2.13	0.48
23:X:5:VAL:CG1	25:Z:109:SER:HB3	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:144:THR:HG23	26:a:37:ARG:O	2.12	0.48
27:b:35:ILE:HG12	27:b:35:ILE:O	2.13	0.48
30:e:94:PRO:HB3	30:e:98:HIS:CD2	2.48	0.48
33:h:96:ALA:O	41:p:63:TYR:CE1	2.62	0.48
33:h:179:ILE:HG22	33:h:180:ASP:N	2.28	0.48
34:i:69:LEU:HG	34:i:71:ALA:HB3	1.94	0.48
36:k:38:VAL:CG1	39:n:39:TYR:HB2	2.43	0.48
45:AA:285:ALA:O	45:AA:359:VAL:HA	2.11	0.48
46:AB:47:LEU:CD2	46:AB:234:ALA:HB1	2.43	0.48
47:AC:196:HIS:NE2	67:AC:402:HEM:ND	2.61	0.48
52:AH:49:GLU:HA	52:AH:52:ASP:OD2	2.13	0.48
47:Ac:72:ASP:HB3	49:Ae:145:ASP:HB3	1.93	0.48
48:Ad:130:VAL:O	48:Ad:175:PHE:HD1	1.95	0.48
62:Ag:102:CDL:H521	62:Ag:102:CDL:H562	1.94	0.48
58:B:304:PC1:H382	8:H:57:MET:HE2	1.95	0.48
4:D:36:GLN:HG3	4:D:38:GLN:HE21	1.78	0.48
4:D:253:LEU:O	4:D:256:ASP:OD1	2.31	0.48
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.48
8:H:19:PHE:CD2	26:a:11:ILE:HG21	2.48	0.48
9:I:180:HIS:HD2	16:P:100:LEU:CD2	2.26	0.48
12:L:56:HIS:CA	40:o:74:PHE:CD1	2.95	0.48
12:L:144:TRP:HH2	12:L:256:GLY:HA2	1.78	0.48
12:L:150:MET:HE3	62:L:704:CDL:H732	1.93	0.48
12:L:350:LEU:HD23	12:L:443:ILE:HD11	1.96	0.48
12:L:372:CYS:SG	12:L:454:ILE:HG22	2.54	0.48
12:L:424:MET:HE2	12:L:502:LEU:CA	2.43	0.48
13:M:351:VAL:HA	33:h:59:PRO:HB3	1.96	0.48
15:O:78:ALA:HB2	15:O:85:HIS:HB2	1.95	0.48
15:O:135:LEU:CD1	63:O:401:ADP:C6	2.96	0.48
15:O:355:LYS:O	29:d:59:HIS:HE1	1.96	0.48
16:P:80:VAL:HB	16:P:103:LEU:HD22	1.94	0.48
16:P:236:VAL:HG23	16:P:271:TYR:O	2.13	0.48
19:S:16:LEU:HD13	19:S:94:VAL:HG12	1.95	0.48
21:V:31:THR:O	21:V:35:LEU:HG	2.12	0.48
21:V:77:VAL:C	21:V:79:GLU:N	2.67	0.48
22:W:93:LEU:O	22:W:94:GLN:C	2.55	0.48
23:X:49:GLU:CG	23:X:50:GLU:N	2.76	0.48
23:X:74:ILE:O	23:X:77:HIS:O	2.31	0.48
23:X:129:THR:HA	27:b:67:PRO:O	2.13	0.48
26:a:3:PHE:CE2	62:a:101:CDL:HA4	2.48	0.48
34:i:19:ARG:HH11	39:n:173:ARG:NH2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:51:HIS:HB3	39:n:63:LEU:HD13	1.95	0.48
45:AA:148:ALA:HA	45:AA:250:LEU:HD21	1.95	0.48
46:AB:64:PHE:CZ	46:AB:394:SER:HA	2.49	0.48
46:AB:177:LEU:HD22	46:AB:270:ALA:HB1	1.96	0.48
50:AF:101:GLU:HB3	50:AF:105:ARG:NH1	2.28	0.48
45:Aa:274:GLU:OE2	45:Aa:276:ARG:NH1	2.44	0.48
48:Ad:212:PHE:CE1	48:Ad:216:THR:HG21	2.47	0.48
49:Ae:200:HIS:O	49:Ae:201:ASP:C	2.55	0.48
1:A:81:THR:N	27:b:46:ASN:HD21	2.10	0.48
2:B:96:GLY:O	2:B:134:ALA:O	2.31	0.48
2:B:99:CYS:HG	56:B:301:SF4:FE1	1.30	0.48
58:B:304:PC1:H241	16:P:310:PHE:HE1	1.79	0.48
3:C:223:VAL:HG23	3:C:225:LEU:HD12	1.88	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
8:H:147:ALA:O	8:H:151:LEU:N	2.42	0.48
8:H:152:SER:O	8:H:153:VAL:C	2.55	0.48
13:M:166:LEU:HD21	13:M:170:HIS:CE1	2.48	0.48
13:M:190:TRP:CE2	24:Y:89:PRO:HG2	2.48	0.48
13:M:311:GLY:HA2	13:M:314:MET:CE	2.42	0.48
15:O:59:VAL:HG22	15:O:157:VAL:CG2	2.43	0.48
22:W:46:VAL:HB	22:W:47:PRO:HD3	1.95	0.48
37:l:167:TYR:OH	37:l:176:LYS:O	2.14	0.48
43:r:27:ARG:CB	43:r:31:ILE:CG2	2.87	0.48
45:AA:101:THR:O	45:AA:102:LYS:C	2.55	0.48
47:AC:51:LEU:HD12	67:AC:401:HEM:CBA	2.43	0.48
48:AD:237:PHE:CZ	48:AD:242:ILE:HA	2.48	0.48
49:AE:222:CYS:SG	47:Ac:268:ILE:CD1	3.01	0.48
49:AE:231:PHE:HD2	49:AE:250:ARG:NH1	2.11	0.48
51:AG:76:ALA:O	51:AG:79:GLU:HB3	2.12	0.48
46:Ab:429:LYS:HA	46:Ab:432:VAL:CG1	2.40	0.48
47:Ac:281:LEU:HD12	47:Ac:290:GLY:HA3	1.95	0.48
47:Ac:317:PHE:HB3	50:Af:27:PHE:HD2	1.78	0.48
48:Ad:181:ASN:O	48:Ad:184:ALA:N	2.46	0.48
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD2	2.47	0.48
49:Ae:174:LEU:HD11	49:Ae:273:VAL:CG1	2.43	0.48
1:A:49:LEU:CB	1:A:50:PRO:HD2	2.17	0.48
1:A:108:GLN:O	1:A:109:LYS:HB2	2.14	0.48
2:B:90:LEU:O	2:B:119:VAL:HA	2.12	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.78	0.48
8:H:51:ASP:C	8:H:51:ASP:OD1	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:68:MET:HG2	8:H:72:ILE:HD13	1.95	0.48
8:H:197:PRO:HB3	8:H:277:TYR:CB	2.43	0.48
12:L:152:PHE:HE1	13:M:412:ILE:HD11	1.79	0.48
12:L:296:ASN:ND2	12:L:425:ARG:HH21	2.12	0.48
12:L:316:THR:HG21	12:L:325:ALA:HA	1.95	0.48
12:L:402:CYS:SG	12:L:403:ASN:N	2.87	0.48
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.47	0.48
13:M:123:GLU:CB	14:N:255:PRO:HG2	2.44	0.48
14:N:321:LYS:HD2	29:d:49:ARG:NE	2.29	0.48
16:P:94:LEU:O	16:P:97:MET:HG2	2.14	0.48
20:T:110:LEU:CD2	20:T:118:ILE:HD12	2.44	0.48
41:p:5:TRP:CZ3	41:p:10:TYR:O	2.66	0.48
47:AC:58:ASP:O	47:AC:62:ALA:N	2.41	0.48
48:AD:214:LEU:HD11	48:AD:237:PHE:CD1	2.48	0.48
51:AG:56:VAL:O	51:AG:57:TYR:C	2.55	0.48
53:AJ:23:LEU:HA	54:AK:27:VAL:CG2	2.44	0.48
45:Aa:160:GLN:HA	45:Aa:163:LYS:NZ	2.29	0.48
48:Ad:277:ALA:O	48:Ad:280:PRO:HD3	2.13	0.48
48:Ad:314:LEU:HB3	50:Af:71:MET:HE1	1.95	0.48
49:Ae:147:LEU:C	49:Ae:147:LEU:HD12	2.38	0.48
1:A:7:ILE:CD1	55:H:401:3PE:H371	2.36	0.48
2:B:97:LEU:CD1	4:D:94:VAL:CG1	2.88	0.48
2:B:104:MET:SD	2:B:122:ARG:NE	2.86	0.48
3:C:149:LEU:CD2	17:Q:64:LEU:HD21	2.43	0.48
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:475:VAL:HG11	7:G:516:LEU:HD23	1.95	0.48
9:I:154:TYR:CA	9:I:169:GLU:OE2	2.61	0.48
10:J:5:ILE:HB	10:J:120:LEU:HD13	1.96	0.48
10:J:88:ILE:HD11	11:K:23:ARG:HH12	1.77	0.48
13:M:216:LEU:HD12	13:M:236:LEU:CD2	2.39	0.48
13:M:307:TRP:CE3	13:M:383:MET:CE	2.97	0.48
14:N:81:LEU:HD23	30:e:60:PHE:HE1	1.78	0.48
18:R:51:ARG:O	18:R:52:GLN:HG3	2.13	0.48
20:T:80:LYS:HB2	20:T:145:VAL:HG11	1.96	0.48
20:T:95:PRO:HG2	20:T:97:LYS:HB3	1.95	0.48
25:Z:97:ILE:CG1	30:e:92:TYR:HD1	2.26	0.48
33:h:73:PHE:O	33:h:77:LEU:N	2.46	0.48
38:m:122:ASP:O	38:m:123:ARG:C	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:195:TYR:OH	46:Ab:261:GLN:HG3	2.12	0.48
47:AC:52:ALA:N	67:AC:401:HEM:HMA2	2.27	0.48
67:AC:402:HEM:HHA	67:AC:402:HEM:O1A	2.12	0.48
48:AD:94:TYR:HD2	48:AD:209:ASP:CG	2.21	0.48
48:AD:96:TRP:CD1	48:AD:96:TRP:H	2.31	0.48
53:AJ:23:LEU:CA	54:AK:27:VAL:CG2	2.91	0.48
46:Ab:113:THR:O	46:Ab:119:MET:HG3	2.13	0.48
46:Ab:286:PHE:CZ	46:Ab:427:ALA:HB1	2.49	0.48
48:Ad:200:ILE:HG12	69:Ad:401:HEC:HMA3	1.95	0.48
49:Ai:43:LEU:O	49:Ai:44:ASP:C	2.56	0.48
4:D:42:GLU:HA	4:D:45:GLU:HG2	1.96	0.48
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.78	0.48
4:D:181:LEU:HD11	4:D:210:MET:CB	2.43	0.48
4:D:181:LEU:HD12	4:D:210:MET:CE	2.43	0.48
5:E:223:CYS:HB3	6:F:132:ARG:NH1	2.28	0.48
6:F:226:LYS:O	6:F:227:PRO:C	2.56	0.48
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.48
10:J:91:PHE:O	10:J:94:LEU:HB3	2.13	0.48
10:J:169:ILE:CD1	14:N:42:PRO:HA	2.44	0.48
12:L:274:LEU:O	12:L:277:MET:HG2	2.14	0.48
12:L:433:THR:HG21	12:L:436:ARG:NH2	2.29	0.48
13:M:42:LEU:HG	13:M:67:ILE:CD1	2.42	0.48
13:M:313:THR:HA	13:M:316:MET:CE	2.43	0.48
14:N:4:ILE:HG23	14:N:5:THR:N	2.29	0.48
14:N:338:PRO:HG3	62:X:201:CDL:H611	1.96	0.48
18:R:67:GLN:HG3	18:R:68:PRO:HD2	1.96	0.48
23:X:170:TRP:CE3	62:X:201:CDL:H521	2.47	0.48
33:h:73:PHE:HE2	33:h:74:TYR:HE1	1.62	0.48
37:l:38:PRO:CB	38:m:75:ASN:ND2	2.70	0.48
46:AB:388:THR:HG23	46:AB:391:GLY:H	1.78	0.48
48:AD:159:ASN:HB3	48:AD:166:MET:HG3	1.94	0.48
45:Aa:341:PHE:HB2	45:Aa:368:MET:CE	2.43	0.48
46:Ab:81:HIS:CD2	46:Ab:158:LEU:HD12	2.48	0.48
46:Ab:159:LYS:HD2	46:Ab:197:MET:HE1	1.95	0.48
46:Ab:201:THR:OG1	46:Ab:204:GLU:HG3	2.14	0.48
46:Ab:388:THR:HG23	46:Ab:391:GLY:H	1.77	0.48
48:Ad:89:LEU:H	52:Ah:70:PHE:HE1	1.60	0.48
2:B:94:THR:HG22	2:B:96:GLY:H	1.79	0.48
2:B:176:SER:O	2:B:177:VAL:HG23	2.14	0.48
5:E:131:ILE:CD1	5:E:185:VAL:HB	2.25	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
6:F:297:LYS:HB2	6:F:333:GLU:HB3	1.95	0.48
7:G:170:LYS:O	7:G:231:LEU:HA	2.13	0.48
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
9:I:62:MET:O	9:I:63:TRP:C	2.56	0.48
10:J:106:LEU:HA	10:J:109:TYR:HB2	1.95	0.48
12:L:141:PHE:HD1	12:L:182:PHE:CD2	2.31	0.48
12:L:319:MET:O	12:L:319:MET:HG2	2.13	0.48
13:M:177:MET:HE1	41:p:86:TYR:CE1	2.49	0.48
13:M:422:HIS:CE1	13:M:425:ASN:OD1	2.66	0.48
14:N:227:ILE:CA	14:N:230:ILE:HG22	2.38	0.48
15:O:245:PHE:CE1	15:O:249:MET:HG3	2.48	0.48
20:T:120:MET:HE1	22:W:43:TYR:CD2	2.49	0.48
20:U:128:PHE:HZ	20:U:148:ILE:HD12	1.76	0.48
25:Z:143:TYR:O	25:Z:144:THR:C	2.55	0.48
30:e:47:ILE:HG13	30:e:47:ILE:O	2.12	0.48
30:e:105:ARG:O	30:e:106:PRO:C	2.56	0.48
34:i:69:LEU:O	34:i:72:VAL:HG22	2.13	0.48
34:i:69:LEU:HD23	34:i:72:VAL:HG13	1.95	0.48
40:o:87:TRP:NE1	40:o:91:GLU:OE1	2.46	0.48
45:AA:341:PHE:CE1	45:AA:356:ALA:HB1	2.48	0.48
47:AC:140:PHE:CZ	47:AC:261:PRO:HA	2.48	0.48
47:AC:145:VAL:HG12	49:Ae:220:LEU:HD13	1.92	0.48
47:AC:153:ILE:HG23	47:AC:154:PRO:HD2	1.96	0.48
51:AG:50:ALA:O	51:AG:54:VAL:HG23	2.13	0.48
51:AG:69:GLN:O	51:AG:72:ARG:HB3	2.14	0.48
45:Aa:339:GLN:O	45:Aa:340:SER:C	2.56	0.48
46:Ab:91:THR:C	46:Ab:93:GLY:H	2.22	0.48
46:Ab:91:THR:C	46:Ab:93:GLY:N	2.69	0.48
47:Ac:32:ASN:ND2	47:Ac:228:ASP:OD1	2.47	0.48
48:Ad:130:VAL:HG12	48:Ad:175:PHE:CE1	2.49	0.48
48:Ad:157:GLY:N	48:Ad:158:PRO:CD	2.77	0.48
48:Ad:279:GLU:HG2	48:Ad:282:HIS:N	2.29	0.48
49:Ae:192:VAL:O	49:Ae:195:LEU:HB2	2.13	0.48
49:Ae:217:CYS:O	49:Ae:218:THR:C	2.56	0.48
54:Ak:9:ARG:O	54:Ak:10:TYR:C	2.56	0.48
4:D:99:LEU:HD22	4:D:106:VAL:HG11	1.95	0.48
4:D:299:GLN:NE2	9:I:36:TYR:CZ	2.80	0.48
5:E:147:ILE:CD1	5:E:195:LEU:HB2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.29	0.48
7:G:183:ILE:HD11	7:G:197:THR:HG23	1.95	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
8:H:140:ILE:HG13	8:H:141:SER:N	2.28	0.48
8:H:154:LEU:O	8:H:155:LEU:C	2.55	0.48
8:H:218:GLY:O	8:H:219:PRO:C	2.57	0.48
8:H:313:GLY:O	8:H:314:VAL:C	2.56	0.48
9:I:41:LYS:HG2	9:I:41:LYS:O	2.13	0.48
10:J:20:ALA:C	10:J:22:LYS:H	2.21	0.48
10:J:28:GLY:O	10:J:31:GLY:N	2.46	0.48
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.49	0.48
12:L:435:PRO:O	36:k:58:ARG:HD2	2.14	0.48
12:L:496:LEU:HD12	12:L:497:GLY:CA	2.44	0.48
12:L:597:LEU:HD21	24:Y:37:ILE:HD12	1.96	0.48
13:M:344:MET:CE	38:m:59:HIS:NE2	2.74	0.48
14:N:146:TYR:CE1	14:N:198:PRO:HG2	2.49	0.48
19:S:87:VAL:O	19:S:88:THR:C	2.55	0.48
23:X:10:LEU:H	23:X:10:LEU:HD12	1.77	0.48
23:X:49:GLU:O	23:X:51:LYS:HD2	2.13	0.48
34:i:83:HIS:CD2	41:p:37:TYR:HE2	2.31	0.48
36:k:69:PHE:CE1	36:k:73:ILE:HD11	2.48	0.48
37:l:167:TYR:HD2	37:l:168:LEU:CD1	2.19	0.48
39:n:144:THR:HG23	39:n:144:THR:O	2.13	0.48
46:AB:109:LYS:O	46:AB:123:VAL:HA	2.14	0.48
48:AD:94:TYR:HB2	48:AD:96:TRP:HE1	1.77	0.48
49:AE:108:GLU:HA	49:AE:111:LYS:HE2	1.96	0.48
52:AH:31:VAL:HG11	52:AH:84:LEU:HB2	1.95	0.48
46:Ab:231:LYS:O	46:Ab:235:GLU:HB3	2.14	0.48
48:Ad:124:CYS:O	48:Ad:125:HIS:CG	2.67	0.48
71:Ad:402:3PH:C3	49:Ae:131:ASN:ND2	2.76	0.48
51:Ag:11:ILE:CG2	51:Ag:12:ARG:N	2.77	0.48
49:Ai:62:ARG:HB3	49:Ai:63:PRO:HD2	1.96	0.48
2:B:97:LEU:HA	4:D:94:VAL:CG2	2.44	0.48
2:B:98:ALA:CB	2:B:101:ALA:H	2.27	0.48
5:E:45:GLU:H	5:E:45:GLU:CD	2.21	0.48
5:E:71:GLU:HG3	44:s:94:GLN:NE2	2.27	0.48
5:E:206:GLU:HB3	5:E:213:PRO:HB3	1.96	0.48
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.96	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:277:MET:HE1	17:Q:153:PRO:HD3	1.96	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:403:VAL:HG23	7:G:432:ILE:CB	2.38	0.48
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.95	0.48
8:H:51:ASP:OD1	8:H:52:ALA:N	2.47	0.48
10:J:124:LEU:HD23	25:Z:137:ASN:HD21	1.64	0.48
13:M:269:MET:HE3	13:M:399:ASN:HB3	1.96	0.48
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.95	0.48
16:P:146:VAL:HG13	16:P:190:GLU:HG3	1.95	0.48
16:P:376:ASN:O	16:P:377:TYR:C	2.57	0.48
17:Q:78:ARG:O	17:Q:80:PHE:HD1	1.96	0.48
32:g:117:ARG:NH2	41:p:10:TYR:OH	2.47	0.48
36:k:18:GLY:O	36:k:19:LYS:C	2.55	0.48
38:m:49:LEU:HD23	39:n:140:LEU:HD21	1.95	0.48
43:r:6:ARG:CA	43:r:9:GLN:HG2	2.42	0.48
45:AA:409:VAL:O	45:AA:410:CYS:C	2.55	0.48
50:AF:39:HIS:O	50:AF:44:VAL:HG21	2.14	0.48
46:Ab:163:ALA:C	49:Ai:43:LEU:CD2	2.82	0.48
47:Ac:153:ILE:HG23	47:Ac:154:PRO:HD2	1.96	0.48
48:Ad:128:ASP:OD1	48:Ad:128:ASP:N	2.46	0.48
52:Ah:32:ARG:HA	52:Ah:80:VAL:HG22	1.96	0.48
52:Ah:47:ARG:HA	52:Ah:50:LEU:CG	2.44	0.48
58:B:304:PC1:H3B1	8:H:57:MET:HE3	1.94	0.48
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.62	0.48
3:C:221:GLU:O	3:C:222:PRO:C	2.56	0.48
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.95	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.48
8:H:17:MET:HG2	8:H:228:TYR:HB2	1.94	0.48
9:I:93:LEU:HD11	9:I:173:PHE:HE2	1.77	0.48
14:N:189:TRP:CZ3	14:N:282:MET:HE3	2.49	0.48
15:O:76:GLU:HG3	15:O:266:PRO:CG	2.44	0.48
16:P:74:GLY:HA2	16:P:102:GLN:OE1	2.14	0.48
16:P:165:ILE:CD1	16:P:253:THR:HG22	2.42	0.48
16:P:169:HIS:HB2	16:P:184:LYS:HE2	1.96	0.48
16:P:285:HIS:HB3	16:P:361:TRP:CE3	2.47	0.48
20:T:119:ILE:HD12	20:T:138:LEU:CD1	2.40	0.48
29:d:100:ASP:HB3	33:h:159:LEU:HD21	1.95	0.48
34:i:90:MET:SD	34:i:97:ILE:HD11	2.54	0.48
37:l:48:ARG:HH22	37:l:64:PRO:HD2	1.79	0.48
43:r:110:GLN:HG2	43:r:113:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:171:THR:HG23	49:AI:64:LEU:HD23	1.95	0.48
46:AB:286:PHE:CZ	46:AB:427:ALA:HB1	2.49	0.48
47:AC:32:ASN:ND2	47:AC:228:ASP:OD1	2.46	0.48
47:AC:211:LEU:HD22	50:AF:37:THR:HA	1.96	0.48
47:AC:269:LYS:CE	47:AC:340:GLY:HA2	2.44	0.48
48:AD:114:PHE:CD2	48:AD:140:TYR:CE1	3.01	0.48
45:Aa:358:PHE:CD1	45:Aa:368:MET:HG2	2.48	0.48
46:Ab:158:LEU:O	46:Ab:159:LYS:C	2.53	0.48
48:Ad:124:CYS:HB2	69:Ad:401:HEC:C3C	2.44	0.48
49:Ae:196:ARG:NH1	49:Ae:252:GLY:O	2.44	0.48
51:Ag:76:ALA:O	51:Ag:77:MET:C	2.57	0.48
4:D:84:PHE:HB3	4:D:96:ARG:O	2.13	0.47
4:D:240:LEU:HG	4:D:244:ILE:CD1	2.44	0.47
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.54	0.47
6:F:134:ASP:CG	6:F:137:LYS:HB2	2.38	0.47
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.47
8:H:1:MET:HE2	26:a:26:ILE:HG23	1.96	0.47
12:L:121:LEU:HD22	12:L:246:LEU:CD2	2.24	0.47
13:M:154:LEU:HD13	14:N:287:LEU:CD2	2.44	0.47
22:W:65:LYS:O	22:W:69:MET:HG2	2.14	0.47
23:X:20:VAL:HB	23:X:24:VAL:HG21	1.95	0.47
23:X:147:ARG:HH22	30:e:39:GLU:HG3	1.78	0.47
26:a:12:MET:O	26:a:12:MET:HG2	2.14	0.47
29:d:119:VAL:O	29:d:120:ARG:C	2.55	0.47
38:m:124:LYS:C	38:m:126:ASN:N	2.70	0.47
55:m:201:3PE:H361	55:m:202:3PE:H341	1.95	0.47
39:n:156:PRO:HD2	39:n:158:ARG:NH1	2.29	0.47
46:AB:170:GLN:CD	46:AB:170:GLN:H	2.21	0.47
68:AC:403:UQ6:H172	68:AC:403:UQ6:H151	1.63	0.47
49:AE:217:CYS:O	49:AE:218:THR:C	2.56	0.47
51:AG:50:ALA:N	51:AG:51:PRO:CD	2.77	0.47
45:Aa:341:PHE:CE1	45:Aa:356:ALA:HB1	2.48	0.47
45:Aa:387:GLU:HB2	45:Aa:390:ARG:HH22	1.78	0.47
47:Ac:304:MET:HA	47:Ac:307:LEU:HD12	1.96	0.47
48:Ad:89:LEU:HG	48:Ad:236:TYR:CE1	2.49	0.47
48:Ad:165:PHE:O	48:Ad:166:MET:HG3	2.13	0.47
49:Ae:166:ALA:HA	49:Ae:174:LEU:C	2.39	0.47
49:Ae:167:PHE:HB2	49:Ae:174:LEU:HD23	1.95	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG11	1.96	0.47
4:D:384:LEU:HD21	7:G:144:MET:HE1	1.95	0.47
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:29:THR:O	11:K:32:CYS:N	2.47	0.47
12:L:3:ILE:HG22	12:L:49:LEU:HD21	1.96	0.47
12:L:54:PHE:CZ	12:L:84:PHE:HB2	2.49	0.47
13:M:94:LEU:O	13:M:98:MET:HG2	2.14	0.47
13:M:176:LEU:HD13	13:M:245:ARG:HH11	1.79	0.47
13:M:336:ARG:HH21	13:M:429:SER:HA	1.78	0.47
15:O:68:SER:C	15:O:70:LYS:N	2.70	0.47
15:O:71:ASN:O	15:O:75:LYS:HE3	2.14	0.47
16:P:59:PHE:HA	16:P:83:PRO:HD2	1.96	0.47
16:P:365:GLU:N	16:P:365:GLU:OE1	2.46	0.47
25:Z:75:PHE:CE2	26:a:47:LEU:HD11	2.50	0.47
25:Z:98:MET:HE3	30:e:83:ARG:CB	2.36	0.47
25:Z:120:LEU:HD23	25:Z:121:ILE:N	2.29	0.47
34:i:79:MET:O	34:i:80:TRP:C	2.57	0.47
44:s:87:LEU:CB	44:s:91:ARG:NH1	2.76	0.47
48:AD:122:SER:O	48:AD:178:PRO:HB3	2.14	0.47
49:AE:111:LYS:O	49:AE:115:TYR:HD1	1.97	0.47
45:Aa:137:SER:HB3	45:Aa:236:GLY:O	2.14	0.47
46:Ab:109:LYS:HD2	46:Ab:124:GLU:OE1	2.14	0.47
47:Ac:220:PHE:HE2	68:Ac:405:UQ6:H4M2	1.77	0.47
3:C:219:VAL:HG11	22:W:113:THR:HG21	1.96	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
7:G:665:PHE:O	7:G:668:ALA:N	2.45	0.47
8:H:42:PRO:HB3	42:q:27:PHE:CZ	2.49	0.47
8:H:87:VAL:O	8:H:96:ILE:HG12	2.14	0.47
8:H:102:ILE:CG2	8:H:150:LEU:HD21	2.40	0.47
12:L:31:ASN:HD22	12:L:34:LEU:HB2	1.80	0.47
13:M:7:PRO:HG3	31:f:20:PHE:HA	1.94	0.47
13:M:147:ILE:HG13	14:N:298:TYR:OH	2.14	0.47
14:N:89:GLN:H	14:N:89:GLN:CD	2.22	0.47
15:O:314:LEU:HD12	15:O:315:PRO:HD3	1.93	0.47
16:P:54:VAL:O	16:P:78:SER:HB3	2.14	0.47
16:P:76:MET:SD	16:P:254:LYS:HE3	2.54	0.47
16:P:307:LEU:O	16:P:308:SER:C	2.54	0.47
23:X:7:LEU:HD22	25:Z:87:LEU:HD12	1.93	0.47
30:e:94:PRO:HB3	30:e:98:HIS:CG	2.48	0.47
34:i:32:GLU:HG3	39:n:115:TYR:HA	1.96	0.47
39:n:81:ILE:HD11	39:n:87:GLY:O	2.14	0.47
39:n:96:CYS:SG	39:n:97:TYR:CE1	3.04	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:185:LEU:O	47:AC:189:ILE:HG13	2.14	0.47
47:AC:296:LEU:O	47:AC:300:ILE:N	2.45	0.47
48:AD:127:MET:CE	48:AD:198:SER:HA	2.44	0.47
48:AD:128:ASP:N	48:AD:128:ASP:OD1	2.46	0.47
48:AD:183:GLU:HA	48:AD:186:ARG:HH21	1.78	0.47
3:C:123:ASN:HB2	21:V:111:GLN:OE1	2.14	0.47
4:D:203:MET:HE3	4:D:258:VAL:HG23	1.95	0.47
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.79	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
7:G:545:LEU:CD2	7:G:547:LEU:HD21	2.44	0.47
8:H:318:MET:HG2	26:a:40:ARG:HD2	1.96	0.47
9:I:152:CYS:SG	56:I:302:SF4:S4	3.12	0.47
12:L:433:THR:CG2	12:L:434:LYS:N	2.78	0.47
12:L:576:LEU:HA	12:L:579:ASN:ND2	2.29	0.47
62:L:704:CDL:H161	13:M:361:MET:HE1	1.96	0.47
55:L:705:3PE:H322	55:L:705:3PE:H351	1.67	0.47
13:M:51:ASN:O	33:h:135:LYS:HD2	2.13	0.47
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.45	0.47
13:M:310:MET:CE	13:M:459:MET:SD	3.02	0.47
13:M:370:PRO:CA	13:M:375:LEU:HD23	2.42	0.47
22:W:84:LEU:HD11	22:W:88:LYS:HE3	1.96	0.47
23:X:48:TRP:O	23:X:51:LYS:HE3	2.15	0.47
29:d:8:HIS:O	29:d:10:PRO:HD3	2.14	0.47
33:h:91:ILE:O	41:p:56:HIS:NE2	2.48	0.47
36:k:84:PHE:CZ	36:k:88:LEU:HD22	2.49	0.47
45:AA:109:LEU:HD21	45:AA:120:LEU:HD21	1.95	0.47
45:AA:339:GLN:O	45:AA:340:SER:C	2.56	0.47
47:AC:141:TRP:CG	47:AC:264:THR:HG1	2.31	0.47
48:AD:98:HIS:HB3	48:AD:105:LEU:HA	1.96	0.47
49:AE:119:ALA:CA	53:AJ:25:ILE:HG12	2.44	0.47
52:AH:61:THR:HG23	52:AH:63:GLU:H	1.78	0.47
46:Ab:38:LEU:CD1	46:Ab:396:ILE:HD13	2.44	0.47
46:Ab:212:HIS:CE1	46:Ab:246:LEU:HB3	2.49	0.47
46:Ab:297:PRO:HA	46:Ab:304:ASN:ND2	2.28	0.47
49:Ae:246:SER:HB3	49:Ae:248:ARG:HE	1.79	0.47
55:A:201:3PE:H272	27:b:23:PHE:HD2	1.78	0.47
2:B:98:ALA:CB	2:B:134:ALA:C	2.82	0.47
2:B:182:ASP:HA	2:B:185:VAL:O	2.14	0.47
3:C:67:ILE:HD13	3:C:98:PHE:CZ	2.49	0.47
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:238:PHE:CD1	9:I:140:ARG:CZ	2.97	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:65:THR:HG21	8:H:71:PHE:HB2	1.96	0.47
11:K:69:CYS:O	11:K:70:GLU:C	2.57	0.47
12:L:277:MET:SD	12:L:318:GLY:HA2	2.54	0.47
12:L:437:PHE:HB2	12:L:438:PRO:HD2	1.96	0.47
13:M:78:MET:HG2	13:M:432:ARG:HG3	1.97	0.47
14:N:1:MET:HE1	14:N:43:MET:SD	2.54	0.47
15:O:52:LYS:HD3	15:O:152:SER:O	2.14	0.47
15:O:343:TYR:CE1	15:O:355:LYS:CB	2.96	0.47
15:O:350:LYS:O	15:O:351:TRP:HB2	2.12	0.47
26:a:3:PHE:HD2	62:a:101:CDL:H132	1.78	0.47
29:d:73:TYR:O	29:d:77:LYS:HB2	2.14	0.47
31:f:37:PHE:O	31:f:38:ARG:C	2.57	0.47
55:i:201:3PE:O22	55:i:201:3PE:H11	2.13	0.47
42:q:43:LYS:O	42:q:44:TYR:HB2	2.13	0.47
47:AC:141:TRP:O	47:AC:145:VAL:HG23	2.14	0.47
49:AI:62:ARG:HB3	49:AI:63:PRO:HD2	1.95	0.47
49:Ae:218:THR:CG2	49:Ae:256:LEU:O	2.61	0.47
1:A:65:PHE:HA	1:A:68:GLU:CD	2.39	0.47
5:E:196:THR:O	5:E:197:PRO:C	2.56	0.47
6:F:313:ASN:OD1	6:F:359:ARG:NH1	2.48	0.47
8:H:230:ASN:HB3	8:H:233:LEU:HD12	1.97	0.47
9:I:77:LEU:O	26:a:2:TRP:HB3	2.14	0.47
12:L:63:ILE:HG23	34:i:97:ILE:CD1	2.45	0.47
12:L:237:MET:HE1	12:L:248:HIS:HB2	1.96	0.47
12:L:420:ALA:HB1	12:L:498:PHE:CD2	2.50	0.47
14:N:120:GLN:O	14:N:176:ARG:NH2	2.48	0.47
15:O:116:LYS:HA	15:O:119:ASP:OD1	2.13	0.47
19:S:35:ASP:O	19:S:38:VAL:HG22	2.15	0.47
20:U:87:LEU:CB	20:U:98:LEU:CD2	2.83	0.47
20:U:133:ILE:HD13	39:n:7:PRO:HD3	1.95	0.47
24:Y:142:LYS:O	24:Y:143:VAL:C	2.57	0.47
34:i:19:ARG:NH1	39:n:173:ARG:HH21	2.11	0.47
34:i:123:PHE:CE2	40:o:61:HIS:HD2	2.32	0.47
37:l:38:PRO:CG	38:m:71:ALA:HB2	2.45	0.47
37:l:44:THR:CG2	37:l:47:GLU:HG3	2.45	0.47
37:l:48:ARG:NH2	37:l:64:PRO:HD2	2.29	0.47
38:m:28:GLU:O	38:m:31:ARG:HB3	2.14	0.47
38:m:124:LYS:C	38:m:126:ASN:H	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:6:ASP:C	41:p:8:ASP:N	2.69	0.47
42:q:69:ASN:CG	42:q:70:GLY:H	2.23	0.47
45:AA:390:ARG:HG3	46:AB:104:GLU:O	2.14	0.47
47:AC:16:HIS:NE2	47:AC:201:HIS:CD2	2.82	0.47
47:AC:44:GLN:O	47:AC:83:HIS:CE1	2.67	0.47
47:AC:141:TRP:CD1	47:AC:264:THR:HA	2.49	0.47
49:AE:130:LYS:HD2	54:AK:34:TRP:CD1	2.49	0.47
45:Aa:292:GLU:OE2	49:Ae:104:LYS:HE3	2.13	0.47
55:Aa:501:3PE:H332	47:Ac:221:HIS:HE1	1.80	0.47
47:Ac:276:PHE:CG	47:Ac:277:ALA:N	2.82	0.47
47:Ac:317:PHE:CD1	50:Af:27:PHE:HB3	2.50	0.47
48:Ad:311:TRP:CZ3	48:Ad:314:LEU:HD12	2.50	0.47
1:A:52:SER:OG	10:J:73:MET:HE3	2.15	0.47
3:C:208:GLU:HG2	3:C:221:GLU:HG3	1.95	0.47
4:D:37:TRP:CE3	13:M:140:THR:HA	2.50	0.47
4:D:123:LEU:HD13	4:D:135:TYR:OH	2.14	0.47
4:D:256:ASP:HB2	25:Z:25:LEU:HD11	1.91	0.47
5:E:71:GLU:CG	44:s:94:GLN:HE21	2.26	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:128:ARG:HA	6:F:131:MET:HE2	1.96	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:258:GLY:O	6:F:259:GLY:C	2.58	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:385:TYR:CE2	7:G:526:LEU:HB2	2.49	0.47
8:H:213:VAL:HG13	8:H:214:GLU:HG2	1.96	0.47
9:I:76:TYR:HE1	9:I:79:ARG:NH2	2.12	0.47
10:J:59:TYR:CD1	10:J:63:MET:SD	3.07	0.47
10:J:130:ASP:CG	25:Z:79:LYS:HE2	2.39	0.47
11:K:75:LEU:O	11:K:79:VAL:HG23	2.15	0.47
12:L:183:ILE:HD13	13:M:400:ILE:HD13	1.96	0.47
12:L:390:TYR:HE2	35:j:68:TRP:HH2	1.61	0.47
12:L:441:ILE:HD13	35:j:48:PRO:HD3	1.97	0.47
12:L:552:LEU:HD22	12:L:553:LEU:HD12	1.97	0.47
62:L:704:CDL:H372	33:h:75:LEU:CD1	2.45	0.47
13:M:57:SER:OG	13:M:113:THR:HG22	2.15	0.47
13:M:231:LEU:CD1	13:M:235:LEU:HD12	2.42	0.47
13:M:305:THR:O	13:M:306:PRO:C	2.58	0.47
13:M:430:HIS:HB3	32:g:73:GLY:HA3	1.97	0.47
13:M:445:ILE:HG23	55:M:502:3PE:H292	1.97	0.47
14:N:1:MET:O	14:N:2:ASN:C	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:LEU:O	14:N:29:MET:N	2.47	0.47
19:S:95:LEU:HD12	19:S:95:LEU:C	2.33	0.47
20:T:116:VAL:O	20:T:120:MET:HG3	2.15	0.47
23:X:48:TRP:CZ3	33:h:184:LYS:O	2.68	0.47
32:g:121:GLU:OE2	41:p:10:TYR:CZ	2.68	0.47
33:h:96:ALA:C	41:p:63:TYR:HE1	2.22	0.47
37:l:42:PRO:HB2	37:l:48:ARG:HG2	1.97	0.47
41:p:65:HIS:O	41:p:66:ARG:C	2.57	0.47
45:AA:174:GLU:C	45:AA:176:ASP:N	2.73	0.47
45:AA:183:VAL:HG21	45:AA:286:HIS:HB2	1.97	0.47
46:AB:429:LYS:O	46:AB:432:VAL:HG12	2.14	0.47
47:AC:304:MET:HA	47:AC:307:LEU:HD12	1.96	0.47
48:AD:183:GLU:CB	48:Ad:161:ASP:HB3	2.44	0.47
49:AE:231:PHE:CD2	49:AE:250:ARG:HG3	2.50	0.47
49:AE:238:CYS:SG	47:Ac:268:ILE:HD11	2.53	0.47
51:AG:31:PHE:CD1	51:AG:32:SER:N	2.83	0.47
45:Aa:92:PHE:CE2	45:Aa:161:ILE:HG23	2.49	0.47
46:Ab:72:GLU:HB3	46:Ab:76:ASN:OD1	2.15	0.47
46:Ab:109:LYS:O	46:Ab:123:VAL:HA	2.15	0.47
48:Ad:223:THR:CG2	52:Ah:55:VAL:HG21	2.45	0.47
49:Ae:159:ILE:HB	49:Ae:210:TRP:CZ3	2.49	0.47
3:C:69:PRO:HD2	21:V:99:PRO:O	2.15	0.47
4:D:320:ILE:CD1	9:I:38:TYR:CD1	2.97	0.47
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.44	0.47
7:G:114:GLU:OE1	43:r:53:TYR:HB3	2.15	0.47
7:G:400:VAL:HG22	7:G:473:MET:CG	2.45	0.47
7:G:648:GLU:O	19:S:22:HIS:CE1	2.68	0.47
8:H:91:MET:HE1	8:H:259:PHE:CZ	2.49	0.47
11:K:57:MET:C	11:K:60:PRO:HD2	2.39	0.47
12:L:23:MET:HE1	62:L:704:CDL:H191	1.96	0.47
12:L:348:HIS:HD2	20:U:69:SER:HB3	1.80	0.47
13:M:122:PHE:HZ	13:M:206:LYS:HD3	1.75	0.47
15:O:204:VAL:HG23	15:O:255:VAL:HG13	1.97	0.47
20:U:120:MET:HE1	39:n:24:LEU:CD1	2.44	0.47
20:U:130:ILE:HG21	20:U:138:LEU:HD11	1.97	0.47
23:X:57:LEU:HD11	25:Z:84:LEU:CD2	2.44	0.47
23:X:141:PRO:O	23:X:142:TYR:HB2	2.14	0.47
23:X:172:VAL:HG23	29:d:30:ARG:NH1	2.30	0.47
62:a:101:CDL:CA3	42:q:10:GLY:HA3	2.43	0.47
28:c:46:LEU:O	28:c:50:ALA:CB	2.63	0.47
31:f:38:ARG:HD3	31:f:56:TRP:NE1	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:121:GLU:OE2	41:p:10:TYR:CE2	2.68	0.47
37:l:118:ASP:OD1	37:l:119:THR:N	2.47	0.47
38:m:14:LEU:HD12	38:m:15:PRO:HD2	1.96	0.47
38:m:18:LEU:HD11	39:n:72:TRP:CB	2.45	0.47
39:n:57:MET:O	39:n:58:MET:C	2.58	0.47
41:p:93:ARG:NH2	41:p:150:TYR:CE1	2.83	0.47
45:AA:463:GLU:HG2	51:AG:6:GLY:H	1.78	0.47
47:AC:262:LEU:HD11	49:Ae:168:LYS:HD2	1.96	0.47
48:AD:129:TYR:HD2	48:AD:198:SER:HB2	1.80	0.47
49:AE:166:ALA:HA	49:AE:174:LEU:O	2.15	0.47
50:AF:26:GLY:C	50:AF:28:ASN:N	2.68	0.47
50:AF:72:ARG:O	50:AF:74:GLN:HG2	2.15	0.47
45:Aa:186:TYR:C	45:Aa:188:HIS:N	2.68	0.47
45:Aa:279:ASP:HA	51:Ag:12:ARG:HA	1.97	0.47
46:Ab:226:SER:O	46:Ab:229:VAL:HG22	2.15	0.47
47:Ac:141:TRP:NE1	47:Ac:263:ASN:O	2.47	0.47
48:Ad:192:ALA:HB1	69:Ad:401:HEC:CGD	2.45	0.47
49:Ae:167:PHE:O	49:Ae:168:LYS:C	2.57	0.47
1:A:55:PHE:HB3	10:J:69:TYR:OH	2.14	0.47
56:B:301:SF4:S2	4:D:138:ARG:HD3	2.55	0.47
4:D:159:LEU:CG	4:D:391:VAL:HG12	2.45	0.47
4:D:392:PRO:HD3	43:r:60:ARG:HG3	1.96	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
6:F:357:MET:HE1	6:F:363:ILE:HD12	1.95	0.47
6:F:364:VAL:HA	6:F:438:LEU:HD11	1.97	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
7:G:544:MET:HA	7:G:565:PHE:O	2.14	0.47
8:H:129:LEU:O	8:H:133:LEU:HG	2.15	0.47
11:K:29:THR:O	11:K:30:LEU:C	2.56	0.47
12:L:357:ARG:NH2	39:n:78:GLN:O	2.48	0.47
12:L:546:LEU:HD22	38:m:72:ARG:NH2	2.29	0.47
13:M:16:TRP:CE3	55:d:201:3PE:H12	2.50	0.47
13:M:196:TRP:HD1	13:M:250:LEU:HB2	1.80	0.47
15:O:129:TYR:CE2	15:O:183:CYS:HB3	2.50	0.47
15:O:135:LEU:HB3	15:O:139:ARG:NH1	2.26	0.47
16:P:40:VAL:O	16:P:42:PRO:HD3	2.15	0.47
16:P:134:TRP:HB3	16:P:312:PRO:CG	2.41	0.47
21:V:6:LYS:HG2	21:V:16:VAL:HG23	1.96	0.47
21:V:44:TYR:O	21:V:48:THR:HG22	2.15	0.47
22:W:28:LEU:O	22:W:32:LYS:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:38:LEU:HG	22:W:70:PHE:HZ	1.80	0.47
25:Z:88:ARG:O	25:Z:92:GLU:HG3	2.14	0.47
33:h:55:PHE:HB2	34:i:28:LEU:HD21	1.95	0.47
41:p:29:PRO:O	41:p:33:LEU:HD13	2.14	0.47
47:AC:29:SER:O	47:AC:30:TRP:C	2.55	0.47
47:AC:176:THR:HB	47:Ac:53:MET:O	2.15	0.47
45:Aa:172:MET:HA	45:Aa:175:ASN:ND2	2.30	0.47
45:Aa:384:THR:HB	54:Ak:9:ARG:HG3	1.97	0.47
45:Aa:387:GLU:HB2	45:Aa:390:ARG:NH2	2.30	0.47
45:Aa:397:ASN:HA	46:Ab:58:LEU:HD11	1.95	0.47
48:Ad:318:LYS:HD2	49:Ae:86:PRO:HB2	1.96	0.47
1:A:72:LEU:HD23	1:A:94:LEU:HD23	1.94	0.47
55:A:201:3PE:H3B2	27:b:26:TRP:CD1	2.50	0.47
2:B:136:THR:HG22	2:B:164:CYS:HB2	1.97	0.47
2:B:146:ARG:NH1	2:B:149:TYR:CD2	2.83	0.47
3:C:168:GLU:HB2	3:C:186:ILE:HG21	1.97	0.47
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.47
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:691:ILE:HG12	7:G:695:TYR:CE2	2.50	0.47
8:H:86:TRP:CD2	8:H:233:LEU:HD21	2.50	0.47
8:H:202:GLU:H	8:H:210:GLY:HA3	1.79	0.47
8:H:202:GLU:O	8:H:203:GLY:C	2.58	0.47
13:M:49:TYR:OH	13:M:457:LEU:HG	2.15	0.47
13:M:165:ILE:HD11	14:N:264:TRP:HE1	1.80	0.47
14:N:307:THR:HG22	14:N:308:ASN:N	2.30	0.47
15:O:78:ALA:CB	15:O:85:HIS:HB2	2.45	0.47
15:O:256:LEU:HD13	15:O:258:TYR:OH	2.15	0.47
16:P:59:PHE:CD2	16:P:152:ILE:HD13	2.49	0.47
20:T:140:CYS:O	20:T:143:GLU:HB2	2.15	0.47
23:X:7:LEU:CD1	25:Z:87:LEU:HD12	2.44	0.47
24:Y:116:GLY:O	24:Y:120:MET:HB2	2.15	0.47
25:Z:75:PHE:HE2	26:a:47:LEU:HD11	1.79	0.47
26:a:22:SER:O	26:a:23:THR:C	2.57	0.47
29:d:59:HIS:CE1	29:d:60:ARG:HG3	2.50	0.47
37:l:127:ASP:O	37:l:128:VAL:C	2.58	0.47
47:Ac:16:HIS:NE2	47:Ac:201:HIS:CD2	2.82	0.47
53:Aj:42:ALA:HA	53:Aj:45:GLU:OE2	2.14	0.47
3:C:232:PHE:HE1	7:G:244:GLU:HG3	1.80	0.46
4:D:47:PHE:CE2	14:N:305:PHE:HZ	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:107:PRO:O	5:E:110:ARG:HB3	2.15	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
7:G:382:ARG:NE	7:G:652:ASN:ND2	2.49	0.46
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.46
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.97	0.46
12:L:73:SER:CB	41:p:100:GLN:HE21	2.25	0.46
12:L:86:SER:OG	12:L:133:SER:HB3	2.15	0.46
13:M:232:ALA:HA	13:M:236:LEU:HD12	1.97	0.46
15:O:232:ALA:O	15:O:235:GLN:HB3	2.14	0.46
20:T:107:ASP:O	20:T:108:LEU:HB2	2.15	0.46
29:d:78:ARG:O	29:d:81:TYR:N	2.48	0.46
29:d:116:PHE:HB2	41:p:157:ALA:HB1	1.96	0.46
35:j:51:THR:O	35:j:52:ARG:C	2.53	0.46
39:n:35:ASP:OD1	39:n:36:LYS:N	2.47	0.46
39:n:50:GLU:O	39:n:51:HIS:C	2.55	0.46
41:p:43:TRP:O	41:p:44:PRO:C	2.58	0.46
45:AA:172:MET:HA	45:AA:175:ASN:ND2	2.30	0.46
47:AC:294:LEU:O	47:AC:297:SER:HB3	2.15	0.46
48:AD:131:ALA:HB3	48:AD:134:HIS:ND1	2.30	0.46
48:AD:159:ASN:N	48:AD:166:MET:HG3	2.29	0.46
48:AD:186:ARG:NE	48:AD:193:LEU:HB2	2.30	0.46
48:AD:255:TYR:HH	48:AD:269:ASP:HB2	1.79	0.46
49:AE:79:SER:OG	49:AE:80:HIS:N	2.38	0.46
45:Aa:104:ARG:HE	45:Aa:112:GLU:CD	2.23	0.46
45:Aa:138:LYS:O	45:Aa:141:PRO:HD2	2.14	0.46
45:Aa:407:THR:HB	45:Aa:408:PRO:HD3	1.96	0.46
7:G:30:ASN:O	7:G:45:PRO:HD3	2.15	0.46
7:G:137:CYS:N	17:Q:88:GLN:HE21	2.13	0.46
7:G:671:LEU:CD2	19:S:45:LYS:HG2	2.44	0.46
11:K:13:SER:O	11:K:17:LEU:HG	2.15	0.46
12:L:172:ILE:O	12:L:176:ARG:HG2	2.16	0.46
12:L:277:MET:CG	12:L:318:GLY:HA2	2.45	0.46
12:L:302:ILE:HG22	12:L:340:PHE:CZ	2.49	0.46
12:L:405:ASN:OD1	37:l:148:HIS:CE1	2.69	0.46
12:L:474:PRO:HD2	40:o:67:LEU:HD21	1.96	0.46
12:L:589:MET:O	12:L:592:LEU:HB3	2.16	0.46
13:M:213:HIS:O	13:M:217:PRO:CD	2.63	0.46
14:N:17:PRO:HG2	14:N:133:TRP:NE1	2.30	0.46
15:O:62:VAL:HG13	15:O:62:VAL:O	2.15	0.46
15:O:82:GLY:O	15:O:155:GLN:NE2	2.48	0.46
15:O:200:PRO:HB3	15:O:252:MET:SD	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:73:LEU:CD2	16:P:250:VAL:HG22	2.45	0.46
17:Q:52:LEU:HA	17:Q:52:LEU:HD23	1.73	0.46
18:R:88:HIS:ND1	18:R:89:PRO:O	2.47	0.46
19:S:24:CYS:N	19:S:58:CYS:HB2	2.30	0.46
22:W:124:LYS:O	22:W:125:PHE:C	2.58	0.46
23:X:15:VAL:O	23:X:17:GLU:HG3	2.15	0.46
27:b:63:MET:HB2	27:b:66:VAL:CG1	2.45	0.46
29:d:51:ARG:O	29:d:52:PRO:C	2.55	0.46
31:f:16:VAL:O	31:f:17:PRO:C	2.57	0.46
31:f:37:PHE:CZ	41:p:83:LEU:HD13	2.50	0.46
31:f:38:ARG:O	31:f:56:TRP:NE1	2.48	0.46
33:h:73:PHE:HD2	33:h:74:TYR:CE1	2.33	0.46
33:h:96:ALA:C	41:p:63:TYR:CE1	2.93	0.46
39:n:133:TRP:O	39:n:137:VAL:HG22	2.15	0.46
41:p:6:ASP:OD1	41:p:8:ASP:HB2	2.16	0.46
45:AA:274:GLU:OE2	45:AA:276:ARG:HD2	2.14	0.46
47:AC:137:GLN:NE2	47:AC:141:TRP:CD1	2.84	0.46
47:AC:137:GLN:N	47:AC:257:MET:O	2.46	0.46
47:AC:145:VAL:HG22	49:Ae:222:CYS:SG	2.54	0.46
48:AD:313:VAL:CA	51:AG:24:GLN:HE22	2.27	0.46
52:AH:76:ARG:O	52:AH:80:VAL:HG23	2.14	0.46
45:Aa:183:VAL:HG21	45:Aa:286:HIS:HB2	1.97	0.46
47:Ac:100:ARG:HH22	67:Ac:402:HEM:HBD1	1.81	0.46
48:Ad:111:ARG:HG3	48:Ad:140:TYR:CE2	2.51	0.46
48:Ad:185:ALA:HB1	48:Ad:194:PRO:CD	2.45	0.46
49:Ae:184:ILE:HD13	49:Ae:208:PRO:HB2	1.97	0.46
53:Aj:39:GLY:O	53:Aj:43:ILE:HG13	2.16	0.46
1:A:7:ILE:HD12	55:H:401:3PE:H292	1.96	0.46
3:C:45:THR:OG1	43:r:57:ARG:CD	2.63	0.46
9:I:85:ASN:HB3	9:I:89:GLU:HG3	1.97	0.46
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.46
12:L:74:MET:HE3	13:M:307:TRP:HH2	1.80	0.46
12:L:581:LYS:HB2	12:L:586:LEU:HD22	1.97	0.46
13:M:4:ILE:HD12	13:M:4:ILE:N	2.30	0.46
13:M:380:PHE:HD1	13:M:380:PHE:N	2.13	0.46
13:M:380:PHE:N	13:M:380:PHE:CD1	2.82	0.46
15:O:38:TYR:CE2	15:O:292:HIS:CD2	3.01	0.46
16:P:229:VAL:HG22	16:P:298:TYR:CD2	2.50	0.46
16:P:293:LEU:HB3	16:P:294:PRO:HD2	1.98	0.46
18:R:72:VAL:HG21	18:R:77:ILE:HG21	1.97	0.46
22:W:22:PRO:HG3	22:W:26:ARG:NH2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:16:ARG:HB3	33:h:178:PHE:CE2	2.50	0.46
31:f:37:PHE:O	33:h:134:GLU:HB3	2.15	0.46
43:r:8:ILE:HA	43:r:11:LEU:HD12	1.98	0.46
48:AD:159:ASN:OD1	48:AD:162:GLY:N	2.48	0.46
45:Aa:66:HIS:CD2	46:Ab:387:GLU:O	2.69	0.46
45:Aa:152:GLN:O	45:Aa:153:ASN:HB2	2.15	0.46
47:Ac:140:PHE:CE1	47:Ac:170:VAL:CG1	2.98	0.46
48:Ad:100:GLY:O	48:Ad:286:LYS:NZ	2.46	0.46
49:Ae:177:ARG:HG2	49:Ae:178:HIS:N	2.29	0.46
49:Ae:179:ARG:HH22	49:Ae:202:LEU:HD23	1.80	0.46
50:Af:29:LYS:HA	50:Af:81:TRP:CD1	2.49	0.46
4:D:234:GLN:HE21	9:I:212:ARG:HB3	1.79	0.46
4:D:412:VAL:HG12	21:V:114:TRP:CZ2	2.51	0.46
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.74	0.46
5:E:131:ILE:N	5:E:169:THR:O	2.49	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
5:E:243:GLY:O	5:E:244:VAL:C	2.58	0.46
6:F:212:LEU:HD12	6:F:212:LEU:O	2.15	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:114:GLU:OE2	43:r:53:TYR:CA	2.51	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
9:I:155:CYS:HG	56:I:302:SF4:FE3	1.32	0.46
12:L:407:TRP:HE1	37:l:140:MET:HE1	1.81	0.46
12:L:515:LYS:HA	39:n:30:TRP:CE3	2.51	0.46
13:M:255:LYS:CE	29:d:117:HIS:HB3	2.46	0.46
14:N:313:MET:HG3	15:O:305:LEU:CD2	2.44	0.46
16:P:73:LEU:HD23	16:P:250:VAL:HG22	1.97	0.46
16:P:169:HIS:H	16:P:184:LYS:CE	2.28	0.46
19:S:62:GLN:O	19:S:64:LYS:HG3	2.15	0.46
20:T:98:LEU:O	20:T:99:SER:C	2.57	0.46
22:W:61:GLN:O	22:W:64:ASP:HB2	2.15	0.46
27:b:28:LEU:O	27:b:31:ILE:HG12	2.15	0.46
34:i:98:VAL:HG13	41:p:115:GLN:HG2	1.98	0.46
42:q:17:HIS:CD2	42:q:35:ILE:HD13	2.50	0.46
48:AD:181:ASN:OD1	48:AD:184:ALA:N	2.49	0.46
51:AG:50:ALA:O	51:AG:51:PRO:C	2.58	0.46
46:Ab:55:TYR:HA	46:Ab:127:ARG:NH1	2.31	0.46
46:Ab:163:ALA:O	49:Ai:43:LEU:HD22	2.15	0.46
47:Ac:36:LEU:HD11	62:Ag:102:CDL:H732	1.98	0.46
47:Ac:253:PRO:HG2	48:Ad:205:HIS:CD2	2.50	0.46
52:Ah:42:VAL:O	52:Ah:46:GLU:N	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:82:HIS:HD2	52:Ah:83:LYS:HE3	1.79	0.46
1:A:73:LEU:HD23	8:H:151:LEU:HD12	1.98	0.46
1:A:79:ILE:HA	1:A:87:MET:CE	2.46	0.46
3:C:79:CYS:SG	43:r:64:VAL:HB	2.56	0.46
3:C:155:ILE:O	3:C:156:VAL:C	2.58	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.15	0.46
6:F:262:PHE:HA	6:F:265:PHE:HD2	1.81	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:661:GLU:O	7:G:661:GLU:CG	2.46	0.46
8:H:157:ASN:HD22	8:H:165:LEU:HD11	1.78	0.46
8:H:230:ASN:HA	8:H:233:LEU:HD12	1.97	0.46
10:J:21:LEU:HD23	55:K:101:3PE:H271	1.96	0.46
12:L:166:THR:HG22	37:l:115:ASN:HA	1.97	0.46
12:L:373:LEU:CD2	12:L:427:ILE:HG22	2.45	0.46
12:L:428:TYR:CD2	12:L:505:ASN:HB3	2.50	0.46
12:L:561:THR:O	55:Y:201:3PE:H381	2.16	0.46
12:L:588:PHE:O	12:L:589:MET:C	2.57	0.46
12:L:594:ASN:OD1	14:N:110:PRO:CB	2.63	0.46
13:M:264:LEU:HD23	38:m:98:LEU:HD11	1.98	0.46
13:M:300:SER:HB2	13:M:308:SER:HB3	1.97	0.46
13:M:348:LEU:O	13:M:351:VAL:N	2.38	0.46
55:N:401:3PE:H3D1	55:N:401:3PE:H2B2	1.98	0.46
15:O:76:GLU:CB	15:O:266:PRO:HB3	2.45	0.46
21:V:24:LEU:O	21:V:25:THR:C	2.58	0.46
21:V:64:ASP:OD2	21:V:67:LYS:HG2	2.15	0.46
62:a:101:CDL:H711	62:a:101:CDL:H321	1.98	0.46
29:d:13:PHE:O	29:d:78:ARG:NE	2.44	0.46
29:d:108:THR:O	29:d:109:TYR:C	2.55	0.46
30:e:20:PHE:HZ	33:h:178:PHE:CB	2.29	0.46
55:m:202:3PE:H392	55:m:202:3PE:H3C1	1.71	0.46
42:q:4:VAL:HG23	42:q:5:GLU:N	2.31	0.46
42:q:60:ARG:HD2	42:q:92:CYS:SG	2.56	0.46
45:Aa:450:TYR:O	45:Aa:451:ASP:HB2	2.15	0.46
55:Ac:403:3PE:HN1	62:Ag:101:CDL:PB2	2.39	0.46
48:Ad:88:GLU:O	48:Ad:89:LEU:C	2.58	0.46
48:Ad:295:MET:HB3	71:Ad:402:3PH:C36	2.45	0.46
49:Ae:160:PRO:HD2	49:Ae:163:LYS:HG3	1.98	0.46
49:Ae:249:ILE:HD11	49:Ae:251:LYS:O	2.15	0.46
52:Ah:42:VAL:HA	52:Ah:45:ARG:CB	2.45	0.46
1:A:85:SER:O	1:A:89:ILE:HG13	2.15	0.46
2:B:122:ARG:O	57:B:302:UQ1:O1	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.45	0.46
5:E:223:CYS:HB3	6:F:132:ARG:HH11	1.79	0.46
6:F:64:LYS:H	6:F:256:ARG:HH21	1.62	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.84	0.46
9:I:114:ILE:HD13	18:R:106:TYR:CD1	2.51	0.46
12:L:21:ILE:HG12	12:L:27:ILE:CG2	2.45	0.46
12:L:225:ALA:CB	12:L:233:LEU:HD12	2.45	0.46
12:L:264:HIS:HA	12:L:267:THR:CG2	2.45	0.46
55:L:701:3PE:H3B2	35:j:71:TRP:CH2	2.50	0.46
13:M:10:MET:C	13:M:13:PRO:HD2	2.41	0.46
13:M:143:LEU:CD2	14:N:303:THR:HG21	2.30	0.46
13:M:158:ILE:HG12	14:N:287:LEU:HD11	1.96	0.46
13:M:173:THR:HG22	33:h:150:ARG:NH1	2.31	0.46
13:M:435:THR:O	13:M:436:LEU:C	2.59	0.46
14:N:154:ILE:HG12	14:N:195:PRO:CG	2.45	0.46
15:O:61:THR:HB	15:O:160:GLU:O	2.15	0.46
15:O:139:ARG:NH2	63:O:401:ADP:N7	2.61	0.46
15:O:339:TYR:CE1	29:d:52:PRO:HA	2.51	0.46
17:Q:69:GLU:HA	17:Q:72:ILE:CG2	2.45	0.46
20:U:105:MET:SD	20:U:139:MET:HE1	2.55	0.46
20:U:114:ASP:O	20:U:117:GLU:N	2.48	0.46
21:V:33:ASP:O	21:V:34:ILE:C	2.59	0.46
25:Z:58:ARG:HG2	27:b:45:ILE:HD11	1.97	0.46
26:a:58:ASN:CB	26:a:60:TYR:CD1	2.89	0.46
28:c:67:LEU:O	28:c:68:GLU:C	2.59	0.46
36:k:55:GLU:OE1	39:n:38:ARG:HB2	2.15	0.46
41:p:6:ASP:O	41:p:8:ASP:N	2.49	0.46
45:AA:74:TRP:C	45:AA:75:ILE:HG13	2.40	0.46
45:AA:287:VAL:HB	45:AA:358:PHE:CZ	2.50	0.46
45:AA:407:THR:HB	45:AA:408:PRO:HD3	1.97	0.46
48:AD:121:CYS:SG	69:AD:401:HEC:CBB	3.03	0.46
48:AD:125:HIS:HE1	48:AD:195:PRO:HD2	1.80	0.46
48:AD:126:SER:O	48:AD:196:ASP:HB3	2.16	0.46
48:AD:156:ASP:HB2	48:AD:167:ARG:O	2.16	0.46
48:AD:263:MET:HB3	52:AH:26:ASP:OD2	2.16	0.46
49:AE:122:THR:CG2	53:AJ:25:ILE:CG2	2.87	0.46
49:AE:246:SER:HB3	49:AE:248:ARG:HE	1.79	0.46
50:AF:26:GLY:O	50:AF:29:LYS:N	2.48	0.46
51:AG:50:ALA:N	51:AG:51:PRO:HD2	2.30	0.46
49:AI:43:LEU:HD12	49:AI:46:LYS:NZ	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:140:LEU:O	45:Aa:141:PRO:C	2.59	0.46
46:Ab:90:THR:HG23	46:Ab:94:ALA:O	2.15	0.46
47:Ac:42:MET:CE	68:Ac:405:UQ6:C19	2.94	0.46
48:Ad:267:ALA:HA	48:Ad:270:VAL:HG12	1.97	0.46
48:Ad:267:ALA:O	48:Ad:268:LYS:C	2.56	0.46
71:Ad:402:3PH:H392	49:Ae:128:ALA:HB3	1.97	0.46
50:Af:85:GLU:CD	50:Af:85:GLU:H	2.24	0.46
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.98	0.46
1:A:49:LEU:N	1:A:49:LEU:CD1	2.78	0.46
4:D:34:ALA:HB3	13:M:86:LYS:HZ2	1.80	0.46
6:F:50:ASP:C	6:F:52:ARG:N	2.73	0.46
7:G:665:PHE:O	7:G:666:GLN:C	2.57	0.46
8:H:197:PRO:O	8:H:279:ARG:HA	2.16	0.46
10:J:133:VAL:HG11	26:a:41:VAL:HG21	1.98	0.46
12:L:101:MET:HE1	12:L:121:LEU:HB2	1.98	0.46
12:L:193:MET:HE1	38:m:125:PHE:CD2	2.51	0.46
12:L:306:THR:HA	12:L:336:LYS:NZ	2.27	0.46
12:L:340:PHE:O	12:L:343:SER:OG	2.33	0.46
12:L:529:PHE:CZ	12:L:533:ILE:HG21	2.50	0.46
13:M:15:THR:HG21	13:M:100:ILE:CD1	2.46	0.46
13:M:105:LEU:CD2	55:N:401:3PE:H2H2	2.46	0.46
13:M:139:GLN:HG3	13:M:141:GLU:H	1.81	0.46
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.98	0.46
15:O:354:LEU:HG	28:c:44:VAL:CG2	2.46	0.46
16:P:99:ASP:CG	16:P:100:LEU:H	2.24	0.46
16:P:303:LYS:O	16:P:307:LEU:HG	2.15	0.46
19:S:24:CYS:CA	19:S:58:CYS:HB2	2.46	0.46
62:a:101:CDL:CB6	42:q:6:VAL:HG21	2.46	0.46
35:j:92:TRP:O	35:j:93:THR:C	2.59	0.46
37:l:57:MET:HE2	37:l:57:MET:HB3	1.75	0.46
37:l:156:VAL:HG11	40:o:95:TYR:CE1	2.48	0.46
38:m:9:ALA:O	38:m:10:PRO:C	2.56	0.46
39:n:136:GLU:O	39:n:139:GLN:N	2.49	0.46
46:AB:225:VAL:HG22	46:AB:229:VAL:CG2	2.46	0.46
48:AD:117:TYR:OH	48:AD:126:SER:HA	2.15	0.46
49:AE:93:ARG:HB3	51:AG:24:GLN:C	2.41	0.46
50:AF:106:GLU:O	50:AF:110:LYS:HG3	2.16	0.46
45:Aa:74:TRP:HB3	45:Aa:418:LEU:CD1	2.46	0.46
45:Aa:74:TRP:C	45:Aa:75:ILE:HG13	2.40	0.46
45:Aa:409:VAL:O	45:Aa:410:CYS:C	2.55	0.46
47:Ac:294:LEU:O	47:Ac:297:SER:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:296:LEU:O	47:Ac:300:ILE:N	2.45	0.46
48:Ad:116:VAL:HG11	48:Ad:270:VAL:HB	1.98	0.46
48:Ad:201:VAL:HG22	48:Ad:278:SER:HB2	1.98	0.46
49:Ae:175:PHE:CE2	49:Ae:215:GLY:HA3	2.51	0.46
49:Ae:265:PHE:HB3	49:Ae:271:VAL:HG23	1.97	0.46
2:B:112:TYR:O	2:B:113:ASP:C	2.56	0.46
4:D:238:LEU:O	4:D:238:LEU:HG	2.16	0.46
4:D:409:VAL:HG13	4:D:422:CYS:SG	2.56	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
8:H:19:PHE:CD2	26:a:11:ILE:CG2	2.98	0.46
8:H:24:GLU:OE2	8:H:195:ARG:NH2	2.49	0.46
10:J:29:GLY:O	10:J:30:LEU:C	2.58	0.46
10:J:75:THR:CG2	11:K:27:MET:HB3	2.46	0.46
10:J:127:GLU:CD	30:e:32:ARG:HG2	2.41	0.46
11:K:57:MET:O	11:K:58:PRO:C	2.58	0.46
12:L:31:ASN:ND2	12:L:34:LEU:HB2	2.31	0.46
12:L:261:VAL:CA	12:L:264:HIS:HD2	2.29	0.46
12:L:439:PRO:HA	36:k:57:TRP:CZ2	2.51	0.46
12:L:550:LEU:O	12:L:554:ASP:HB3	2.16	0.46
13:M:319:HIS:CA	13:M:322:THR:HG22	2.41	0.46
16:P:220:TYR:CD1	16:P:223:PHE:HE1	2.34	0.46
16:P:229:VAL:C	16:P:231:LEU:N	2.73	0.46
16:P:235:THR:CG2	16:P:323:HIS:O	2.63	0.46
20:U:90:TYR:CD1	36:k:51:TRP:CE2	3.04	0.46
23:X:145:ARG:HD2	23:X:146:ALA:O	2.15	0.46
25:Z:97:ILE:HG13	30:e:92:TYR:CD1	2.51	0.46
62:a:101:CDL:HB4	43:r:5:THR:OG1	2.15	0.46
28:c:38:LYS:HA	28:c:39:PRO:HD3	1.58	0.46
34:i:123:PHE:CD2	40:o:61:HIS:HD2	2.32	0.46
37:l:35:ASP:O	37:l:54:LYS:HD3	2.15	0.46
37:l:117:VAL:CG1	37:l:118:ASP:N	2.79	0.46
38:m:15:PRO:HG2	38:m:18:LEU:HD12	1.97	0.46
39:n:61:THR:O	39:n:65:ARG:HG3	2.15	0.46
45:AA:120:LEU:HD13	45:AA:133:ILE:HG12	1.97	0.46
45:AA:286:HIS:CG	45:AA:359:VAL:HG22	2.51	0.46
46:AB:284:ASN:HB3	46:AB:419:VAL:CG2	2.45	0.46
47:AC:269:LYS:HE3	47:AC:340:GLY:HA2	1.97	0.46
48:AD:105:LEU:CB	48:AD:110:ILE:HD11	2.42	0.46
48:AD:321:TYR:HB2	50:AF:61:PHE:CE1	2.50	0.46
52:AH:51:CYS:O	52:AH:54:ARG:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:287:VAL:HB	45:Aa:358:PHE:CZ	2.50	0.46
46:Ab:284:ASN:HB3	46:Ab:419:VAL:CG2	2.45	0.46
47:Ac:146:ILE:CG1	70:Ac:404:U10:C4M	2.69	0.46
47:Ac:280:ILE:O	47:Ac:281:LEU:C	2.58	0.46
48:Ad:292:MET:SD	48:Ad:292:MET:C	2.98	0.46
48:Ad:312:SER:O	48:Ad:313:VAL:C	2.58	0.46
49:Ae:166:ALA:CA	49:Ae:175:PHE:HA	2.44	0.46
49:Ae:205:VAL:HG12	49:Ae:211:VAL:HG23	1.98	0.46
1:A:52:SER:H	10:J:73:MET:HE3	1.78	0.46
2:B:81:LEU:CD1	8:H:53:MET:SD	3.04	0.46
2:B:175:TYR:CE2	4:D:117:HIS:HE1	2.34	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.16	0.46
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:182:CYS:SG	56:G:802:SF4:S1	3.14	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:381:LEU:HD23	19:S:55:ILE:HG12	1.98	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:65:THR:HG22	8:H:67:SER:H	1.80	0.46
9:I:87:PRO:HG2	9:I:88:PHE:CE2	2.50	0.46
10:J:13:LEU:HD22	10:J:99:GLU:OE1	2.16	0.46
12:L:142:ILE:HA	13:M:370:PRO:CB	2.45	0.46
13:M:56:PHE:CE1	13:M:108:MET:HG2	2.47	0.46
14:N:123:PRO:HG2	14:N:126:MET:CG	2.40	0.46
14:N:241:LEU:O	14:N:244:ILE:HG22	2.15	0.46
14:N:277:ILE:HG22	14:N:278:MET:H	1.79	0.46
15:O:132:GLN:HE22	63:O:401:ADP:HN62	1.64	0.46
15:O:140:LEU:HD11	15:O:198:TYR:CE2	2.51	0.46
15:O:204:VAL:CG2	15:O:255:VAL:HG22	2.46	0.46
16:P:151:ALA:O	16:P:154:GLN:HB3	2.16	0.46
16:P:276:LEU:CD2	16:P:280:ILE:HD11	2.46	0.46
24:Y:74:LEU:HD23	24:Y:74:LEU:C	2.41	0.46
25:Z:108:GLU:O	25:Z:109:SER:C	2.57	0.46
26:a:4:GLU:C	26:a:7:PRO:HD2	2.40	0.46
32:g:77:ASP:HA	32:g:78:PRO:HD3	1.70	0.46
33:h:69:ARG:O	33:h:73:PHE:CB	2.63	0.46
33:h:82:VAL:O	33:h:85:GLY:N	2.49	0.46
36:k:39:GLN:NE2	36:k:49:ASP:HB3	2.31	0.46
41:p:50:GLU:CG	41:p:54:ARG:HH21	2.28	0.46
42:q:4:VAL:HG23	42:q:5:GLU:H	1.81	0.46
47:AC:138:MET:HB2	47:AC:254:ASP:CB	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:141:TRP:CZ3	49:Ae:223:VAL:HG23	2.50	0.46
50:AF:49:ARG:HH22	50:AF:50:ARG:HE	1.62	0.46
49:AI:71:ASN:HB2	49:AI:73:PRO:HD2	1.97	0.46
46:Ab:66:LYS:HA	46:Ab:118:ASN:OD1	2.16	0.46
50:Af:83:LYS:HB3	50:Af:85:GLU:OE2	2.15	0.46
5:E:184:MET:HE2	5:E:184:MET:HB3	1.74	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:330:LEU:HD12	7:G:544:MET:HE1	1.98	0.46
7:G:330:LEU:CA	7:G:544:MET:HE1	2.46	0.46
7:G:405:THR:O	7:G:407:PRO:HD3	2.16	0.46
7:G:651:PRO:CB	19:S:57:GLU:O	2.62	0.46
8:H:118:TRP:CZ2	10:J:30:LEU:HD22	2.51	0.46
8:H:121:TRP:CH2	10:J:27:TYR:HE1	2.24	0.46
8:H:233:LEU:O	8:H:236:ALA:N	2.48	0.46
12:L:135:ASN:O	12:L:198:LEU:HD13	2.16	0.46
12:L:324:LEU:HA	12:L:327:LEU:HD12	1.97	0.46
12:L:339:LEU:HD11	12:L:376:GLY:HA3	1.98	0.46
12:L:364:LYS:O	35:j:47:PHE:HZ	1.99	0.46
12:L:445:GLU:OE2	35:j:54:GLN:CG	2.62	0.46
12:L:598:ILE:HB	55:L:703:3PE:C2G	2.46	0.46
62:L:704:CDL:H141	62:L:704:CDL:H112	1.73	0.46
13:M:116:ILE:HD12	13:M:119:TYR:HB3	1.98	0.46
13:M:208:PRO:CD	13:M:236:LEU:HD22	2.38	0.46
14:N:37:LEU:HD21	14:N:60:PHE:CD1	2.51	0.46
15:O:68:SER:OG	15:O:70:LYS:HB3	2.16	0.46
16:P:354:ARG:HD2	16:P:362:LEU:O	2.16	0.46
21:V:51:ILE:O	21:V:52:THR:C	2.58	0.46
22:W:77:THR:O	22:W:79:PRO:HD3	2.16	0.46
29:d:94:ILE:HD13	33:h:152:LYS:CE	2.46	0.46
33:h:95:GLU:OE1	33:h:114:LYS:HD3	2.16	0.46
36:k:69:PHE:CZ	36:k:73:ILE:HG13	2.52	0.46
40:o:71:ARG:HB3	40:o:71:ARG:NH1	2.27	0.46
42:q:17:HIS:ND1	42:q:26:VAL:HG21	2.30	0.46
45:AA:74:TRP:HB3	45:AA:418:LEU:CD1	2.46	0.46
46:AB:425:VAL:HG12	46:AB:429:LYS:HZ1	1.81	0.46
47:AC:121:PHE:CZ	47:AC:299:LEU:HG	2.51	0.46
47:AC:152:ALA:O	47:AC:153:ILE:C	2.58	0.46
47:AC:184:ILE:HG23	47:AC:185:LEU:N	2.31	0.46
47:AC:260:ASN:O	47:AC:262:LEU:N	2.48	0.46
48:AD:218:TYR:CE1	48:AD:232:TYR:HB2	2.51	0.46
48:AD:235:PRO:HB3	52:AH:70:PHE:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:131:ASN:O	49:AE:135:GLN:HG2	2.16	0.46
49:AE:231:PHE:CE2	49:AE:250:ARG:HB3	2.51	0.46
51:AG:46:ILE:C	51:AG:48:ARG:N	2.74	0.46
45:Aa:109:LEU:CD1	45:Aa:110:GLU:H	2.24	0.46
45:Aa:286:HIS:CG	45:Aa:359:VAL:HG22	2.51	0.46
47:Ac:233:LEU:HD23	48:Ad:300:LEU:HA	1.96	0.46
47:Ac:278:TYR:CE2	47:Ac:282:ARG:HD2	2.51	0.46
48:Ad:112:ARG:O	48:Ad:116:VAL:HG23	2.16	0.46
48:Ad:155:GLN:CD	48:Ad:165:PHE:HB2	2.41	0.46
48:Ad:185:ALA:O	48:Ad:189:ASN:HB2	2.16	0.46
49:Ae:217:CYS:C	49:Ae:219:HIS:N	2.72	0.46
52:Ah:47:ARG:HB3	52:Ah:47:ARG:NH1	2.30	0.46
1:A:65:PHE:HA	1:A:68:GLU:CG	2.46	0.45
2:B:207:GLN:HA	2:B:210:ARG:NH2	2.30	0.45
6:F:157:TYR:CG	6:F:212:LEU:HD11	2.51	0.45
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.45
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.98	0.45
7:G:651:PRO:HD2	19:S:56:ARG:HB3	1.96	0.45
10:J:43:VAL:HG13	11:K:49:LEU:HD11	1.98	0.45
10:J:104:CYS:O	10:J:107:ASN:HB2	2.16	0.45
10:J:120:LEU:HA	10:J:123:TRP:CZ3	2.52	0.45
11:K:26:LEU:O	11:K:29:THR:N	2.48	0.45
12:L:12:PHE:O	12:L:16:LEU:HG	2.15	0.45
12:L:195:SER:O	12:L:201:ILE:HD11	2.16	0.45
13:M:61:LEU:C	13:M:64:PRO:HD2	2.41	0.45
13:M:393:ILE:O	13:M:397:GLY:N	2.49	0.45
15:O:72:LYS:O	15:O:75:LYS:HG2	2.16	0.45
15:O:76:GLU:HB3	15:O:266:PRO:CB	2.46	0.45
15:O:344:ASN:OD1	15:O:346:GLU:HG2	2.15	0.45
16:P:131:GLY:HA3	64:P:401:NDP:O3D	2.15	0.45
20:T:99:SER:HB2	20:T:102:SER:CB	2.33	0.45
20:U:118:ILE:O	20:U:122:MET:HG2	2.16	0.45
20:U:124:ASP:CG	39:n:25:ARG:HH12	2.25	0.45
21:V:31:THR:C	21:V:33:ASP:N	2.73	0.45
23:X:128:VAL:HG12	27:b:54:PRO:HB2	1.99	0.45
27:b:80:TRP:O	27:b:81:LEU:C	2.59	0.45
30:e:42:GLU:CG	33:h:176:LYS:HE2	2.46	0.45
31:f:49:ARG:HG2	31:f:52:GLU:HG3	1.98	0.45
37:l:166:LEU:HD12	37:l:170:ARG:HH22	1.81	0.45
38:m:49:LEU:CD2	39:n:140:LEU:CD2	2.94	0.45
39:n:37:TYR:O	39:n:38:ARG:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:44:MET:O	39:n:45:ARG:C	2.54	0.45
41:p:24:THR:HG22	41:p:26:LEU:N	2.30	0.45
46:AB:195:TYR:CD2	46:Ab:262:ASN:C	2.94	0.45
47:AC:51:LEU:HA	47:AC:51:LEU:HD13	1.76	0.45
52:AH:82:HIS:HB3	52:AH:83:LYS:NZ	2.29	0.45
45:Aa:294:PRO:HB3	45:Aa:448:TYR:OH	2.16	0.45
45:Aa:478:LEU:HD23	53:Aj:18:THR:CG2	2.44	0.45
46:Ab:81:HIS:HE2	46:Ab:161:ASP:HB3	1.81	0.45
48:Ad:112:ARG:HE	48:Ad:269:ASP:CG	2.24	0.45
48:Ad:158:PRO:HG3	48:Ad:167:ARG:CB	2.45	0.45
49:Ae:242:HIS:CD2	49:Ae:251:LYS:HD3	2.51	0.45
4:D:266:ARG:HH11	9:I:66:LEU:HG	1.81	0.45
4:D:345:GLU:CD	25:Z:19:ILE:HG12	2.41	0.45
4:D:348:LEU:HB3	25:Z:16:TYR:CE2	2.52	0.45
4:D:460:GLU:O	4:D:463:ARG:HG2	2.16	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.31	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
7:G:97:MET:SD	7:G:100:TRP:CZ2	3.09	0.45
7:G:176:CYS:SG	56:G:802:SF4:S1	3.14	0.45
8:H:111:LEU:HD21	10:J:60:LEU:CD1	2.44	0.45
8:H:243:LEU:HB3	8:H:262:GLU:OE1	2.16	0.45
12:L:204:SER:HA	12:L:207:ASN:ND2	2.31	0.45
12:L:475:THR:O	12:L:476:SER:HB2	2.16	0.45
12:L:508:THR:HG22	39:n:33:HIS:HD2	1.81	0.45
12:L:552:LEU:HD12	37:l:70:MET:CE	2.36	0.45
12:L:591:PHE:N	12:L:591:PHE:CD1	2.83	0.45
13:M:6:LEU:HD21	31:f:22:PHE:HD2	1.81	0.45
13:M:42:LEU:HD21	13:M:67:ILE:HD12	1.97	0.45
13:M:105:LEU:HD21	55:N:401:3PE:H2H2	1.98	0.45
14:N:133:TRP:CE3	14:N:136:ILE:HD12	2.51	0.45
14:N:300:THR:CG2	14:N:301:SER:N	2.79	0.45
16:P:141:PHE:HD1	16:P:145:PHE:HE2	1.64	0.45
16:P:203:PRO:HG2	64:P:401:NDP:C6N	2.47	0.45
16:P:255:ASP:OD1	16:P:256:PRO:HD2	2.16	0.45
21:V:79:GLU:O	21:V:80:VAL:C	2.59	0.45
25:Z:85:GLN:CD	30:e:105:ARG:HD3	2.35	0.45
45:AA:92:PHE:HE1	45:AA:165:ARG:N	2.15	0.45
45:AA:188:HIS:NE2	45:AA:348:TYR:OH	2.47	0.45
46:AB:418:SER:O	46:AB:419:VAL:C	2.59	0.45
47:AC:48:GLY:CA	67:AC:401:HEM:C1B	2.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:135:TRP:CH2	47:AC:140:PHE:CE1	3.04	0.45
48:AD:207:GLY:O	48:AD:208:GLU:C	2.58	0.45
48:AD:226:SER:O	48:AD:227:LEU:C	2.59	0.45
48:AD:237:PHE:CG	48:AD:238:PRO:HD2	2.51	0.45
48:AD:264:SER:CB	52:AH:28:LEU:HB2	2.34	0.45
49:AE:177:ARG:HD2	49:AE:234:TYR:CZ	2.51	0.45
50:AF:95:LEU:O	50:AF:99:ILE:HG12	2.16	0.45
48:Ad:207:GLY:O	48:Ad:208:GLU:C	2.58	0.45
49:Ae:130:LYS:HD3	53:Aj:33:GLU:OE1	2.17	0.45
2:B:174:SER:HB3	4:D:123:LEU:HD11	1.99	0.45
4:D:79:ASN:ND2	4:D:102:SER:HB2	2.32	0.45
4:D:211:PHE:O	4:D:212:GLU:C	2.56	0.45
4:D:326:CYS:CB	4:D:453:THR:HG21	2.47	0.45
5:E:179:CYS:O	5:E:180:VAL:C	2.59	0.45
5:E:241:GLY:O	5:E:244:VAL:HG23	2.17	0.45
6:F:47:GLY:O	6:F:48:ARG:HB3	2.16	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.46	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:382:ARG:HA	7:G:385:TYR:CE1	2.51	0.45
9:I:135:ARG:O	9:I:136:ALA:HB3	2.16	0.45
10:J:99:GLU:HG3	10:J:100:VAL:N	2.32	0.45
55:K:101:3PE:H351	24:Y:43:VAL:HG12	1.99	0.45
12:L:47:SER:O	12:L:50:PRO:HD2	2.16	0.45
12:L:56:HIS:CA	40:o:74:PHE:CE1	3.00	0.45
12:L:302:ILE:HG22	12:L:340:PHE:CE2	2.51	0.45
12:L:532:ILE:HG23	12:L:533:ILE:N	2.31	0.45
13:M:22:LYS:HG2	13:M:22:LYS:O	2.17	0.45
13:M:186:LEU:HD22	13:M:250:LEU:HA	1.98	0.45
13:M:249:ILE:O	13:M:250:LEU:CG	2.47	0.45
13:M:282:LEU:HD11	13:M:410:MET:HE3	1.96	0.45
14:N:26:LEU:HG	14:N:85:MET:SD	2.56	0.45
14:N:215:MET:SD	14:N:244:ILE:HD11	2.56	0.45
15:O:306:ASN:O	15:O:309:THR:HG22	2.16	0.45
15:O:342:GLY:O	15:O:355:LYS:NZ	2.50	0.45
16:P:338:LEU:HD12	16:P:338:LEU:HA	1.73	0.45
20:T:140:CYS:HB2	20:T:143:GLU:HG2	1.98	0.45
21:V:43:ALA:O	21:V:44:TYR:C	2.60	0.45
24:Y:75:THR:HB	24:Y:95:GLY:HA2	1.98	0.45
30:e:19:MET:HE2	30:e:19:MET:HB3	1.85	0.45
34:i:103:ARG:O	41:p:18:PRO:HG3	2.17	0.45
55:i:201:3PE:H2E1	55:i:201:3PE:H362	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:63:LEU:O	40:o:64:ILE:C	2.59	0.45
41:p:107:GLN:O	41:p:111:LYS:HG3	2.16	0.45
41:p:173:GLU:O	41:p:174:ALA:C	2.59	0.45
45:AA:82:GLU:O	45:AA:199:GLN:NE2	2.50	0.45
45:AA:410:CYS:O	45:AA:411:GLU:C	2.58	0.45
47:AC:202:GLU:CD	47:Ac:9:PRO:HG3	2.42	0.45
48:AD:114:PHE:HD2	48:AD:140:TYR:CE1	2.33	0.45
46:Ab:306:THR:O	46:Ab:307:SER:C	2.58	0.45
47:Ac:312:GLN:HG2	50:Af:37:THR:O	2.16	0.45
48:Ad:121:CYS:C	48:Ad:123:SER:N	2.73	0.45
48:Ad:123:SER:O	48:Ad:178:PRO:HB3	2.17	0.45
48:Ad:158:PRO:CG	48:Ad:166:MET:H	2.29	0.45
53:Aj:9:ARG:O	53:Aj:13:LEU:HD23	2.15	0.45
2:B:154:GLU:O	2:B:155:PRO:C	2.57	0.45
3:C:226:ALA:O	17:Q:116:SER:OG	2.31	0.45
4:D:133:LEU:HD11	4:D:148:GLU:HB3	1.98	0.45
4:D:163:PRO:HG2	4:D:168:GLN:NE2	2.32	0.45
6:F:109:ARG:NH2	6:F:232:ASP:O	2.45	0.45
7:G:49:VAL:HB	7:G:91:ALA:HA	1.98	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:142:TYR:CD1	8:H:289:LEU:HD13	2.51	0.45
10:J:28:GLY:O	10:J:29:GLY:C	2.59	0.45
12:L:60:GLU:HG2	12:L:83:ASP:HA	1.98	0.45
12:L:277:MET:HG3	12:L:318:GLY:CA	2.46	0.45
12:L:358:LYS:HZ1	39:n:34:ARG:HH12	1.63	0.45
12:L:366:MET:SD	12:L:443:ILE:HG21	2.57	0.45
55:L:701:3PE:H3B2	55:L:701:3PE:H381	1.70	0.45
13:M:65:LEU:O	13:M:66:ILE:C	2.59	0.45
13:M:207:MET:O	13:M:208:PRO:C	2.59	0.45
13:M:283:LYS:HG3	13:M:327:PHE:HE1	1.78	0.45
13:M:309:PHE:O	13:M:312:ALA:HB3	2.16	0.45
16:P:106:LEU:HB2	18:R:50:ASP:OD2	2.16	0.45
16:P:227:PRO:HB3	16:P:291:TYR:CE1	2.51	0.45
20:U:102:SER:O	20:U:141:PRO:HD3	2.16	0.45
22:W:31:ALA:O	22:W:32:LYS:C	2.58	0.45
22:W:36:ARG:O	22:W:40:ARG:HG3	2.16	0.45
24:Y:19:GLN:HE21	24:Y:22:ARG:CG	2.15	0.45
24:Y:39:SER:HB2	24:Y:58:VAL:HA	1.98	0.45
30:e:18:PHE:O	30:e:18:PHE:CD2	2.69	0.45
36:k:57:TRP:O	36:k:58:ARG:C	2.59	0.45
37:l:110:ASP:O	37:l:116:ARG:NH1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:170:VAL:O	47:AC:170:VAL:HG13	2.16	0.45
49:AE:217:CYS:C	49:AE:219:HIS:N	2.72	0.45
50:AF:83:LYS:HB3	50:AF:85:GLU:OE2	2.17	0.45
45:Aa:246:ALA:O	45:Aa:249:HIS:O	2.34	0.45
45:Aa:341:PHE:CZ	45:Aa:372:LEU:CD1	2.98	0.45
47:Ac:30:TRP:HZ3	47:Ac:96:LEU:HD22	1.81	0.45
47:Ac:233:LEU:CD2	48:Ad:300:LEU:HA	2.46	0.45
48:Ad:307:LYS:O	48:Ad:311:TRP:HB2	2.16	0.45
49:Ae:248:ARG:HG2	49:Ae:257:ASN:ND2	2.31	0.45
4:D:87:GLN:O	4:D:88:HIS:C	2.57	0.45
5:E:180:VAL:HG13	5:E:181:ASN:N	2.31	0.45
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:629:ILE:HD11	22:W:122:LEU:HD21	1.98	0.45
8:H:149:ILE:HG21	8:H:185:TRP:HB2	1.98	0.45
8:H:151:LEU:HD23	8:H:151:LEU:C	2.41	0.45
9:I:116:CYS:HB2	9:I:118:LEU:H	1.80	0.45
12:L:210:LEU:HD23	12:L:210:LEU:C	2.41	0.45
12:L:310:LEU:HA	12:L:313:MET:HB2	1.99	0.45
12:L:407:TRP:HE1	37:l:140:MET:HE3	1.82	0.45
12:L:591:PHE:N	12:L:591:PHE:HD1	2.15	0.45
13:M:42:LEU:HD11	13:M:67:ILE:HD12	1.99	0.45
13:M:122:PHE:CZ	13:M:206:LYS:CD	2.95	0.45
13:M:453:LEU:CD1	13:M:454:ILE:CG2	2.84	0.45
14:N:155:LEU:O	14:N:159:ILE:HG22	2.16	0.45
15:O:351:TRP:HB3	28:c:39:PRO:CG	2.43	0.45
16:P:188:GLU:HG3	16:P:202:ARG:HH21	1.82	0.45
18:R:97:LYS:CE	18:R:100:LYS:HD3	2.45	0.45
20:T:133:ILE:HG13	20:T:137:LYS:NZ	2.30	0.45
21:V:35:LEU:HD22	21:V:48:THR:HG21	1.98	0.45
23:X:167:PHE:HB3	23:X:170:TRP:HD1	1.77	0.45
26:a:7:PRO:HG3	62:a:101:CDL:H152	1.98	0.45
29:d:54:MET:HE2	29:d:54:MET:HB3	1.89	0.45
55:i:201:3PE:H2E1	55:i:201:3PE:C34	2.41	0.45
36:k:26:ARG:O	36:k:27:GLN:C	2.57	0.45
37:l:38:PRO:HD2	38:m:70:TYR:CD2	2.52	0.45
42:q:24:LEU:O	42:q:28:PHE:HB2	2.16	0.45
45:AA:358:PHE:CD1	45:AA:368:MET:HG2	2.52	0.45
46:AB:278:ILE:HB	46:AB:331:SER:HA	1.98	0.45
47:AC:53:MET:C	47:AC:55:TYR:N	2.74	0.45
47:AC:53:MET:HE2	47:Ac:180:ALA:HB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:126:THR:CG2	67:AC:401:HEM:HBC2	2.45	0.45
47:AC:140:PHE:HE2	47:AC:141:TRP:CH2	2.34	0.45
48:AD:111:ARG:HA	48:AD:140:TYR:HE1	1.81	0.45
49:AE:241:SER:OG	49:AE:254:ALA:HB2	2.17	0.45
50:AF:99:ILE:O	50:AF:103:LYS:HG2	2.17	0.45
52:AH:52:ASP:HA	52:AH:55:VAL:HG23	1.98	0.45
46:Ab:297:PRO:HB3	46:Ab:304:ASN:ND2	2.26	0.45
47:Ac:170:VAL:HG13	47:Ac:170:VAL:O	2.16	0.45
47:Ac:262:LEU:HD12	47:Ac:262:LEU:N	2.32	0.45
48:Ad:159:ASN:N	48:Ad:164:MET:HB3	2.31	0.45
49:Ae:196:ARG:HH22	49:Ae:252:GLY:N	2.14	0.45
49:Ae:228:ALA:CB	49:Ae:235:TYR:HB3	2.46	0.45
49:Ae:272:VAL:HG12	49:Ae:274:GLY:N	2.32	0.45
52:Ah:47:ARG:HA	52:Ah:50:LEU:HG	1.99	0.45
1:A:24:LEU:HD22	58:B:304:PC1:H352	1.98	0.45
2:B:104:MET:HE3	2:B:104:MET:HB3	1.84	0.45
4:D:137:ASP:OD1	4:D:138:ARG:N	2.50	0.45
4:D:362:LYS:O	4:D:384:LEU:HD21	2.17	0.45
5:E:142:ARG:CB	5:E:182:ALA:HB3	2.46	0.45
5:E:241:GLY:HA2	6:F:63:TYR:CE2	2.51	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:157:ASN:HD22	8:H:165:LEU:CD1	2.29	0.45
8:H:200:LEU:HD23	8:H:282:TYR:CD1	2.49	0.45
8:H:206:GLU:HG3	8:H:207:LEU:H	1.79	0.45
10:J:22:LYS:CE	11:K:18:GLY:O	2.65	0.45
12:L:515:LYS:HG2	39:n:30:TRP:CD2	2.51	0.45
14:N:293:TYR:O	14:N:297:ILE:HG12	2.16	0.45
15:O:112:CYS:HB3	15:O:131:LEU:HA	1.97	0.45
17:Q:163:ASN:OD1	17:Q:164:PHE:CG	2.69	0.45
20:T:123:GLU:HA	20:T:128:PHE:O	2.16	0.45
25:Z:69:ILE:HD12	27:b:54:PRO:HD3	1.98	0.45
33:h:91:ILE:O	41:p:56:HIS:CD2	2.70	0.45
36:k:48:ARG:HG3	36:k:48:ARG:O	2.16	0.45
41:p:28:ASN:HA	41:p:29:PRO:HD3	1.86	0.45
41:p:49:ARG:O	41:p:50:GLU:C	2.57	0.45
45:AA:384:THR:HG23	45:AA:384:THR:O	2.15	0.45
46:AB:355:TYR:OH	46:AB:436:LYS:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:48:GLY:C	67:AC:401:HEM:HMB3	2.41	0.45
47:AC:150:LEU:CD1	47:AC:164:ILE:HD12	2.46	0.45
47:AC:218:ILE:HD11	47:AC:224:TYR:CE2	2.52	0.45
48:AD:147:ALA:O	48:AD:151:GLU:HG2	2.17	0.45
52:AH:35:CYS:HA	52:AH:38:LEU:HD13	1.98	0.45
46:Ab:278:ILE:HB	46:Ab:331:SER:HA	1.98	0.45
46:Ab:305:THR:O	46:Ab:311:GLN:HG3	2.17	0.45
48:Ad:92:PRO:HG2	48:Ad:94:TYR:CE1	2.52	0.45
48:Ad:240:GLN:HE21	52:Ah:70:PHE:HZ	1.63	0.45
49:Ae:111:LYS:HE3	53:Aj:11:TYR:CZ	2.52	0.45
49:Ae:177:ARG:HB3	49:Ae:211:VAL:HG13	1.98	0.45
1:A:13:LEU:HD21	8:H:14:LEU:CD1	2.46	0.45
1:A:24:LEU:HD13	58:B:304:PC1:H3B2	1.99	0.45
2:B:92:PRO:CB	2:B:130:VAL:HG13	2.45	0.45
2:B:137:LEU:HD13	2:B:145:LEU:HD22	1.99	0.45
3:C:229:PHE:CD1	9:I:126:GLN:HG3	2.43	0.45
4:D:80:MET:HE2	4:D:101:LEU:HD12	1.99	0.45
4:D:144:MET:SD	4:D:222:MET:CG	2.98	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
10:J:17:LEU:O	10:J:21:LEU:HG	2.16	0.45
11:K:85:TYR:OH	11:K:95:LEU:HD11	2.17	0.45
12:L:74:MET:HE3	12:L:74:MET:HB2	1.76	0.45
12:L:81:LYS:CA	12:L:135:ASN:HD21	2.29	0.45
12:L:145:GLU:CG	13:M:370:PRO:HD3	2.47	0.45
12:L:241:THR:N	12:L:242:PRO:HD2	2.31	0.45
12:L:246:LEU:C	12:L:246:LEU:CD1	2.90	0.45
12:L:387:THR:HA	12:L:465:GLY:HA3	1.98	0.45
62:L:704:CDL:H322	33:h:71:MET:HE1	1.99	0.45
13:M:25:THR:HG22	32:g:84:ASN:CG	2.42	0.45
13:M:187:ASP:H	13:M:192:ASN:ND2	2.15	0.45
14:N:109:ALA:HB3	14:N:110:PRO:CD	2.46	0.45
14:N:153:ILE:O	14:N:154:ILE:C	2.58	0.45
55:N:401:3PE:H2I2	62:X:201:CDL:C60	2.46	0.45
15:O:265:ASP:O	15:O:266:PRO:C	2.58	0.45
15:O:351:TRP:HB2	15:O:355:LYS:HE3	1.98	0.45
16:P:81:ILE:HD11	18:R:46:VAL:HG21	1.97	0.45
16:P:128:ASN:HD22	16:P:166:HIS:CD2	2.35	0.45
16:P:168:SER:O	16:P:203:PRO:HD2	2.16	0.45
20:T:140:CYS:O	20:T:141:PRO:C	2.59	0.45
21:V:48:THR:HA	21:V:51:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:65:VAL:O	21:V:66:LYS:C	2.60	0.45
23:X:168:PHE:O	23:X:169:PHE:CG	2.69	0.45
24:Y:88:ASP:H	24:Y:128:LYS:HZ3	1.63	0.45
32:g:67:LYS:O	32:g:68:ASN:C	2.60	0.45
38:m:25:VAL:O	38:m:26:SER:C	2.56	0.45
44:s:94:GLN:OE1	44:s:94:GLN:N	2.49	0.45
45:AA:92:PHE:CZ	45:AA:161:ILE:HG23	2.52	0.45
45:AA:96:LEU:HD13	45:AA:156:LEU:HB3	1.98	0.45
47:AC:59:THR:CG2	47:AC:172:LYS:HG2	2.46	0.45
48:Ad:298:LEU:C	48:Ad:301:PRO:HD2	2.41	0.45
52:Ah:64:ASP:HB3	52:Ah:66:THR:HG23	1.98	0.45
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.98	0.45
4:D:256:ASP:OD1	4:D:257:GLU:N	2.50	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.45
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.52	0.45
7:G:241:ARG:NH1	9:I:140:ARG:HH22	2.15	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
8:H:142:TYR:CE1	8:H:285:LEU:HD11	2.51	0.45
8:H:148:ILE:HG21	8:H:297:THR:HG22	1.98	0.45
8:H:228:TYR:N	8:H:228:TYR:CD1	2.85	0.45
10:J:12:PHE:HE2	11:K:42:ILE:HD11	1.82	0.45
12:L:100:ILE:O	12:L:104:SER:N	2.42	0.45
12:L:226:GLN:HG3	12:L:314:MET:HE2	1.98	0.45
12:L:524:THR:HG22	39:n:78:GLN:HG3	1.99	0.45
12:L:565:SER:OG	55:Y:201:3PE:H331	2.16	0.45
13:M:3:LYS:HA	13:M:7:PRO:HD2	1.99	0.45
14:N:89:GLN:HB3	30:e:60:PHE:CZ	2.52	0.45
15:O:66:ILE:HD11	15:O:218:ILE:HG13	1.97	0.45
16:P:315:THR:O	16:P:319:VAL:HG23	2.16	0.45
28:c:65:ASP:O	28:c:66:VAL:C	2.56	0.45
34:i:4:TYR:HE1	39:n:4:CYS:SG	2.40	0.45
34:i:88:TYR:CE2	41:p:49:ARG:HB2	2.52	0.45
39:n:146:PRO:O	39:n:147:ASP:C	2.60	0.45
40:o:44:GLN:O	40:o:45:GLU:C	2.58	0.45
47:AC:117:VAL:HG21	47:AC:302:ALA:HB2	1.99	0.45
47:AC:276:PHE:O	47:AC:279:ALA:HB3	2.17	0.45
48:AD:124:CYS:HB3	48:AD:194:PRO:CB	2.47	0.45
48:AD:214:LEU:HA	48:AD:234:ASN:HD21	1.81	0.45
49:AE:237:PRO:HB2	47:Ac:266:PRO:O	2.17	0.45
45:Aa:373:GLN:NE2	45:Aa:471:ILE:O	2.49	0.45
46:Ab:170:GLN:HG2	49:Ai:60:ALA:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:201:THR:H	46:Ab:204:GLU:CD	2.25	0.45
48:Ad:306:MET:O	48:Ad:307:LYS:C	2.60	0.45
53:Aj:11:TYR:HA	53:Aj:15:PHE:HB2	1.97	0.45
2:B:153:PRO:O	2:B:156:ARG:HB3	2.16	0.45
3:C:126:GLU:O	3:C:128:VAL:HG23	2.17	0.45
4:D:226:TYR:CZ	4:D:232:VAL:HB	2.52	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.52	0.45
8:H:213:VAL:HG13	8:H:214:GLU:N	2.32	0.45
11:K:73:VAL:HG21	14:N:38:LEU:CD2	2.47	0.45
12:L:295:GLN:NE2	12:L:524:THR:O	2.50	0.45
13:M:43:TRP:HZ2	33:h:122:ALA:HB2	1.82	0.45
13:M:87:ASP:HB3	13:M:91:LEU:HB2	1.99	0.45
13:M:272:THR:O	13:M:275:ILE:HG13	2.17	0.45
14:N:214:PRO:HB2	14:N:247:MET:SD	2.56	0.45
15:O:129:TYR:CD2	15:O:183:CYS:HB3	2.52	0.45
15:O:230:THR:HG22	15:O:232:ALA:N	2.32	0.45
16:P:88:VAL:O	16:P:91:ILE:HG12	2.17	0.45
16:P:171:ASN:OD1	16:P:171:ASN:O	2.34	0.45
16:P:221:ARG:HD2	16:P:286:ARG:CD	2.43	0.45
16:P:293:LEU:HD12	16:P:298:TYR:OH	2.16	0.45
17:Q:53:ILE:HG22	22:W:20:VAL:O	2.17	0.45
17:Q:112:MET:HG2	17:Q:114:TRP:CE2	2.52	0.45
18:R:44:ARG:HB3	18:R:47:ARG:HH12	1.82	0.45
23:X:27:ALA:HB1	23:X:85:TYR:CD2	2.52	0.45
29:d:11:LEU:HD11	30:e:4:LEU:HD12	1.98	0.45
29:d:13:PHE:CE2	29:d:14:LEU:HD23	2.52	0.45
29:d:78:ARG:O	29:d:79:GLN:C	2.59	0.45
33:h:73:PHE:CE2	33:h:74:TYR:HE1	2.35	0.45
39:n:101:GLU:HG2	39:n:122:ARG:HH12	1.81	0.45
39:n:145:SER:O	39:n:146:PRO:C	2.58	0.45
41:p:110:LEU:O	41:p:111:LYS:C	2.58	0.45
42:q:37:THR:O	42:q:49:TYR:HA	2.17	0.45
45:AA:387:GLU:HB2	45:AA:390:ARG:HH12	1.82	0.45
46:AB:47:LEU:HD11	46:AB:238:LEU:HD13	1.98	0.45
46:AB:341:ILE:HD12	49:AI:59:ALA:HB2	1.97	0.45
47:AC:223:TYR:CE1	48:AD:314:LEU:HG	2.52	0.45
48:AD:268:LYS:HD2	52:AH:88:LEU:HD13	1.97	0.45
50:AF:56:TYR:O	50:AF:60:MET:HG2	2.17	0.45
51:AG:39:LEU:HA	51:AG:42:THR:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:38:LEU:HG	46:Ab:396:ILE:HD13	1.99	0.45
46:Ab:148:ARG:HG3	46:Ab:149:TRP:N	2.32	0.45
50:Af:53:GLU:OE2	51:Ag:12:ARG:NH1	2.49	0.45
51:Ag:38:VAL:HA	51:Ag:41:ARG:HD3	1.99	0.45
2:B:140:LYS:HD2	4:D:115:LEU:HD23	1.99	0.45
3:C:118:VAL:HB	3:C:121:ARG:HD2	1.98	0.45
4:D:100:GLU:HB2	4:D:107:ARG:HB3	1.99	0.45
4:D:168:GLN:HB3	4:D:310:VAL:HG13	1.99	0.45
4:D:304:LYS:HD3	4:D:318:VAL:CG2	2.47	0.45
5:E:73:HIS:CE1	17:Q:166:TRP:CD2	3.05	0.45
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.91	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:381:LEU:HD22	19:S:55:ILE:CD1	2.47	0.45
8:H:227:GLU:C	8:H:228:TYR:HD1	2.25	0.45
10:J:97:ILE:O	10:J:100:VAL:HB	2.17	0.45
12:L:527:GLY:O	12:L:528:PHE:HB2	2.17	0.45
13:M:73:LEU:HB3	13:M:103:GLN:OE1	2.16	0.45
13:M:129:THR:CG2	13:M:235:LEU:CD1	2.95	0.45
13:M:192:ASN:C	13:M:194:LEU:N	2.72	0.45
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.81	0.45
14:N:163:PHE:CZ	14:N:285:MET:HG3	2.52	0.45
14:N:217:MET:HA	14:N:220:MET:SD	2.57	0.45
14:N:258:THR:CB	14:N:333:SER:O	2.64	0.45
16:P:318:LYS:HA	16:P:321:ARG:HG2	1.97	0.45
18:R:46:VAL:O	18:R:47:ARG:C	2.58	0.45
18:R:54:GLU:O	42:q:127:TYR:OH	2.24	0.45
20:T:102:SER:HB2	20:T:107:ASP:CB	2.47	0.45
22:W:31:ALA:C	22:W:33:ARG:N	2.74	0.45
22:W:33:ARG:NH2	22:W:37:GLU:OE2	2.50	0.45
22:W:86:VAL:O	22:W:90:LYS:N	2.41	0.45
23:X:125:LEU:HB2	25:Z:66:GLU:HB3	1.99	0.45
24:Y:83:ARG:HH12	24:Y:90:LEU:HD13	1.82	0.45
26:a:52:ARG:CG	26:a:57:VAL:O	2.55	0.45
30:e:70:TYR:O	30:e:71:LYS:C	2.60	0.45
32:g:64:VAL:HG11	32:g:71:PHE:CE1	2.52	0.45
33:h:87:THR:HG22	62:h:201:CDL:C51	2.46	0.45
39:n:98:LYS:HD3	39:n:176:GLU:O	2.17	0.45
45:AA:246:ALA:O	45:AA:249:HIS:O	2.34	0.45
47:AC:10:LEU:HD22	47:Ac:195:VAL:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:69:ILE:HA	47:AC:73:VAL:CG2	2.47	0.45
47:AC:376:MET:CE	50:AF:18:ARG:HA	2.47	0.45
48:AD:135:LEU:HD13	48:AD:140:TYR:HB2	1.99	0.45
48:AD:310:LYS:HD2	48:AD:310:LYS:N	2.32	0.45
45:Aa:99:LYS:HE2	46:Ab:301:ARG:O	2.18	0.45
45:Aa:402:HIS:NE2	45:Aa:403:LEU:CD1	2.75	0.45
46:Ab:115:THR:HG23	46:Ab:118:ASN:N	2.27	0.45
47:Ac:150:LEU:CD1	47:Ac:164:ILE:HD12	2.46	0.45
47:Ac:280:ILE:O	47:Ac:283:SER:N	2.50	0.45
48:Ad:211:VAL:HG11	48:Ad:274:LEU:HD12	1.99	0.45
49:Ae:156:LEU:HG	49:Ae:271:VAL:CG1	2.47	0.45
52:Ah:49:GLU:O	52:Ah:50:LEU:C	2.60	0.45
4:D:174:PHE:O	4:D:178:THR:HG23	2.17	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:136:VAL:HG23	10:J:69:TYR:HE1	1.82	0.44
10:J:169:ILE:HG23	14:N:45:ILE:HD11	1.99	0.44
11:K:61:ILE:O	11:K:62:THR:C	2.58	0.44
12:L:231:PRO:C	12:L:234:PRO:HD2	2.41	0.44
12:L:424:MET:HG3	12:L:505:ASN:HD21	1.82	0.44
13:M:42:LEU:CG	13:M:67:ILE:CD1	2.95	0.44
13:M:42:LEU:CG	13:M:67:ILE:HD11	2.43	0.44
14:N:154:ILE:CD1	14:N:195:PRO:HG2	2.47	0.44
22:W:65:LYS:HE3	22:W:69:MET:SD	2.56	0.44
22:W:69:MET:C	22:W:71:MET:H	2.24	0.44
23:X:137:LEU:HD22	23:X:139:GLU:CD	2.42	0.44
24:Y:20:CYS:O	24:Y:21:HIS:C	2.60	0.44
27:b:78:LEU:C	27:b:80:TRP:H	2.23	0.44
27:b:80:TRP:CG	27:b:81:LEU:H	2.35	0.44
62:h:201:CDL:H162	62:h:201:CDL:H191	1.75	0.44
36:k:47:LEU:HD12	39:n:43:LEU:HD23	1.99	0.44
42:q:48:TYR:OH	42:q:83:PRO:HD2	2.18	0.44
43:r:57:ARG:HG3	43:r:57:ARG:O	2.16	0.44
45:AA:365:ILE:HG21	45:AA:465:LEU:HB2	1.98	0.44
45:AA:388:VAL:O	45:AA:392:LYS:HG3	2.17	0.44
47:AC:176:THR:O	47:AC:179:PHE:HB3	2.17	0.44
48:AD:157:GLY:N	48:AD:167:ARG:O	2.51	0.44
48:AD:279:GLU:C	48:AD:281:GLU:H	2.25	0.44
49:AE:93:ARG:HG2	51:AG:23:GLU:O	2.17	0.44
52:AH:47:ARG:HH21	52:AH:71:ASP:CB	2.24	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AJ:27:VAL:O	53:AJ:30:LEU:HB3	2.17	0.44
45:Aa:178:SER:O	45:Aa:179:MET:C	2.60	0.44
46:Ab:170:GLN:HG3	46:Ab:339:TYR:OH	2.17	0.44
47:Ac:245:PHE:HE2	48:Ad:293:LEU:HG	1.82	0.44
47:Ac:256:TYR:HB2	48:Ad:203:ALA:HA	1.99	0.44
47:Ac:341:GLN:HE21	47:Ac:342:PRO:HD2	1.82	0.44
48:Ad:219:CYS:SG	48:Ad:220:GLU:N	2.90	0.44
49:Ae:155:LYS:NZ	49:Ae:157:SER:HB3	2.32	0.44
1:A:70:ALA:HB2	10:J:58:ILE:HG13	1.98	0.44
58:B:303:PC1:H341	58:B:303:PC1:C22	2.45	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:136:HIS:O	6:F:137:LYS:C	2.59	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:284:GLU:CD	17:Q:84:ARG:NH2	2.75	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:74:ALA:N	8:H:75:PRO:HD2	2.32	0.44
10:J:133:VAL:CG1	26:a:41:VAL:HG21	2.47	0.44
55:K:101:3PE:H3F1	12:L:596:ILE:HG21	1.98	0.44
12:L:54:PHE:CB	12:L:87:ILE:HD11	2.47	0.44
12:L:117:PHE:CE1	12:L:243:VAL:CG2	3.00	0.44
12:L:149:ILE:CG2	13:M:364:LEU:HD21	2.47	0.44
12:L:366:MET:SD	12:L:443:ILE:CG2	3.06	0.44
12:L:598:ILE:HD11	14:N:153:ILE:CG1	2.47	0.44
14:N:220:MET:O	14:N:221:LEU:C	2.60	0.44
16:P:92:MET:C	16:P:94:LEU:N	2.74	0.44
16:P:192:ARG:NE	16:P:200:ILE:HD12	2.31	0.44
16:P:294:PRO:HG2	16:P:297:VAL:HG23	1.99	0.44
21:V:31:THR:O	21:V:33:ASP:N	2.50	0.44
21:V:50:GLN:NE2	43:r:94:ALA:H	2.15	0.44
23:X:140:ASN:OD1	23:X:144:SER:N	2.49	0.44
25:Z:104:TRP:CH2	30:e:79:ILE:HG12	2.52	0.44
32:g:69:PRO:HB2	39:n:109:PRO:CD	2.47	0.44
33:h:55:PHE:C	33:h:55:PHE:CD1	2.94	0.44
33:h:120:TRP:NE1	33:h:124:ASN:ND2	2.64	0.44
39:n:97:TYR:HB2	39:n:178:PRO:HB2	1.99	0.44
45:AA:165:ARG:NH2	45:AA:211:LEU:O	2.51	0.44
45:AA:463:GLU:OE2	51:AG:8:LEU:CG	2.65	0.44
47:AC:48:GLY:CA	47:AC:83:HIS:CE1	3.00	0.44
51:AG:45:ARG:O	51:AG:49:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:107:ASN:ND2	45:Aa:111:LYS:HD2	2.33	0.44
45:Aa:294:PRO:HB2	45:Aa:298:ASN:HB3	1.98	0.44
46:Ab:178:HIS:CE1	46:Ab:330:TYR:HH	2.32	0.44
47:Ac:218:ILE:HD11	47:Ac:224:TYR:CE2	2.52	0.44
47:Ac:237:LEU:HD22	48:Ad:300:LEU:HD11	1.98	0.44
48:Ad:223:THR:HG21	52:Ah:55:VAL:HB	1.98	0.44
1:A:80:GLN:CA	27:b:46:ASN:ND2	2.61	0.44
2:B:197:THR:O	2:B:200:ALA:HB3	2.17	0.44
4:D:116:LEU:O	4:D:116:LEU:CG	2.62	0.44
4:D:212:GLU:OE1	43:r:27:ARG:NH2	2.50	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.58	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
10:J:94:LEU:HD23	10:J:94:LEU:C	2.42	0.44
12:L:155:ILE:HG12	12:L:248:HIS:CE1	2.53	0.44
14:N:87:GLN:O	14:N:88:GLN:C	2.59	0.44
14:N:250:SER:O	14:N:259:GLY:HA3	2.17	0.44
16:P:266:THR:CG2	16:P:329:PRO:HB3	2.47	0.44
19:S:20:ARG:CG	19:S:66:TRP:HB2	2.47	0.44
22:W:98:LYS:HD3	22:W:100:TRP:CZ2	2.53	0.44
23:X:139:GLU:O	23:X:140:ASN:C	2.60	0.44
26:a:66:LEU:HD13	26:a:66:LEU:O	2.17	0.44
33:h:56:VAL:O	33:h:58:LYS:HG3	2.16	0.44
37:l:119:THR:CG2	38:m:13:THR:HG23	2.48	0.44
46:AB:45:ASN:ND2	46:AB:239:ASN:CA	2.74	0.44
46:AB:255:GLY:HA3	46:AB:435:LYS:HE2	2.00	0.44
47:AC:169:SER:HB2	49:Ae:172:LYS:HZ1	1.82	0.44
48:AD:110:ILE:CG1	48:AD:272:THR:HG22	2.47	0.44
51:AG:45:ARG:HA	51:AG:48:ARG:CZ	2.48	0.44
46:Ab:142:THR:HA	46:Ab:241:ARG:HH12	1.82	0.44
47:Ac:294:LEU:HD21	70:Ac:404:U10:C1M	2.47	0.44
47:Ac:368:ILE:O	47:Ac:372:ILE:HG13	2.17	0.44
48:Ad:146:LYS:O	48:Ad:149:ALA:HB3	2.18	0.44
48:Ad:183:GLU:HG3	48:Ad:184:ALA:N	2.32	0.44
49:Ae:239:HIS:CE1	49:Ae:253:PRO:CG	2.87	0.44
1:A:24:LEU:O	1:A:25:PRO:C	2.56	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:309:ASN:OD1	7:G:310:GLU:N	2.51	0.44
7:G:388:ASN:N	7:G:514:ASN:CB	2.69	0.44
12:L:2:ASN:O	12:L:3:ILE:C	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:56:HIS:N	40:o:74:PHE:CE1	2.85	0.44
12:L:197:GLU:HG3	41:p:111:LYS:HE2	1.98	0.44
12:L:211:ILE:HA	55:m:201:3PE:H272	1.99	0.44
12:L:348:HIS:CD2	20:U:69:SER:CB	3.00	0.44
12:L:524:THR:CG2	39:n:78:GLN:HG3	2.48	0.44
55:L:702:3PE:H362	55:L:702:3PE:H331	1.45	0.44
13:M:24:TRP:CE3	13:M:81:GLN:HG2	2.52	0.44
13:M:26:ASN:OD1	31:f:13:HIS:HE1	2.00	0.44
13:M:29:SER:HB3	32:g:91:PHE:CE2	2.50	0.44
13:M:177:MET:HB3	33:h:140:LEU:HD21	2.00	0.44
13:M:200:MET:HE2	13:M:250:LEU:HD21	2.00	0.44
13:M:415:GLN:O	13:M:416:ARG:CG	2.64	0.44
55:M:501:3PE:H292	14:N:284:MET:HG3	1.99	0.44
14:N:275:CYS:SG	24:Y:139:PRO:HD2	2.58	0.44
15:O:262:GLU:HB3	15:O:268:LYS:NZ	2.33	0.44
15:O:336:GLY:HA2	15:O:344:ASN:HB3	1.99	0.44
15:O:351:TRP:O	15:O:355:LYS:HG2	2.16	0.44
16:P:370:LYS:HD3	16:P:371:PRO:O	2.16	0.44
19:S:59:SER:O	19:S:60:GLU:C	2.59	0.44
21:V:56:LEU:O	21:V:60:LYS:HG2	2.18	0.44
24:Y:7:PHE:CZ	24:Y:26:ILE:HG12	2.52	0.44
24:Y:141:PRO:HB2	33:h:161:ARG:NH1	2.33	0.44
35:j:89:PRO:O	40:o:103:GLU:HG2	2.18	0.44
39:n:45:ARG:O	39:n:49:GLU:N	2.37	0.44
40:o:110:GLN:O	40:o:111:ARG:C	2.59	0.44
41:p:6:ASP:HB3	41:p:9:VAL:CG2	2.39	0.44
42:q:43:LYS:HG3	42:q:44:TYR:CD2	2.53	0.44
45:AA:384:THR:HG22	45:AA:387:GLU:CB	2.45	0.44
45:AA:392:LYS:O	45:AA:396:ARG:HG3	2.17	0.44
49:AE:168:LYS:HZ3	49:AE:171:GLY:HA2	1.81	0.44
49:AE:226:ALA:HB2	49:AE:234:TYR:HE1	1.80	0.44
49:AE:239:HIS:CD2	47:Ac:278:TYR:HH	2.30	0.44
50:AF:90:TYR:O	50:AF:93:PRO:HD2	2.17	0.44
45:Aa:109:LEU:CG	45:Aa:110:GLU:H	2.31	0.44
45:Aa:389:THR:O	45:Aa:390:ARG:C	2.59	0.44
46:Ab:123:VAL:HG12	46:Ab:137:LEU:HD13	1.98	0.44
48:Ad:237:PHE:CD1	48:Ad:238:PRO:HD2	2.53	0.44
48:Ad:262:THR:HB	52:Ah:26:ASP:CB	2.47	0.44
49:Ae:263:TYR:O	49:Ae:264:GLU:C	2.59	0.44
2:B:79:ASP:OD1	2:B:80:ASP:N	2.51	0.44
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:ASP:OD1	3:C:153:ASP:N	2.50	0.44
4:D:142:VAL:HG11	4:D:185:MET:CB	2.48	0.44
4:D:325:ASP:O	4:D:326:CYS:C	2.58	0.44
5:E:79:LEU:HB2	5:E:80:PRO:HD3	2.00	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.44
7:G:75:CYS:SG	59:G:803:FES:S2	3.15	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:308:ARG:NH1	7:G:578:PRO:O	2.50	0.44
7:G:629:ILE:HD11	22:W:122:LEU:HD11	2.00	0.44
8:H:62:ARG:HD2	8:H:68:MET:HB2	2.00	0.44
8:H:187:ILE:HD11	9:I:63:TRP:CH2	2.53	0.44
8:H:193:THR:O	8:H:194:ASN:C	2.58	0.44
9:I:98:ARG:NH1	9:I:155:CYS:O	2.50	0.44
10:J:103:ILE:O	10:J:107:ASN:N	2.50	0.44
11:K:33:LEU:HA	11:K:36:MET:HE2	2.00	0.44
12:L:485:PHE:CD1	12:L:485:PHE:N	2.84	0.44
13:M:18:SER:OG	13:M:26:ASN:ND2	2.51	0.44
13:M:424:ILE:O	13:M:424:ILE:CG2	2.65	0.44
14:N:122:ILE:HD11	14:N:127:GLY:HA2	1.98	0.44
14:N:208:TYR:O	14:N:212:THR:HG22	2.18	0.44
15:O:169:PHE:CD2	63:O:401:ADP:N6	2.86	0.44
15:O:211:VAL:N	15:O:212:PRO:CD	2.80	0.44
16:P:331:ASP:O	16:P:332:LEU:HD23	2.18	0.44
20:T:103:HIS:O	20:T:107:ASP:N	2.51	0.44
21:V:62:GLU:HA	21:V:63:PRO:HD3	1.82	0.44
30:e:38:LYS:NZ	33:h:181:HIS:HD2	2.15	0.44
30:e:91:LYS:NZ	30:e:91:LYS:HB3	2.32	0.44
37:l:88:PRO:HB2	39:n:86:PRO:HB2	1.98	0.44
40:o:49:ALA:O	40:o:50:GLN:C	2.60	0.44
45:AA:294:PRO:HB2	45:AA:298:ASN:HB3	1.98	0.44
45:AA:402:HIS:NE2	45:AA:403:LEU:CD1	2.75	0.44
47:AC:58:ASP:C	47:AC:60:MET:N	2.72	0.44
48:AD:230:GLY:O	48:AD:243:GLY:HA2	2.17	0.44
48:AD:244:MET:HG3	69:AD:401:HEC:NA	2.32	0.44
45:Aa:249:HIS:O	45:Aa:250:LEU:CB	2.64	0.44
45:Aa:392:LYS:O	45:Aa:396:ARG:HG3	2.17	0.44
47:Ac:152:ALA:O	47:Ac:153:ILE:C	2.58	0.44
48:Ad:291:LYS:HB3	71:Ad:402:3PH:C3	2.44	0.44
48:Ad:314:LEU:HB3	50:Af:71:MET:CE	2.47	0.44
52:Ah:34:HIS:O	52:Ah:37:GLN:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:ILE:CG2	4:D:432:LEU:HD21	2.48	0.44
4:D:256:ASP:C	4:D:259:GLU:HB3	2.43	0.44
4:D:259:GLU:HG2	25:Z:25:LEU:HD13	2.00	0.44
4:D:259:GLU:CD	4:D:263:THR:HG1	2.26	0.44
4:D:378:LEU:HD22	7:G:126:LEU:HB2	1.99	0.44
5:E:247:GLY:HA2	6:F:257:ARG:O	2.17	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:195:ARG:HH12	8:H:274:ARG:HB2	1.82	0.44
10:J:136:GLU:HG3	10:J:136:GLU:O	2.18	0.44
12:L:66:TRP:CZ3	12:L:68:TRP:HD1	2.34	0.44
62:L:704:CDL:H132	13:M:361:MET:HE1	1.98	0.44
13:M:22:LYS:HG2	13:M:26:ASN:ND2	2.33	0.44
13:M:154:LEU:HD13	14:N:287:LEU:HD22	2.00	0.44
14:N:254:LEU:HA	14:N:255:PRO:HD3	1.60	0.44
16:P:114:ASP:O	16:P:118:LYS:HG2	2.18	0.44
16:P:265:PHE:CD2	16:P:335:LEU:HD21	2.52	0.44
20:T:99:SER:C	20:T:101:ASN:N	2.75	0.44
21:V:39:PRO:O	21:V:40:LYS:C	2.60	0.44
22:W:104:THR:HG22	22:W:108:ARG:HE	1.82	0.44
29:d:109:TYR:HB3	41:p:156:LEU:HD21	1.99	0.44
46:Ab:262:ASN:HA	46:Ab:195:TYR:CD1	2.53	0.44
47:AC:195:VAL:HG12	47:AC:199:PHE:HD2	1.83	0.44
47:AC:343:VAL:CG2	49:Ae:239:HIS:HD2	2.29	0.44
47:AC:376:MET:HE3	50:AF:18:ARG:HG2	1.99	0.44
48:AD:120:VAL:HG11	48:AD:247:PRO:HB2	1.98	0.44
48:AD:159:ASN:HB3	48:AD:166:MET:CG	2.47	0.44
48:AD:185:ALA:HB1	48:AD:194:PRO:HD2	2.00	0.44
48:AD:304:TYR:CE2	51:AG:27:PHE:HZ	2.35	0.44
49:AE:255:PRO:HG2	47:Ac:287:LYS:HZ1	1.81	0.44
45:Aa:384:THR:HG21	54:Ak:9:ARG:HD2	2.00	0.44
45:Aa:401:SER:O	45:Aa:404:ASP:N	2.51	0.44
46:Ab:155:ARG:HD2	46:Ab:198:GLY:H	1.82	0.44
46:Ab:160:ILE:O	46:Ab:163:ALA:HB3	2.18	0.44
46:Ab:225:VAL:HG22	46:Ab:229:VAL:CG2	2.48	0.44
48:Ad:128:ASP:O	48:Ad:174:TYR:HB3	2.17	0.44
49:Ae:152:ILE:C	49:Ae:153:GLU:CD	2.86	0.44
51:Ag:25:ARG:NH2	51:Ag:29:SER:H	2.16	0.44
1:A:52:SER:CA	10:J:73:MET:HE3	2.48	0.44
2:B:154:GLU:O	16:P:89:TYR:OH	2.27	0.44
2:B:192:PRO:HD3	9:I:176:SER:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:LEU:HD22	22:W:91:MET:HE1	1.99	0.44
4:D:133:LEU:O	4:D:134:PRO:C	2.59	0.44
4:D:150:ALA:O	4:D:151:TYR:C	2.57	0.44
4:D:292:MET:HA	4:D:329:ARG:HD3	1.98	0.44
4:D:319:PRO:HG3	4:D:336:GLU:HG3	2.00	0.44
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.44
5:E:228:GLY:H	6:F:284:HIS:CG	2.35	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:267:THR:HB	17:Q:115:ALA:HB2	1.98	0.44
12:L:529:PHE:O	12:L:533:ILE:HG22	2.16	0.44
12:L:537:THR:N	12:L:538:PRO:HD2	2.32	0.44
12:L:556:ILE:CG2	38:m:80:PHE:CE2	3.00	0.44
12:L:594:ASN:CG	14:N:110:PRO:CB	2.88	0.44
55:L:705:3PE:H11	55:L:705:3PE:H121	1.99	0.44
13:M:154:LEU:HA	13:M:154:LEU:HD23	1.84	0.44
13:M:186:LEU:HD13	13:M:250:LEU:HA	2.00	0.44
13:M:421:ASN:ND2	38:m:47:TYR:OH	2.51	0.44
15:O:148:GLU:HG3	15:O:295:ARG:NH1	2.32	0.44
15:O:272:ASP:O	15:O:275:TYR:HB2	2.18	0.44
16:P:97:MET:HE2	16:P:97:MET:HB3	1.83	0.44
23:X:49:GLU:CG	23:X:50:GLU:H	2.30	0.44
25:Z:89:GLU:O	30:e:97:HIS:NE2	2.50	0.44
28:c:61:THR:HG22	28:c:65:ASP:OD2	2.18	0.44
29:d:27:ASN:O	29:d:28:ASP:C	2.61	0.44
46:AB:39:GLU:HG3	46:AB:227:HIS:ND1	2.32	0.44
46:AB:195:TYR:CZ	46:Ab:261:GLN:HG3	2.52	0.44
46:AB:233:VAL:HA	46:AB:236:GLN:CG	2.47	0.44
47:AC:105:GLY:HA3	47:AC:313:ARG:O	2.18	0.44
47:AC:257:MET:O	47:AC:258:PRO:C	2.60	0.44
48:AD:132:TYR:CE2	48:AD:149:ALA:HA	2.53	0.44
53:AJ:23:LEU:HD13	54:AK:27:VAL:CB	2.47	0.44
45:Aa:47:GLU:OE1	45:Aa:47:GLU:N	2.51	0.44
45:Aa:139:ASP:O	45:Aa:140:LEU:C	2.59	0.44
45:Aa:174:GLU:C	45:Aa:176:ASP:N	2.73	0.44
45:Aa:375:GLN:O	45:Aa:376:TRP:C	2.58	0.44
45:Aa:410:CYS:O	45:Aa:411:GLU:C	2.59	0.44
48:Ad:94:TYR:HB3	48:Ad:95:PRO:HD2	2.00	0.44
48:Ad:201:VAL:HG11	48:Ad:275:ARG:N	2.32	0.44
48:Ad:299:LEU:HD21	49:Ae:124:GLY:C	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:195:LEU:HD13	49:Ae:248:ARG:HD2	1.99	0.44
49:Ae:267:SER:O	49:Ae:268:ASP:C	2.61	0.44
50:Af:97:GLU:HA	50:Af:100:ARG:NH1	2.33	0.44
51:Ag:12:ARG:HB3	51:Ag:13:HIS:CD2	2.52	0.44
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.44
6:F:261:TRP:HZ3	6:F:262:PHE:CE2	2.35	0.44
8:H:84:SER:O	8:H:87:VAL:HG13	2.18	0.44
8:H:112:SER:O	8:H:113:VAL:C	2.59	0.44
9:I:152:CYS:SG	56:I:302:SF4:S2	3.16	0.44
10:J:95:GLY:O	10:J:96:VAL:C	2.60	0.44
12:L:68:TRP:HE3	12:L:76:LEU:HD21	1.82	0.44
12:L:247:LEU:HD12	12:L:247:LEU:C	2.41	0.44
12:L:563:PRO:HG3	13:M:152:TYR:OH	2.18	0.44
13:M:42:LEU:CD1	13:M:67:ILE:CD1	2.96	0.44
13:M:126:LEU:HD11	13:M:153:THR:HG21	2.00	0.44
13:M:344:MET:HE3	13:M:423:MET:CE	2.48	0.44
13:M:446:LEU:CD1	32:g:97:LEU:HD12	2.47	0.44
14:N:35:PHE:O	14:N:36:SER:C	2.59	0.44
14:N:227:ILE:HG13	14:N:228:ASN:N	2.32	0.44
15:O:238:GLU:HG3	15:O:242:LYS:HD3	1.99	0.44
16:P:263:PHE:CE1	16:P:333:PRO:HB2	2.51	0.44
16:P:270:ARG:O	16:P:375:VAL:N	2.37	0.44
16:P:321:ARG:HA	16:P:325:SER:HB2	2.00	0.44
21:V:82:LEU:HG	21:V:86:LYS:HE2	2.00	0.44
23:X:73:GLN:O	23:X:77:HIS:N	2.51	0.44
28:c:33:GLU:CD	28:c:33:GLU:H	2.26	0.44
29:d:57:GLY:O	29:d:60:ARG:N	2.51	0.44
30:e:20:PHE:CZ	33:h:178:PHE:CB	3.01	0.44
39:n:149:ILE:HD12	39:n:149:ILE:N	2.33	0.44
40:o:118:LYS:HD2	40:o:118:LYS:HA	1.85	0.44
42:q:9:ARG:O	42:q:13:GLN:HG3	2.18	0.44
42:q:41:GLU:HG3	42:q:47:LYS:HD3	2.00	0.44
46:AB:63:LEU:HD12	46:AB:220:LEU:HD13	2.00	0.44
46:AB:155:ARG:HD2	46:AB:198:GLY:H	1.83	0.44
46:AB:230:LEU:O	46:AB:233:VAL:HG22	2.18	0.44
47:AC:8:HIS:HE2	47:Ac:199:PHE:HE1	1.65	0.44
47:AC:125:ALA:O	47:AC:129:MET:HG2	2.18	0.44
47:AC:148:ASN:HB2	49:Ae:220:LEU:C	2.43	0.44
48:AD:164:MET:HG3	48:AD:165:PHE:N	2.30	0.44
48:AD:213:SER:O	48:AD:217:GLY:N	2.50	0.44
48:AD:248:ILE:HA	48:AD:252:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:107:ASN:HA	45:Aa:110:GLU:HG2	2.00	0.44
45:Aa:230:VAL:HG21	45:Aa:417:LEU:HB3	2.00	0.44
48:Ad:186:ARG:HG2	48:Ad:191:GLY:O	2.17	0.44
49:Ae:142:ALA:HB1	49:Ae:147:LEU:HD23	1.95	0.44
51:Ag:19:LEU:HG	51:Ag:20:SER:N	2.33	0.44
51:Ag:74:ASN:O	51:Ag:75:PRO:C	2.60	0.44
1:A:102:LEU:HD12	1:A:111:LEU:HD21	1.99	0.44
2:B:153:PRO:CG	8:H:58:LYS:HE3	2.47	0.44
2:B:202:LEU:HD21	9:I:86:TYR:CB	2.48	0.44
3:C:149:LEU:HD21	17:Q:64:LEU:HD21	1.86	0.44
3:C:229:PHE:CE1	9:I:126:GLN:CG	2.71	0.44
4:D:36:GLN:NE2	4:D:38:GLN:NE2	2.62	0.44
4:D:326:CYS:HB3	4:D:453:THR:HG21	1.99	0.44
5:E:133:VAL:HG22	5:E:185:VAL:HG12	2.00	0.44
5:E:240:PRO:CB	6:F:60:GLY:HA3	2.46	0.44
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
7:G:662:THR:HB	19:S:25:GLN:NE2	2.33	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:121:TRP:NE1	10:J:76:GLU:CD	2.60	0.44
8:H:201:THR:C	8:H:203:GLY:N	2.70	0.44
10:J:125:MET:O	25:Z:121:ILE:CD1	2.41	0.44
10:J:132:GLY:HA2	25:Z:68:ARG:HH12	1.70	0.44
10:J:165:ILE:HD13	14:N:38:LEU:HB3	1.99	0.44
11:K:57:MET:O	11:K:60:PRO:HD2	2.18	0.44
12:L:53:MET:HE2	12:L:53:MET:HB3	1.78	0.44
12:L:152:PHE:HD2	12:L:153:LEU:HD12	1.83	0.44
12:L:186:MET:HE1	13:M:379:LEU:HD21	2.00	0.44
12:L:305:SER:OG	12:L:336:LYS:HE2	2.18	0.44
12:L:586:LEU:HA	12:L:589:MET:HE3	1.99	0.44
12:L:598:ILE:HD11	14:N:153:ILE:CD1	2.48	0.44
13:M:8:SER:O	13:M:11:LEU:HB2	2.18	0.44
14:N:146:TYR:O	14:N:147:PRO:C	2.53	0.44
16:P:146:VAL:O	16:P:147:ASN:C	2.60	0.44
16:P:275:HIS:CE1	16:P:373:LYS:HE2	2.53	0.44
24:Y:120:MET:HE2	24:Y:120:MET:HB3	1.90	0.44
32:g:140:PHE:HZ	41:p:152:ALA:HB1	1.83	0.44
33:h:83:ILE:HG12	62:h:201:CDL:H561	2.00	0.44
37:l:58:ARG:HD2	38:m:35:GLU:OE1	2.18	0.44
40:o:5:LEU:HB3	40:o:9:TYR:CD2	2.53	0.44
41:p:140:GLN:HG2	41:p:144:LEU:CD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:165:GLU:C	41:p:167:ARG:H	2.26	0.44
45:AA:311:ILE:CG2	45:AA:341:PHE:CZ	3.01	0.44
46:AB:307:SER:O	46:AB:308:LEU:C	2.59	0.44
47:AC:53:MET:C	47:AC:55:TYR:H	2.26	0.44
48:AD:95:PRO:HD2	52:AH:85:PHE:CD1	2.52	0.44
51:AG:79:GLU:HA	52:AH:61:THR:HA	2.00	0.44
45:Aa:183:VAL:HG21	45:Aa:286:HIS:CB	2.48	0.44
46:Ab:142:THR:HA	46:Ab:241:ARG:HH22	1.82	0.44
46:Ab:173:ILE:O	46:Ab:174:ILE:C	2.59	0.44
46:Ab:426:LYS:HA	46:Ab:429:LYS:HZ3	1.83	0.44
48:Ad:311:TRP:HZ3	50:Af:71:MET:SD	2.41	0.44
4:D:126:TYR:HA	4:D:418:ARG:HH11	1.83	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43
6:F:257:ARG:HB3	6:F:262:PHE:HE1	1.82	0.43
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.43
8:H:91:MET:HE1	8:H:259:PHE:CE1	2.53	0.43
8:H:184:MET:CG	8:H:293:PHE:CE2	2.87	0.43
55:H:401:3PE:H2A1	55:H:401:3PE:H2D2	1.80	0.43
10:J:13:LEU:HD11	11:K:10:MET:SD	2.58	0.43
11:K:26:LEU:HG	11:K:30:LEU:HD13	1.98	0.43
12:L:72:ASN:ND2	13:M:459:MET:HG2	2.33	0.43
12:L:172:ILE:HD13	12:L:172:ILE:HA	1.89	0.43
12:L:348:HIS:CD2	20:U:69:SER:HB3	2.53	0.43
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.43
13:M:98:MET:SD	55:N:401:3PE:H3C1	2.58	0.43
14:N:12:THR:CG2	14:N:39:ALA:HB2	2.48	0.43
14:N:120:GLN:HE22	14:N:174:GLN:HB3	1.83	0.43
14:N:146:TYR:CD1	14:N:198:PRO:HG2	2.53	0.43
14:N:175:MET:HE2	14:N:175:MET:HB2	1.85	0.43
14:N:323:ASN:N	14:N:323:ASN:OD1	2.49	0.43
15:O:40:LEU:O	15:O:44:ILE:HG13	2.18	0.43
15:O:72:LYS:O	15:O:76:GLU:HG2	2.16	0.43
16:P:223:PHE:CZ	16:P:227:PRO:HG3	2.53	0.43
23:X:137:LEU:HD23	23:X:138:PRO:N	2.33	0.43
23:X:169:PHE:HE1	62:X:201:CDL:H551	1.82	0.43
24:Y:7:PHE:O	24:Y:8:PHE:C	2.61	0.43
24:Y:12:HIS:CD2	24:Y:131:LYS:HE2	2.53	0.43
26:a:57:VAL:O	26:a:57:VAL:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:42:GLU:CD	33:h:176:LYS:HE2	2.42	0.43
34:i:19:ARG:HA	39:n:171:VAL:HG13	2.00	0.43
38:m:45:ARG:O	38:m:45:ARG:CG	2.61	0.43
45:AA:78:GLY:H	45:AA:81:TYR:HD2	1.65	0.43
46:AB:138:LEU:CD1	46:AB:233:VAL:HB	2.47	0.43
46:AB:411:THR:O	46:AB:414:GLN:HG2	2.18	0.43
47:AC:341:GLN:HE21	47:AC:342:PRO:HD2	1.82	0.43
48:AD:170:LYS:HE3	48:AD:170:LYS:HB2	1.82	0.43
48:AD:218:TYR:HA	48:AD:234:ASN:HA	2.00	0.43
45:Aa:120:LEU:HD23	46:Ab:299:ILE:CG2	2.48	0.43
46:Ab:236:GLN:HG3	46:Ab:237:PHE:N	2.33	0.43
47:Ac:146:ILE:HG12	70:Ac:404:U10:H4M3	1.94	0.43
47:Ac:253:PRO:O	48:Ad:203:ALA:HA	2.18	0.43
48:Ad:292:MET:CA	71:Ad:402:3PH:H331	2.43	0.43
49:Ae:153:GLU:C	49:Ae:154:ILE:HD12	2.43	0.43
49:Ae:225:ILE:N	49:Ae:235:TYR:O	2.51	0.43
1:A:58:VAL:HG21	1:A:113:TRP:CZ2	2.53	0.43
4:D:138:ARG:HG2	4:D:223:HIS:CE1	2.53	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:382:CYS:SG	56:F:502:SF4:S1	3.13	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.58	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.43
7:G:611:THR:CG2	17:Q:104:ARG:C	2.91	0.43
8:H:97:ASN:O	55:H:401:3PE:H111	2.17	0.43
8:H:138:GLN:HG3	8:H:285:LEU:HD21	1.99	0.43
8:H:277:TYR:OH	9:I:66:LEU:O	2.29	0.43
55:L:703:3PE:P	24:Y:46:ASN:HD22	2.41	0.43
16:P:81:ILE:HG12	18:R:46:VAL:HG11	1.99	0.43
16:P:231:LEU:HB2	16:P:233:PHE:HD1	1.82	0.43
16:P:304:LEU:HA	16:P:307:LEU:HG	2.00	0.43
17:Q:55:VAL:HG22	22:W:20:VAL:HG21	1.99	0.43
17:Q:59:LEU:N	17:Q:59:LEU:CD1	2.78	0.43
19:S:85:ASP:OD1	19:S:86:GLU:N	2.51	0.43
24:Y:89:PRO:HG3	24:Y:129:ILE:HG12	1.99	0.43
25:Z:101:VAL:CB	25:Z:102:PRO:HD2	2.45	0.43
25:Z:128:ARG:O	25:Z:129:THR:C	2.61	0.43
27:b:37:PRO:O	27:b:40:LYS:NZ	2.51	0.43
37:l:142:PHE:O	37:l:145:TRP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:103:MET:HE1	41:p:135:VAL:HG12	1.98	0.43
46:AB:166:PHE:CD1	46:AB:172:ARG:HG2	2.52	0.43
47:AC:50:PHE:HB2	47:AC:79:ILE:HG21	1.99	0.43
47:AC:52:ALA:CA	67:AC:401:HEM:HMA2	2.49	0.43
47:AC:68:HIS:CD2	47:AC:72:ASP:HB2	2.53	0.43
47:AC:182:HIS:CE1	67:AC:401:HEM:C4C	3.06	0.43
47:AC:185:LEU:HA	47:AC:188:ILE:HD12	1.99	0.43
49:AE:127:TYR:CE1	53:AJ:37:ASP:OD1	2.71	0.43
49:AE:164:ASN:HB3	49:AE:226:ALA:HB2	2.00	0.43
50:AF:33:MET:HE1	50:AF:88:LYS:HG2	1.99	0.43
51:AG:33:LYS:O	51:AG:36:PRO:HD2	2.18	0.43
45:Aa:78:GLY:H	45:Aa:81:TYR:HD2	1.65	0.43
45:Aa:186:TYR:OH	49:Ae:80:HIS:CB	2.66	0.43
45:Aa:271:THR:HG22	45:Aa:273:SER:OG	2.18	0.43
46:Ab:106:VAL:CG2	46:Ab:133:LEU:HD21	2.47	0.43
46:Ab:112:VAL:HG22	46:Ab:121:TYR:CD2	2.52	0.43
46:Ab:300:LYS:HE2	46:Ab:301:ARG:HH11	1.83	0.43
46:Ab:312:SER:HA	46:Ab:315:LYS:HE3	1.99	0.43
48:Ad:223:THR:HG21	52:Ah:52:ASP:HA	1.99	0.43
1:A:72:LEU:O	8:H:151:LEU:HD11	2.19	0.43
58:B:304:PC1:H241	16:P:310:PHE:CE1	2.53	0.43
3:C:117:ASP:OD1	3:C:124:ARG:HB2	2.18	0.43
4:D:129:TYR:CE2	4:D:391:VAL:HG22	2.54	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
8:H:124:ASN:HD22	8:H:124:ASN:HA	1.63	0.43
8:H:318:MET:HB2	8:H:318:MET:HE3	1.92	0.43
9:I:57:ALA:O	9:I:61:LEU:HB2	2.18	0.43
10:J:30:LEU:O	10:J:34:VAL:HG23	2.17	0.43
10:J:55:VAL:HG13	10:J:56:PHE:N	2.33	0.43
10:J:77:GLU:OE1	11:K:87:THR:HA	2.18	0.43
12:L:141:PHE:CB	12:L:182:PHE:CE2	2.81	0.43
12:L:496:LEU:CD1	12:L:497:GLY:N	2.73	0.43
62:L:704:CDL:H792	62:L:704:CDL:H581	2.00	0.43
13:M:123:GLU:CD	14:N:255:PRO:CG	2.91	0.43
13:M:353:PRO:HG3	33:h:61:LEU:CD2	2.48	0.43
14:N:338:PRO:HG2	29:d:33:TYR:CZ	2.52	0.43
17:Q:75:ARG:NH1	17:Q:102:ASP:OD1	2.51	0.43
22:W:45:GLU:O	22:W:46:VAL:C	2.59	0.43
24:Y:19:GLN:OE1	24:Y:19:GLN:HA	2.17	0.43
28:c:55:TRP:HE1	29:d:66:THR:CG2	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:57:TYR:HD2	29:d:70:PHE:CZ	2.35	0.43
29:d:72:GLY:O	29:d:73:TYR:C	2.60	0.43
29:d:78:ARG:HG2	29:d:82:LEU:HD23	2.00	0.43
30:e:38:LYS:HB3	30:e:38:LYS:HE2	1.74	0.43
32:g:58:GLU:CD	32:g:59:PRO:HD2	2.44	0.43
37:l:41:TYR:HD2	37:l:43:ARG:HD3	1.82	0.43
46:AB:173:ILE:HD11	46:AB:439:ALA:C	2.44	0.43
47:AC:265:PRO:O	47:AC:266:PRO:C	2.62	0.43
48:AD:95:PRO:HG2	52:AH:85:PHE:CG	2.53	0.43
50:AF:22:TYR:CZ	50:AF:84:TYR:HA	2.53	0.43
51:AG:76:ALA:HA	51:AG:79:GLU:HB3	2.00	0.43
45:Aa:162:GLU:HA	45:Aa:165:ARG:NH1	2.32	0.43
45:Aa:172:MET:HE1	45:Aa:205:SER:HA	2.00	0.43
45:Aa:385:GLU:OE2	54:Ak:12:GLU:OE2	2.36	0.43
46:Ab:130:ILE:HA	46:Ab:133:LEU:HB2	2.00	0.43
46:Ab:164:VAL:N	49:Ai:43:LEU:HD22	2.33	0.43
46:Ab:411:THR:O	46:Ab:414:GLN:HG2	2.19	0.43
48:Ad:121:CYS:HB3	69:Ad:401:HEC:CHC	2.49	0.43
48:Ad:219:CYS:O	48:Ad:233:PHE:HD2	2.01	0.43
48:Ad:262:THR:O	48:Ad:263:MET:C	2.59	0.43
48:Ad:299:LEU:HD12	71:Ad:402:3PH:H372	1.98	0.43
51:Ag:29:SER:CB	51:Ag:32:SER:HB2	2.38	0.43
52:Ah:49:GLU:O	52:Ah:53:ASN:N	2.33	0.43
1:A:79:ILE:HG13	1:A:87:MET:HE1	2.01	0.43
1:A:87:MET:O	1:A:88:MET:C	2.60	0.43
4:D:137:ASP:HB2	4:D:223:HIS:HA	1.99	0.43
4:D:142:VAL:HG12	4:D:182:ASN:HA	2.01	0.43
5:E:196:THR:O	5:E:199:ASP:N	2.51	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.61	0.43
10:J:155:ALA:HB1	11:K:65:VAL:HG11	2.00	0.43
12:L:92:VAL:HG21	12:L:330:CYS:HB3	2.00	0.43
12:L:226:GLN:OE1	12:L:284:THR:CG2	2.66	0.43
12:L:386:LEU:HA	35:j:68:TRP:HZ3	1.82	0.43
12:L:427:ILE:HG13	12:L:428:TYR:N	2.33	0.43
13:M:321:LEU:HD23	13:M:321:LEU:HA	1.81	0.43
15:O:214:VAL:O	15:O:218:ILE:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:232:GLY:O	16:P:273:LEU:HB3	2.18	0.43
20:U:137:LYS:HD3	34:i:4:TYR:CD1	2.53	0.43
23:X:165:THR:N	23:X:172:VAL:HG11	2.33	0.43
24:Y:26:ILE:O	24:Y:30:LEU:HG	2.17	0.43
29:d:116:PHE:HB2	41:p:157:ALA:CB	2.48	0.43
30:e:101:ARG:HH21	30:e:104:PRO:CD	2.31	0.43
32:g:139:TYR:HB2	41:p:142:ARG:NH2	2.34	0.43
33:h:127:ASP:OD1	33:h:127:ASP:C	2.61	0.43
35:j:44:TYR:CG	36:k:22:LEU:HD22	2.54	0.43
39:n:131:GLU:O	39:n:131:GLU:HG2	2.17	0.43
42:q:26:VAL:HG13	42:q:30:ALA:HB3	2.00	0.43
42:q:68:MET:HE2	42:q:71:LYS:HD3	1.99	0.43
45:AA:183:VAL:HG21	45:AA:286:HIS:CB	2.48	0.43
46:AB:148:ARG:NH2	50:Af:50:ARG:O	2.52	0.43
47:AC:45:ILE:HG23	67:AC:401:HEM:HAB	2.00	0.43
47:AC:278:TYR:CE2	47:AC:282:ARG:HD2	2.53	0.43
49:AE:132:VAL:O	49:AE:136:PHE:HB2	2.18	0.43
49:AE:235:TYR:CE1	49:AE:240:GLY:HA2	2.53	0.43
50:AF:110:LYS:HA	54:Ak:10:TYR:HE1	1.84	0.43
51:AG:20:SER:O	51:AG:24:GLN:HG2	2.19	0.43
51:AG:29:SER:HB2	51:AG:32:SER:HB3	2.00	0.43
52:AH:58:ARG:HB3	52:AH:61:THR:HG21	2.00	0.43
45:Aa:311:ILE:CG2	45:Aa:341:PHE:CZ	3.01	0.43
46:Ab:297:PRO:CB	46:Ab:304:ASN:CG	2.91	0.43
47:Ac:138:MET:CE	47:Ac:268:ILE:HG23	2.49	0.43
48:Ad:183:GLU:N	48:Ad:186:ARG:HH21	2.17	0.43
48:Ad:302:LEU:O	48:Ad:305:ALA:HB3	2.19	0.43
1:A:33:LYS:NZ	2:B:154:GLU:HB2	2.33	0.43
2:B:108:ALA:N	2:B:114:MET:HE3	2.33	0.43
2:B:170:TYR:CD2	4:D:135:TYR:CE1	3.06	0.43
2:B:224:ARG:HG3	16:P:136:THR:HG21	2.00	0.43
4:D:172:VAL:HG21	4:D:310:VAL:CG2	2.49	0.43
4:D:211:PHE:HD1	4:D:221:ARG:O	2.01	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.41	0.43
5:E:162:THR:HG21	5:E:166:LYS:HA	2.01	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.34	0.43
6:F:36:LYS:CB	6:F:38:GLU:HG2	2.42	0.43
6:F:119:GLU:H	6:F:159:ARG:HD2	1.83	0.43
7:G:291:ARG:HD2	7:G:292:PHE:CE2	2.54	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:617:ARG:HH22	22:W:128:GLY:H	1.64	0.43
8:H:100:LEU:HD21	10:J:50:PHE:HA	2.01	0.43
11:K:32:CYS:O	11:K:33:LEU:C	2.59	0.43
12:L:22:SER:HA	12:L:27:ILE:HG21	2.00	0.43
13:M:348:LEU:O	13:M:349:GLN:C	2.60	0.43
14:N:186:HIS:O	14:N:190:MET:HG3	2.18	0.43
14:N:319:LYS:HA	15:O:302:THR:CG2	2.43	0.43
15:O:315:PRO:O	32:g:53:TRP:HA	2.19	0.43
15:O:332:ARG:O	15:O:338:LYS:HA	2.19	0.43
16:P:111:ARG:NH1	16:P:138:ASN:HB3	2.33	0.43
16:P:283:MET:HG2	16:P:353:LEU:HD12	1.99	0.43
21:V:56:LEU:HG	21:V:60:LYS:HE3	2.01	0.43
24:Y:19:GLN:O	24:Y:23:LYS:HG2	2.19	0.43
26:a:18:ILE:O	26:a:22:SER:HB3	2.18	0.43
32:g:89:PHE:HB3	33:h:74:TYR:HD2	1.84	0.43
37:l:38:PRO:HD2	38:m:70:TYR:HD2	1.82	0.43
41:p:75:THR:HG22	41:p:156:LEU:HD13	2.00	0.43
46:AB:109:LYS:HD2	49:AI:71:ASN:ND2	2.31	0.43
46:AB:138:LEU:HD22	46:AB:238:LEU:HG	2.01	0.43
47:AC:269:LYS:HE3	47:AC:275:LEU:HD21	2.01	0.43
47:AC:277:ALA:HA	47:AC:280:ILE:HD12	2.00	0.43
48:AD:98:HIS:O	48:AD:286:LYS:NZ	2.52	0.43
48:AD:279:GLU:C	48:AD:281:GLU:N	2.75	0.43
45:Aa:71:VAL:HG21	45:Aa:140:LEU:CD1	2.48	0.43
45:Aa:110:GLU:HB2	46:Ab:299:ILE:CD1	2.35	0.43
46:Ab:297:PRO:HB3	46:Ab:304:ASN:CG	2.43	0.43
48:Ad:222:PRO:HB3	52:Ah:69:LEU:HD13	1.98	0.43
51:Ag:48:ARG:HH21	55:Ag:103:3PE:H322	1.83	0.43
1:A:56:PHE:CZ	11:K:75:LEU:HB3	2.54	0.43
1:A:96:THR:O	1:A:97:ILE:C	2.61	0.43
4:D:188:THR:O	4:D:192:LEU:HD13	2.18	0.43
4:D:265:ASN:O	4:D:266:ARG:C	2.61	0.43
6:F:398:ARG:HH21	7:G:155:GLU:HG3	1.83	0.43
12:L:60:GLU:C	12:L:61:TYR:CD1	2.97	0.43
12:L:81:LYS:HD3	12:L:262:ARG:NH1	2.34	0.43
12:L:136:ASN:HD21	62:h:201:CDL:C27	2.18	0.43
12:L:246:LEU:HD12	12:L:247:LEU:CB	2.49	0.43
12:L:327:LEU:HD21	12:L:472:ILE:HD13	2.00	0.43
12:L:427:ILE:CD1	36:k:69:PHE:CE1	3.01	0.43
13:M:16:TRP:CD1	55:d:201:3PE:H361	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:207:MET:SD	13:M:240:SER:CA	3.06	0.43
13:M:304:GLN:HA	13:M:309:PHE:HE1	1.83	0.43
14:N:11:PHE:O	14:N:15:LEU:N	2.50	0.43
14:N:240:MET:O	14:N:240:MET:HG2	2.18	0.43
14:N:279:ALA:HA	14:N:282:MET:HE2	2.00	0.43
15:O:68:SER:O	15:O:69:GLY:C	2.59	0.43
15:O:239:ASN:HA	15:O:242:LYS:HE2	2.01	0.43
16:P:187:GLY:O	16:P:188:GLU:C	2.62	0.43
16:P:276:LEU:CD2	16:P:280:ILE:CD1	2.95	0.43
19:S:44:LEU:CD2	19:S:91:MET:HG2	2.48	0.43
32:g:117:ARG:NE	41:p:10:TYR:OH	2.51	0.43
37:l:97:LEU:O	37:l:98:ARG:C	2.60	0.43
42:q:66:THR:HG23	42:q:74:PHE:HD1	1.83	0.43
45:AA:80:ARG:NH2	45:AA:268:CYS:SG	2.92	0.43
46:AB:130:ILE:HA	46:AB:133:LEU:HB2	2.01	0.43
46:AB:177:LEU:HD22	46:AB:270:ALA:CB	2.49	0.43
47:AC:53:MET:HG2	47:Ac:180:ALA:HB2	2.01	0.43
47:AC:100:ARG:HH12	67:AC:402:HEM:CBD	2.30	0.43
48:AD:94:TYR:HB3	52:AH:85:PHE:CZ	2.54	0.43
48:AD:112:ARG:HB3	48:AD:255:TYR:CE1	2.53	0.43
48:AD:248:ILE:HD12	48:AD:266:VAL:HG11	2.00	0.43
48:AD:312:SER:O	48:AD:313:VAL:C	2.59	0.43
49:AE:114:SER:HB2	51:AG:22:PHE:HE2	1.83	0.43
49:AE:166:ALA:HB2	49:AE:175:PHE:HD1	1.84	0.43
45:Aa:142:LYS:HE2	45:Aa:142:LYS:HB2	1.86	0.43
46:Ab:418:SER:O	46:Ab:419:VAL:C	2.59	0.43
49:Ae:161:GLU:HA	49:Ae:178:HIS:CD2	2.54	0.43
62:Ag:101:CDL:CA5	62:Ag:101:CDL:H512	2.49	0.43
2:B:74:VAL:O	2:B:78:LEU:HG	2.19	0.43
2:B:199:GLU:O	2:B:200:ALA:C	2.60	0.43
4:D:72:LEU:O	4:D:72:LEU:HD12	2.18	0.43
6:F:157:TYR:CG	6:F:212:LEU:CD1	3.01	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:184:ARG:O	7:G:185:PHE:C	2.60	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
7:G:651:PRO:HG2	19:S:57:GLU:O	2.19	0.43
8:H:61:MET:O	8:H:63:PRO:HD3	2.18	0.43
8:H:231:ILE:O	8:H:231:ILE:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:PHE:O	10:J:68:GLY:C	2.59	0.43
10:J:120:LEU:HA	10:J:123:TRP:CE3	2.53	0.43
12:L:70:THR:O	12:L:75:GLU:HA	2.18	0.43
12:L:217:LEU:CD1	12:L:273:ILE:HG23	2.49	0.43
13:M:73:LEU:HD23	13:M:103:GLN:HE22	1.84	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.19	0.43
14:N:219:LEU:CD2	14:N:230:ILE:HD12	2.49	0.43
15:O:209:VAL:HA	15:O:210:PRO:HD3	1.80	0.43
20:U:73:PRO:HG3	33:h:52:LYS:NZ	2.34	0.43
22:W:87:ILE:O	22:W:88:LYS:C	2.61	0.43
26:a:49:GLU:O	26:a:50:ARG:C	2.60	0.43
34:i:11:ARG:HD2	39:n:154:LEU:O	2.19	0.43
37:l:152:SER:HA	40:o:5:LEU:CD2	2.43	0.43
38:m:5:LYS:HB2	38:m:5:LYS:HE3	1.73	0.43
38:m:34:VAL:O	38:m:34:VAL:HG12	2.16	0.43
55:m:202:3PE:H252	55:m:202:3PE:H381	1.99	0.43
41:p:118:GLY:O	41:p:119:GLU:HB2	2.19	0.43
42:q:41:GLU:HG2	42:q:42:ASP:H	1.84	0.43
45:AA:371:PHE:O	45:AA:375:GLN:HG2	2.19	0.43
47:AC:128:PHE:CE1	47:AC:143:ALA:HA	2.52	0.43
47:AC:133:LEU:HD23	47:AC:133:LEU:HA	1.85	0.43
47:AC:264:THR:HG22	49:Ae:225:ILE:HD11	2.01	0.43
67:AC:402:HEM:HBA1	68:AC:403:UQ6:C4	2.48	0.43
48:AD:242:ILE:CG2	48:AD:243:GLY:N	2.82	0.43
48:AD:247:PRO:HB3	69:AD:401:HEC:CMC	2.33	0.43
49:AE:162:GLY:O	49:AE:227:ASN:OD1	2.36	0.43
45:Aa:74:TRP:CZ3	45:Aa:232:ALA:HB3	2.54	0.43
48:Ad:117:TYR:CD2	48:Ad:121:CYS:SG	3.11	0.43
49:Ae:122:THR:CG2	53:Aj:25:ILE:HG21	2.48	0.43
49:Ae:200:HIS:O	49:Ae:203:ASP:N	2.51	0.43
49:Ae:242:HIS:HD2	49:Ae:251:LYS:HB3	1.83	0.43
52:Ah:42:VAL:O	52:Ah:45:ARG:HB3	2.18	0.43
1:A:55:PHE:CD1	10:J:69:TYR:OH	2.69	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:61:PRO:HB3	7:G:146:PHE:CD2	2.53	0.43
7:G:114:GLU:CD	43:r:53:TYR:HD1	2.26	0.43
7:G:165:ILE:CG2	7:G:169:VAL:HB	2.48	0.43
8:H:142:TYR:CD2	8:H:289:LEU:HD12	2.54	0.43
12:L:296:ASN:HD21	12:L:425:ARG:HH21	1.65	0.43
13:M:1:MET:HB3	13:M:1:MET:HE3	1.73	0.43
13:M:119:TYR:HD1	13:M:160:LEU:HD22	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:39:ALA:O	14:N:42:PRO:HD2	2.19	0.43
14:N:309:ASN:N	15:O:317:ILE:O	2.49	0.43
16:P:134:TRP:CZ2	16:P:311:GLU:HG2	2.54	0.43
16:P:226:VAL:HG21	16:P:277:VAL:CG1	2.49	0.43
20:T:147:TYR:O	20:T:148:ILE:C	2.61	0.43
20:U:115:GLN:O	20:U:116:VAL:C	2.61	0.43
22:W:42:TRP:CE2	66:W:201:EHZ:O1	2.71	0.43
23:X:131:VAL:HG23	23:X:131:VAL:O	2.19	0.43
24:Y:115:MET:O	24:Y:119:TYR:HD2	2.02	0.43
25:Z:87:LEU:HA	25:Z:90:ASN:HB2	2.01	0.43
25:Z:120:LEU:O	25:Z:121:ILE:C	2.61	0.43
26:a:37:ARG:NH1	26:a:59:ARG:HD2	2.34	0.43
34:i:123:PHE:CE2	40:o:61:HIS:CD2	3.06	0.43
40:o:13:ALA:O	40:o:14:SER:C	2.60	0.43
45:AA:96:LEU:HB3	45:AA:156:LEU:HD22	2.01	0.43
45:AA:152:GLN:O	45:AA:153:ASN:HB2	2.17	0.43
45:AA:182:VAL:HG13	45:AA:186:TYR:CZ	2.53	0.43
46:AB:332:ASP:OD1	46:AB:332:ASP:N	2.52	0.43
47:AC:193:ALA:O	47:AC:196:HIS:HB3	2.19	0.43
46:Ab:61:ILE:HG22	46:Ab:220:LEU:HD11	2.01	0.43
46:Ab:236:GLN:HG3	46:Ab:237:PHE:H	1.84	0.43
47:Ac:33:PHE:O	47:Ac:36:LEU:HB2	2.19	0.43
48:Ad:131:ALA:O	48:Ad:134:HIS:N	2.52	0.43
48:Ad:152:VAL:CG1	48:Ad:176:PRO:HG3	2.49	0.43
48:Ad:219:CYS:O	48:Ad:220:GLU:C	2.61	0.43
52:Ah:72:PHE:CE2	52:Ah:76:ARG:NE	2.85	0.43
1:A:56:PHE:HD1	10:J:70:THR:HG1	1.56	0.43
3:C:53:THR:O	3:C:54:HIS:C	2.60	0.43
3:C:120:THR:CG2	3:C:121:ARG:H	2.32	0.43
5:E:145:ASP:O	5:E:146:SER:C	2.62	0.43
7:G:246:ARG:NH1	17:Q:106:ARG:HE	2.17	0.43
7:G:571:HIS:HD2	7:G:572:HIS:NE2	2.09	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
7:G:651:PRO:O	7:G:654:VAL:HG12	2.19	0.43
7:G:664:TYR:OH	19:S:23:LEU:HD11	2.18	0.43
8:H:283:ASP:N	8:H:283:ASP:OD1	2.52	0.43
9:I:71:GLY:O	43:r:15:ALA:HB1	2.19	0.43
10:J:124:LEU:HG	25:Z:137:ASN:HD21	1.84	0.43
12:L:138:PHE:CD1	62:h:201:CDL:H271	2.54	0.43
12:L:145:GLU:HG3	13:M:369:LEU:HD12	2.01	0.43
12:L:253:VAL:HG21	12:L:310:LEU:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:446:ASN:O	12:L:447:ASP:C	2.57	0.43
12:L:493:ILE:O	12:L:496:LEU:HG	2.19	0.43
12:L:526:LEU:HD12	12:L:526:LEU:N	2.34	0.43
13:M:51:ASN:ND2	33:h:136:THR:HG23	2.34	0.43
13:M:63:THR:N	13:M:64:PRO:CD	2.81	0.43
13:M:208:PRO:HG2	13:M:216:LEU:CD1	2.44	0.43
14:N:12:THR:HG22	14:N:39:ALA:HB2	2.00	0.43
14:N:193:ILE:HD11	14:N:269:GLU:CB	2.49	0.43
15:O:75:LYS:HE2	15:O:75:LYS:HB3	1.76	0.43
16:P:92:MET:C	16:P:94:LEU:H	2.26	0.43
18:R:72:VAL:HG11	18:R:77:ILE:CG2	2.49	0.43
21:V:31:THR:O	21:V:32:LEU:C	2.61	0.43
23:X:48:TRP:CD2	27:b:55:VAL:HG22	2.54	0.43
23:X:151:ASN:OD1	33:h:170:GLN:NE2	2.52	0.43
29:d:101:PHE:CZ	33:h:156:VAL:HG22	2.54	0.43
30:e:49:GLY:O	30:e:50:THR:C	2.61	0.43
33:h:90:ASN:OD1	33:h:115:HIS:NE2	2.52	0.43
34:i:111:LEU:CD2	41:p:19:ALA:HB2	2.48	0.43
34:i:123:PHE:CD2	40:o:61:HIS:CD2	3.07	0.43
39:n:81:ILE:HD12	39:n:87:GLY:C	2.44	0.43
40:o:57:ASP:OD2	40:o:59:CYS:HB2	2.19	0.43
41:p:73:ASP:O	41:p:74:ILE:C	2.59	0.43
43:r:5:THR:CG2	43:r:7:VAL:HG12	2.46	0.43
45:AA:92:PHE:CE2	45:AA:161:ILE:HG23	2.53	0.43
45:AA:178:SER:O	45:AA:179:MET:C	2.60	0.43
47:AC:18:PHE:HE1	68:AC:403:UQ6:C8	2.32	0.43
48:AD:237:PHE:CD1	48:AD:242:ILE:HG13	2.54	0.43
48:AD:262:THR:O	48:AD:263:MET:C	2.61	0.43
51:AG:51:PRO:O	51:AG:54:VAL:HB	2.18	0.43
52:AH:43:LYS:O	52:AH:47:ARG:HG3	2.19	0.43
49:AI:72:VAL:N	49:AI:73:PRO:HD2	2.34	0.43
45:Aa:71:VAL:HG21	45:Aa:140:LEU:HD12	2.01	0.43
47:Ac:77:TRP:CZ2	48:Ad:284:HIS:HD2	2.35	0.43
47:Ac:140:PHE:HE2	47:Ac:141:TRP:CH2	2.36	0.43
47:Ac:253:PRO:CG	48:Ad:205:HIS:CG	3.02	0.43
47:Ac:278:TYR:O	47:Ac:279:ALA:C	2.61	0.43
49:Ae:112:GLY:O	49:Ae:116:LEU:HB2	2.19	0.43
49:Ae:167:PHE:HE2	49:Ae:176:VAL:HG21	1.83	0.43
49:Ae:197:ASP:HB3	49:Ae:257:ASN:OD1	2.19	0.43
49:Ae:222:CYS:HB2	49:Ae:236:CYS:SG	2.59	0.43
49:Ae:271:VAL:HG22	49:Ae:273:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:O	1:A:35:ASN:C	2.59	0.43
2:B:171:TYR:CE1	4:D:135:TYR:CD1	3.06	0.43
3:C:127:ILE:H	3:C:127:ILE:HD12	1.83	0.43
3:C:219:VAL:HG21	22:W:113:THR:HG21	2.01	0.43
5:E:138:PRO:HG3	6:F:355:ILE:HD13	1.99	0.43
5:E:144:SER:O	5:E:147:ILE:HB	2.19	0.43
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.43
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.43
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
8:H:114:TYR:HE2	10:J:60:LEU:HD11	1.83	0.43
10:J:50:PHE:O	10:J:54:MET:HG2	2.18	0.43
12:L:193:MET:CE	38:m:125:PHE:CD2	3.02	0.43
12:L:246:LEU:CD1	12:L:247:LEU:N	2.68	0.43
13:M:29:SER:CB	32:g:91:PHE:HD2	2.24	0.43
13:M:100:ILE:O	13:M:103:GLN:HG2	2.19	0.43
14:N:154:ILE:HD12	14:N:155:LEU:N	2.33	0.43
14:N:193:ILE:HD12	14:N:266:ILE:HA	2.01	0.43
14:N:239:ALA:HB1	29:d:47:MET:HG2	2.01	0.43
15:O:224:PRO:O	15:O:228:LYS:NZ	2.52	0.43
15:O:303:GLU:O	15:O:304:VAL:C	2.59	0.43
17:Q:132:GLU:H	17:Q:132:GLU:CD	2.27	0.43
18:R:72:VAL:HG11	18:R:77:ILE:HG22	2.01	0.43
22:W:104:THR:HG22	22:W:108:ARG:NE	2.34	0.43
23:X:18:VAL:CG1	23:X:20:VAL:HG22	2.44	0.43
23:X:130:LYS:HE2	23:X:130:LYS:HB3	1.79	0.43
24:Y:8:PHE:CD1	24:Y:30:LEU:HD21	2.53	0.43
26:a:18:ILE:H	26:a:19:PRO:HD3	1.84	0.43
26:a:48:MET:HG3	26:a:59:ARG:CD	2.48	0.43
42:q:14:VAL:HG13	42:q:23:LEU:HG	2.01	0.43
46:AB:195:TYR:OH	46:Ab:261:GLN:CG	2.66	0.43
47:AC:33:PHE:O	47:AC:36:LEU:HB2	2.19	0.43
48:AD:242:ILE:HG12	48:AD:244:MET:CB	2.49	0.43
52:AH:55:VAL:CG2	52:AH:65:CYS:HB2	2.49	0.43
52:AH:85:PHE:O	52:AH:88:LEU:HB2	2.18	0.43
48:Ad:183:GLU:CA	48:Ad:186:ARG:HH21	2.32	0.43
3:C:184:ARG:NH2	4:D:112:HIS:HE2	2.17	0.42
4:D:218:SER:OG	4:D:219:GLY:N	2.51	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:LEU:HG	6:F:46:TYR:CE1	2.54	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.58	0.42
7:G:304:GLU:CG	7:G:305:PRO:HD2	2.47	0.42
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.42
8:H:102:ILE:HG22	8:H:150:LEU:HD11	2.00	0.42
8:H:249:ILE:HG12	23:X:99:HIS:CE1	2.54	0.42
8:H:307:LEU:HD23	8:H:310:PHE:HZ	1.84	0.42
8:H:309:ILE:HG22	27:b:39:THR:HG23	2.01	0.42
11:K:50:ASN:C	11:K:50:ASN:OD1	2.62	0.42
12:L:60:GLU:N	12:L:60:GLU:OE2	2.52	0.42
12:L:335:PHE:O	12:L:339:LEU:HD13	2.18	0.42
13:M:68:LEU:HD23	13:M:234:ILE:CD1	2.49	0.42
13:M:367:LEU:C	13:M:367:LEU:HD12	2.44	0.42
14:N:105:LYS:HE3	14:N:105:LYS:HB3	1.79	0.42
14:N:174:GLN:O	14:N:178:ILE:HG13	2.18	0.42
14:N:219:LEU:HD23	14:N:230:ILE:HD12	2.01	0.42
15:O:243:LYS:HB2	15:O:243:LYS:HE2	1.64	0.42
16:P:72:HIS:O	16:P:73:LEU:C	2.61	0.42
20:U:142:GLN:O	20:U:143:GLU:C	2.60	0.42
22:W:98:LYS:HD3	22:W:100:TRP:CE2	2.53	0.42
33:h:59:PRO:O	33:h:61:LEU:HG	2.19	0.42
33:h:129:PRO:HD2	33:h:130:GLU:OE1	2.18	0.42
33:h:163:ARG:CG	33:h:165:ASP:HB2	2.33	0.42
34:i:93:LYS:HD3	55:i:201:3PE:C12	2.46	0.42
34:i:93:LYS:HE3	34:i:96:THR:HG21	2.01	0.42
36:k:28:TRP:CE3	36:k:60:MET:HG2	2.54	0.42
45:AA:68:THR:HG22	45:AA:136:LEU:HD23	2.00	0.42
46:AB:286:PHE:CD1	46:AB:427:ALA:HB1	2.54	0.42
48:AD:126:SER:HB3	48:AD:177:LYS:HA	2.01	0.42
48:AD:135:LEU:CA	48:AD:276:TRP:HH2	2.20	0.42
48:AD:159:ASN:CB	48:AD:166:MET:HG3	2.48	0.42
48:AD:227:LEU:HD21	48:AD:241:ALA:HA	2.00	0.42
49:AE:249:ILE:HG12	49:AE:254:ALA:HB3	2.01	0.42
52:AH:46:GLU:O	52:AH:50:LEU:HG	2.19	0.42
45:Aa:172:MET:HA	45:Aa:175:ASN:CG	2.44	0.42
45:Aa:410:CYS:O	45:Aa:413:ILE:N	2.52	0.42
46:Ab:177:LEU:HD21	46:Ab:272:VAL:HG13	2.01	0.42
46:Ab:286:PHE:CD1	46:Ab:427:ALA:HB1	2.54	0.42
52:Ah:24:LEU:HD12	52:Ah:25:VAL:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:72:PHE:CE2	52:Ah:76:ARG:HD3	2.49	0.42
52:Ah:79:CYS:O	52:Ah:82:HIS:N	2.46	0.42
53:Aj:23:LEU:CD1	54:Ak:27:VAL:HG22	2.48	0.42
2:B:108:ALA:HB2	2:B:114:MET:HE3	2.01	0.42
2:B:122:ARG:HB3	57:B:302:UQ1:H72	1.98	0.42
4:D:159:LEU:HG	4:D:391:VAL:HG12	2.01	0.42
5:E:78:VAL:HG21	6:F:218:GLY:O	2.20	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:304:GLU:HB3	7:G:316:TYR:HD1	1.83	0.42
7:G:480:ALA:O	7:G:481:LEU:C	2.63	0.42
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.18	0.42
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.54	0.42
8:H:231:ILE:HG23	8:H:270:PHE:CD2	2.54	0.42
12:L:5:THR:O	12:L:6:THR:C	2.62	0.42
12:L:38:THR:O	12:L:41:LYS:HB3	2.19	0.42
12:L:214:MET:HG2	55:m:201:3PE:H291	2.01	0.42
12:L:591:PHE:HE1	14:N:113:PHE:HD2	1.66	0.42
13:M:72:LEU:HD12	13:M:234:ILE:HG12	2.01	0.42
13:M:214:LEU:C	13:M:217:PRO:HD2	2.44	0.42
14:N:170:LEU:HD12	14:N:292:PHE:CD2	2.54	0.42
15:O:58:ARG:O	15:O:157:VAL:N	2.45	0.42
15:O:63:ASP:OD2	15:O:165:SER:HB2	2.20	0.42
15:O:117:PHE:HD1	15:O:128:SER:CA	2.31	0.42
15:O:310:ILE:HG23	15:O:312:VAL:HG23	2.01	0.42
15:O:323:GLN:HB2	32:g:56:ASP:OD1	2.18	0.42
16:P:271:TYR:CA	16:P:375:VAL:HG22	2.50	0.42
16:P:309:PRO:HG2	16:P:310:PHE:CD2	2.54	0.42
17:Q:69:GLU:O	17:Q:72:ILE:CG2	2.62	0.42
20:T:105:MET:HE1	20:T:115:GLN:HG3	1.99	0.42
20:U:74:LEU:HD11	20:U:82:ARG:NH1	2.33	0.42
23:X:119:ARG:NH1	25:Z:63:GLU:OE2	2.52	0.42
27:b:31:ILE:O	27:b:35:ILE:HG22	2.18	0.42
34:i:22:TRP:O	34:i:26:GLN:HG2	2.19	0.42
34:i:81:PHE:O	34:i:82:VAL:C	2.60	0.42
40:o:46:MET:HE2	40:o:60:ALA:HB3	2.00	0.42
47:AC:113:TRP:O	47:AC:117:VAL:N	2.48	0.42
48:AD:221:PRO:HB2	48:AD:225:VAL:CG1	2.44	0.42
48:AD:221:PRO:HB3	48:AD:233:PHE:CG	2.54	0.42
48:AD:227:LEU:CD2	48:AD:241:ALA:HA	2.48	0.42
50:AF:77:PRO:O	50:AF:78:LYS:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AH:65:CYS:HA	52:AH:68:GLU:OE1	2.18	0.42
46:Ab:161:ASP:C	46:Ab:163:ALA:N	2.75	0.42
46:Ab:378:LEU:HD23	46:Ab:416:ILE:CG2	2.49	0.42
47:Ac:190:ALA:HB1	68:Ac:405:UQ6:C21	2.49	0.42
48:Ad:99:ARG:HA	48:Ad:99:ARG:HD3	1.94	0.42
48:Ad:186:ARG:HA	48:Ad:191:GLY:CA	2.49	0.42
48:Ad:270:VAL:HG13	48:Ad:271:ALA:N	2.34	0.42
49:Ae:205:VAL:CG1	49:Ae:211:VAL:HG23	2.49	0.42
49:Ae:243:TYR:CD2	49:Ae:258:LEU:HG	2.54	0.42
4:D:96:ARG:HB2	4:D:112:HIS:HB2	2.01	0.42
4:D:97:LEU:O	4:D:97:LEU:CG	2.52	0.42
4:D:141:TYR:HB2	4:D:222:MET:CE	2.49	0.42
4:D:236:LEU:HD22	4:D:240:LEU:CD2	2.41	0.42
6:F:41:ILE:HD13	6:F:250:VAL:HG12	2.02	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
6:F:363:ILE:HG23	6:F:364:VAL:N	2.33	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.42
8:H:45:ILE:CD1	26:a:11:ILE:CD1	2.91	0.42
8:H:85:LEU:CD2	8:H:108:THR:HB	2.49	0.42
8:H:179:TRP:NE1	25:Z:43:LEU:HD12	2.34	0.42
8:H:195:ARG:HG3	8:H:196:ALA:N	2.34	0.42
8:H:303:TRP:HA	27:b:29:ALA:HB2	2.01	0.42
9:I:135:ARG:HD2	18:R:61:ILE:CG1	2.49	0.42
12:L:272:PHE:O	12:L:275:THR:HG22	2.19	0.42
12:L:275:THR:HG23	12:L:276:THR:N	2.34	0.42
12:L:444:ASN:HB2	35:j:40:ILE:HG21	2.01	0.42
12:L:489:THR:HG23	12:L:490:ALA:N	2.34	0.42
12:L:591:PHE:O	12:L:595:ILE:HG13	2.19	0.42
13:M:14:LEU:HD21	13:M:26:ASN:CB	2.50	0.42
14:N:80:GLN:O	14:N:81:LEU:HG	2.19	0.42
15:O:170:LEU:HD21	15:O:184:VAL:HG13	2.00	0.42
15:O:209:VAL:CG1	15:O:260:SER:HB2	2.31	0.42
15:O:351:TRP:CB	28:c:39:PRO:HG3	2.45	0.42
16:P:144:VAL:HG23	16:P:145:PHE:CD2	2.54	0.42
17:Q:130:ALA:O	17:Q:131:LYS:C	2.62	0.42
22:W:23:ILE:HD12	22:W:80:ARG:O	2.19	0.42
22:W:69:MET:O	22:W:71:MET:N	2.53	0.42
22:W:87:ILE:CG2	22:W:91:MET:HE3	2.45	0.42
24:Y:68:ILE:HG22	24:Y:102:THR:OG1	2.19	0.42
25:Z:143:TYR:O	25:Z:144:THR:HB	2.14	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:14:VAL:HA	26:a:17:VAL:HG22	2.00	0.42
30:e:89:GLU:HB2	30:e:91:LYS:HG2	2.00	0.42
37:l:57:MET:HG2	37:l:104:PRO:CG	2.49	0.42
39:n:45:ARG:O	39:n:46:ALA:C	2.61	0.42
39:n:85:SER:O	39:n:86:PRO:C	2.60	0.42
39:n:163:LEU:HA	39:n:164:PRO:HD2	1.75	0.42
41:p:43:TRP:NE1	41:p:47:LEU:HD11	2.33	0.42
47:AC:47:THR:CB	47:AC:83:HIS:HD1	2.32	0.42
47:AC:177:ARG:NH2	49:Ae:140:MET:O	2.51	0.42
48:AD:116:VAL:HG11	48:AD:270:VAL:HB	2.02	0.42
48:AD:242:ILE:C	48:AD:244:MET:H	2.27	0.42
45:Aa:281:ALA:HA	51:Ag:10:ARG:HH12	1.84	0.42
46:Ab:346:ALA:O	46:Ab:347:ALA:C	2.62	0.42
68:Ac:405:UQ6:H151	68:Ac:405:UQ6:H172	1.79	0.42
49:Ae:122:THR:O	49:Ae:123:VAL:C	2.61	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.66	0.42
3:C:227:GLN:NE2	9:I:129:THR:HG21	2.34	0.42
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.84	0.42
4:D:234:GLN:NE2	9:I:212:ARG:HB3	2.35	0.42
4:D:261:MET:CE	9:I:73:THR:CG2	2.90	0.42
5:E:73:HIS:HE1	17:Q:166:TRP:CG	2.38	0.42
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.85	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.28	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.20	0.42
8:H:84:SER:C	8:H:86:TRP:H	2.27	0.42
8:H:190:LEU:HG	8:H:196:ALA:HB3	2.01	0.42
10:J:44:LEU:HD13	10:J:49:SER:HA	2.01	0.42
12:L:81:LYS:HD3	12:L:262:ARG:HH11	1.83	0.42
13:M:200:MET:CE	13:M:247:SER:HB2	2.46	0.42
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.42
15:O:121:PRO:HB3	15:O:178:TYR:HE1	1.83	0.42
15:O:297:LEU:C	15:O:297:LEU:HD23	2.44	0.42
16:P:140:ASP:O	16:P:141:PHE:C	2.62	0.42
19:S:35:ASP:O	19:S:36:PHE:C	2.60	0.42
25:Z:30:LEU:HD12	25:Z:30:LEU:H	1.84	0.42
30:e:82:GLN:O	30:e:86:LEU:HG	2.20	0.42
30:e:101:ARG:HE	30:e:104:PRO:HD2	1.83	0.42
41:p:6:ASP:C	41:p:8:ASP:H	2.27	0.42
41:p:36:ALA:O	41:p:37:TYR:C	2.60	0.42
45:AA:99:LYS:HG3	45:AA:160:GLN:CG	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:396:ILE:HG12	46:AB:406:TYR:HE1	1.85	0.42
47:AC:171:ASP:CG	47:AC:172:LYS:N	2.76	0.42
47:AC:208:PRO:HB2	47:AC:316:MET:HE3	2.01	0.42
47:AC:345:HIS:O	51:AG:67:PHE:HD1	2.02	0.42
47:AC:376:MET:CE	50:AF:18:ARG:HG2	2.49	0.42
48:AD:214:LEU:CD1	48:AD:237:PHE:HB2	2.49	0.42
49:Ae:271:VAL:O	49:Ae:271:VAL:HG13	2.19	0.42
4:D:264:ASN:HB2	9:I:65:GLU:OE2	2.19	0.42
4:D:385:TYR:HD2	9:I:122:ILE:CD1	2.31	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
6:F:257:ARG:HG2	6:F:258:GLY:H	1.84	0.42
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.42
7:G:65:TYR:HB2	7:G:92:CYS:SG	2.59	0.42
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.50	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
7:G:670:GLU:HB2	19:S:42:VAL:HG23	2.01	0.42
8:H:100:LEU:HB3	10:J:53:LEU:HD12	2.01	0.42
8:H:111:LEU:HD23	10:J:60:LEU:HD12	2.01	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.01	0.42
12:L:21:ILE:HG23	12:L:27:ILE:CG2	2.50	0.42
12:L:189:PHE:CZ	12:L:212:PRO:HB2	2.55	0.42
13:M:206:LYS:HA	13:M:215:TRP:CZ2	2.54	0.42
13:M:293:HIS:O	13:M:294:MET:HE2	2.20	0.42
13:M:347:GLY:O	13:M:348:LEU:C	2.63	0.42
14:N:80:GLN:O	14:N:80:GLN:HG2	2.19	0.42
14:N:241:LEU:HG	14:N:301:SER:OG	2.19	0.42
15:O:180:ARG:HH22	32:g:51:MET:HE3	1.84	0.42
16:P:75:ARG:C	16:P:77:GLY:H	2.28	0.42
18:R:43:TYR:C	18:R:45:ARG:H	2.26	0.42
20:T:104:PHE:O	20:T:110:LEU:HB2	2.20	0.42
21:V:62:GLU:OE2	21:V:64:ASP:HB3	2.19	0.42
24:Y:141:PRO:HB2	33:h:161:ARG:NE	2.35	0.42
25:Z:111:PHE:CD1	25:Z:117:VAL:HG21	2.55	0.42
32:g:119:GLU:OE1	32:g:122:ARG:NH1	2.53	0.42
33:h:111:GLU:O	41:p:63:TYR:HA	2.18	0.42
38:m:15:PRO:HG2	38:m:18:LEU:HB2	2.01	0.42
38:m:41:ALA:HA	39:n:152:GLU:HG2	2.01	0.42
40:o:53:LEU:HD11	41:p:122:GLN:HG3	2.02	0.42
45:AA:193:GLN:NE2	49:AE:85:VAL:HG11	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:141:TRP:CD1	47:AC:265:PRO:CD	2.98	0.42
47:AC:256:TYR:CZ	48:AD:202:ARG:HD3	2.54	0.42
48:AD:220:GLU:O	48:AD:222:PRO:HD3	2.19	0.42
48:AD:232:TYR:HB2	48:AD:242:ILE:CG2	2.49	0.42
48:AD:247:PRO:O	48:AD:252:VAL:HG21	2.19	0.42
51:AG:46:ILE:HD12	51:AG:49:VAL:HB	2.02	0.42
46:Ab:38:LEU:CG	46:Ab:396:ILE:HD13	2.50	0.42
46:Ab:166:PHE:HE1	46:Ab:191:TYR:CD2	2.38	0.42
47:Ac:181:PHE:HA	47:Ac:184:ILE:HG22	2.00	0.42
49:Ae:115:TYR:HB3	53:Aj:21:PHE:HE1	1.85	0.42
49:Ae:271:VAL:O	49:Ae:273:VAL:HG23	2.18	0.42
55:A:201:3PE:H252	55:A:201:3PE:H281	1.80	0.42
2:B:87:ARG:HH12	58:B:303:PC1:P	2.43	0.42
2:B:94:THR:H	57:B:302:UQ1:C11	2.19	0.42
2:B:202:LEU:HD21	9:I:86:TYR:CG	2.53	0.42
58:B:303:PC1:H142	42:q:77:VAL:HG12	2.02	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:110:PRO:CB	6:F:152:ARG:HE	2.19	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.42
7:G:480:ALA:O	7:G:483:ARG:HG3	2.20	0.42
13:M:77:LEU:O	13:M:81:GLN:HG3	2.19	0.42
13:M:118:PHE:HE2	13:M:203:PHE:CE1	2.37	0.42
13:M:230:ILE:HG23	13:M:235:LEU:HD11	2.01	0.42
14:N:109:ALA:HB3	14:N:110:PRO:HD3	2.00	0.42
14:N:148:LEU:HD12	14:N:148:LEU:N	2.34	0.42
15:O:242:LYS:HE2	15:O:242:LYS:HB2	1.92	0.42
17:Q:98:LYS:NZ	17:Q:127:THR:OG1	2.52	0.42
17:Q:99:MET:HB2	17:Q:128:PHE:HE2	1.84	0.42
17:Q:126:LEU:CD1	17:Q:137:PHE:CE2	3.03	0.42
20:T:107:ASP:C	20:T:108:LEU:HD12	2.45	0.42
23:X:41:LYS:HB3	23:X:131:VAL:HG11	2.02	0.42
25:Z:12:PRO:CD	25:Z:16:TYR:CZ	3.02	0.42
25:Z:93:GLU:HG3	30:e:97:HIS:HD1	1.78	0.42
26:a:58:ASN:O	26:a:59:ARG:C	2.61	0.42
27:b:69:HIS:H	27:b:72:ASP:CG	2.28	0.42
28:c:65:ASP:OD2	29:d:77:LYS:NZ	2.50	0.42
32:g:112:MET:HE1	41:p:94:ARG:HG3	2.02	0.42
32:g:147:LEU:O	32:g:148:PRO:C	2.62	0.42
34:i:32:GLU:OE2	39:n:118:TYR:N	2.52	0.42
34:i:94:PRO:HG3	41:p:10:TYR:CD2	2.52	0.42
35:j:96:GLU:HG2	35:j:97:LEU:HD23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:38:PRO:C	38:m:75:ASN:HD21	2.25	0.42
37:l:62:TYR:CE2	37:l:64:PRO:HG3	2.55	0.42
37:l:120:SER:O	37:l:121:PRO:C	2.60	0.42
39:n:139:GLN:HA	39:n:142:GLU:HG2	2.01	0.42
40:o:3:ALA:O	40:o:4:HIS:C	2.61	0.42
44:s:87:LEU:CB	44:s:91:ARG:HH12	2.31	0.42
45:AA:187:LEU:O	45:AA:188:HIS:C	2.62	0.42
46:AB:39:GLU:OE2	46:AB:227:HIS:HB2	2.19	0.42
46:AB:319:GLN:O	46:AB:320:PRO:C	2.62	0.42
48:AD:233:PHE:CD1	48:AD:240:GLN:HB3	2.54	0.42
49:AE:222:CYS:HB2	49:AE:236:CYS:SG	2.59	0.42
53:AJ:20:THR:O	53:AJ:24:THR:HG22	2.19	0.42
53:AJ:23:LEU:HD21	54:AK:23:MET:SD	2.52	0.42
46:Ab:61:ILE:HA	46:Ab:222:GLY:HA2	2.00	0.42
46:Ab:147:ARG:HD3	46:Ab:149:TRP:CZ2	2.54	0.42
47:Ac:215:ALA:HB2	50:Af:60:MET:HE3	2.01	0.42
48:Ad:299:LEU:HD12	71:Ad:402:3PH:H371	1.96	0.42
49:Ae:271:VAL:HG22	49:Ae:273:VAL:CG2	2.49	0.42
50:Af:102:ARG:HA	50:Af:105:ARG:CZ	2.49	0.42
52:Ah:33:GLU:O	52:Ah:34:HIS:C	2.62	0.42
53:Aj:43:ILE:O	53:Aj:47:ILE:HG13	2.20	0.42
2:B:79:ASP:OD1	2:B:79:ASP:C	2.62	0.42
2:B:92:PRO:CB	2:B:130:VAL:CG1	2.98	0.42
2:B:140:LYS:CD	4:D:115:LEU:HD23	2.49	0.42
2:B:193:GLY:HA2	9:I:154:TYR:CE1	2.55	0.42
2:B:224:ARG:HH21	16:P:85:ARG:NH1	2.17	0.42
4:D:266:ARG:NH2	9:I:59:ARG:O	2.52	0.42
6:F:44:ASN:O	6:F:45:LEU:C	2.62	0.42
6:F:315:LEU:HD22	6:F:363:ILE:HD13	2.02	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
10:J:84:SER:HB3	10:J:87:LEU:HG	2.02	0.42
12:L:52:LEU:HB2	41:p:30:ILE:HD11	2.01	0.42
12:L:220:ALA:HB2	12:L:260:LEU:CD1	2.49	0.42
12:L:405:ASN:HB2	12:L:408:ALA:HB3	2.01	0.42
12:L:534:HIS:O	12:L:538:PRO:CG	2.60	0.42
12:L:568:THR:O	12:L:569:LEU:C	2.61	0.42
13:M:207:MET:HE3	13:M:240:SER:HB2	2.02	0.42
13:M:210:TYR:O	13:M:213:HIS:HD2	2.02	0.42
14:N:226:THR:HG22	14:N:228:ASN:N	2.34	0.42
14:N:331:ILE:HG23	14:N:335:MET:HE3	2.01	0.42
18:R:31:ILE:CG2	18:R:35:GLY:HA2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:32:THR:C	18:R:34:THR:N	2.76	0.42
19:S:16:LEU:HD11	19:S:19:ILE:HG12	2.02	0.42
20:U:72:PRO:CD	35:j:42:PRO:CG	2.96	0.42
21:V:11:LEU:H	21:V:11:LEU:HD12	1.84	0.42
21:V:24:LEU:HD23	21:V:24:LEU:HA	1.90	0.42
22:W:59:VAL:HG12	22:W:63:ARG:HD2	2.01	0.42
23:X:32:TYR:CE1	23:X:67:ALA:HB2	2.55	0.42
24:Y:45:LEU:O	24:Y:46:ASN:C	2.62	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CD2	2.55	0.42
33:h:188:ASP:O	33:h:189:ASN:C	2.63	0.42
37:l:167:TYR:CG	37:l:178:PRO:HG3	2.55	0.42
39:n:110:SER:O	39:n:113:ALA:HB3	2.20	0.42
39:n:132:SER:O	39:n:133:TRP:C	2.62	0.42
41:p:6:ASP:O	41:p:7:LYS:C	2.63	0.42
45:AA:112:GLU:HB3	45:AA:142:LYS:NZ	2.34	0.42
47:AC:141:TRP:HA	47:AC:141:TRP:CE3	2.54	0.42
48:AD:186:ARG:HD2	48:AD:191:GLY:O	2.20	0.42
52:AH:58:ARG:HB3	52:AH:61:THR:CG2	2.48	0.42
54:AK:23:MET:HG3	54:AK:27:VAL:HG23	2.00	0.42
45:Aa:114:GLU:OE1	46:Ab:298:HIS:ND1	2.52	0.42
45:Aa:136:LEU:HD22	46:Ab:383:LEU:HD12	2.02	0.42
45:Aa:276:ARG:O	51:Ag:16:SER:N	2.53	0.42
46:Ab:103:ILE:HB	49:Ai:70:LEU:CD2	2.50	0.42
49:Ae:83:VAL:HG22	49:Ae:84:LYS:N	2.34	0.42
49:Ae:175:PHE:HE2	49:Ae:215:GLY:HA3	1.85	0.42
52:Ah:73:LEU:CD2	52:Ah:76:ARG:HH21	2.33	0.42
52:Ah:73:LEU:HD22	52:Ah:76:ARG:HH21	1.83	0.42
49:Ai:72:VAL:N	49:Ai:73:PRO:HD2	2.33	0.42
1:A:5:THR:OG1	8:H:2:PHE:HE2	2.02	0.42
1:A:13:LEU:O	1:A:17:LEU:HG	2.19	0.42
5:E:190:ASN:HB3	5:E:192:TYR:CE1	2.55	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:21:THR:HG21	61:H:400:UQ9:H15A	2.02	0.42
8:H:102:ILE:CG1	8:H:162:LEU:HD23	2.50	0.42
8:H:231:ILE:HG23	8:H:270:PHE:HD2	1.83	0.42
9:I:79:ARG:HH21	43:r:20:LEU:CD1	2.33	0.42
9:I:128:ILE:HG22	9:I:130:ILE:HG23	2.01	0.42
9:I:182:GLU:HA	42:q:124:TYR:HD2	1.84	0.42
11:K:59:ILE:HB	11:K:60:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:66:TRP:CZ3	62:h:201:CDL:H181	2.54	0.42
12:L:226:GLN:OE1	12:L:281:GLY:HA2	2.20	0.42
12:L:277:MET:CG	12:L:318:GLY:CA	2.98	0.42
12:L:346:ILE:HG21	12:L:362:ILE:HD11	2.02	0.42
12:L:364:LYS:CE	36:k:67:ILE:HD11	2.41	0.42
12:L:396:ILE:HD13	12:L:396:ILE:HA	1.89	0.42
13:M:123:GLU:OE2	13:M:154:LEU:HD21	2.20	0.42
13:M:191:SER:O	13:M:194:LEU:HB2	2.20	0.42
13:M:428:PRO:HD3	39:n:106:TYR:CG	2.55	0.42
14:N:154:ILE:HD11	14:N:155:LEU:HG	2.02	0.42
14:N:340:ALA:N	14:N:341:PRO:CD	2.83	0.42
16:P:110:ALA:HB1	16:P:148:ILE:CD1	2.48	0.42
16:P:220:TYR:HA	16:P:223:PHE:CE1	2.55	0.42
19:S:32:GLY:HA2	19:S:35:ASP:CG	2.44	0.42
20:T:90:TYR:HD2	20:T:93:ILE:CB	2.32	0.42
20:U:87:LEU:HD12	20:U:98:LEU:HD21	2.00	0.42
24:Y:76:THR:CG2	24:Y:92:TYR:HA	2.48	0.42
24:Y:91:ASN:HD22	24:Y:91:ASN:HA	1.71	0.42
29:d:114:GLU:O	29:d:114:GLU:HG2	2.18	0.42
30:e:36:PHE:O	30:e:37:GLU:C	2.62	0.42
35:j:44:TYR:CE2	35:j:45:ARG:HG3	2.54	0.42
35:j:99:ILE:CD1	40:o:107:ARG:HB2	2.50	0.42
38:m:91:ALA:HB2	55:m:203:3PE:H272	2.00	0.42
39:n:100:PRO:HB2	39:n:102:TRP:NE1	2.35	0.42
45:AA:62:GLU:CD	45:AA:423:ARG:HH12	2.23	0.42
45:AA:62:GLU:HB2	45:AA:413:ILE:HD11	2.02	0.42
45:AA:401:SER:O	45:AA:404:ASP:N	2.51	0.42
46:AB:378:LEU:HD23	46:AB:416:ILE:CG2	2.49	0.42
47:AC:195:VAL:HG12	47:AC:199:PHE:CD2	2.55	0.42
48:AD:109:SER:O	48:AD:110:ILE:C	2.62	0.42
48:AD:110:ILE:HD13	48:AD:276:TRP:HB2	2.01	0.42
48:AD:200:ILE:HG23	48:AD:201:VAL:N	2.35	0.42
48:AD:214:LEU:O	48:AD:234:ASN:ND2	2.52	0.42
54:AK:31:GLY:O	54:AK:34:TRP:HE3	2.02	0.42
46:Ab:60:ARG:CG	46:Ab:393:LEU:HD13	2.50	0.42
46:Ab:66:LYS:HB3	46:Ab:71:TYR:CE2	2.55	0.42
46:Ab:180:VAL:CG2	46:Ab:258:ILE:HG23	2.49	0.42
46:Ab:225:VAL:HG22	46:Ab:226:SER:N	2.35	0.42
47:Ac:71:ARG:NH2	48:Ad:199:TYR:CE1	2.86	0.42
53:Aj:34:ARG:CZ	53:Aj:38:GLN:HB2	2.50	0.42
1:A:52:SER:CB	1:A:55:PHE:CE2	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:LEU:CD2	4:D:391:VAL:HG12	2.48	0.42
4:D:184:ILE:HD12	4:D:210:MET:HE1	2.02	0.42
7:G:114:GLU:OE2	43:r:54:TYR:N	2.51	0.42
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.42
7:G:545:LEU:HD21	7:G:547:LEU:CD2	2.50	0.42
8:H:118:TRP:CE2	10:J:30:LEU:HD22	2.54	0.42
8:H:308:PRO:O	8:H:312:ALA:N	2.53	0.42
12:L:51:LEU:HA	12:L:87:ILE:HD12	2.02	0.42
12:L:463:PHE:CE2	35:j:64:LEU:HD21	2.54	0.42
13:M:216:LEU:CG	13:M:220:HIS:CE1	2.88	0.42
14:N:180:ALA:O	14:N:184:ILE:HG13	2.20	0.42
14:N:315:THR:O	14:N:316:HIS:C	2.61	0.42
14:N:338:PRO:HA	23:X:170:TRP:HZ3	1.84	0.42
15:O:195:LEU:N	15:O:196:PRO:HD2	2.35	0.42
15:O:272:ASP:HA	15:O:275:TYR:HD2	1.85	0.42
16:P:96:LEU:HD12	16:P:97:MET:CA	2.49	0.42
16:P:230:SER:C	16:P:232:GLY:N	2.77	0.42
20:T:85:TYR:CZ	20:T:89:LEU:HD11	2.55	0.42
20:T:90:TYR:OH	20:T:92:LYS:HD3	2.20	0.42
21:V:37:HIS:HB2	21:V:95:LEU:HD11	2.01	0.42
23:X:147:ARG:NH1	30:e:39:GLU:HG3	2.31	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CE2	2.54	0.42
55:d:201:3PE:O31	55:d:201:3PE:H342	2.19	0.42
40:o:104:ARG:O	40:o:108:LEU:HG	2.20	0.42
41:p:9:VAL:O	41:p:109:ARG:NH2	2.51	0.42
45:AA:279:ASP:OD1	51:AG:12:ARG:NE	2.49	0.42
45:AA:397:ASN:ND2	46:AB:126:ILE:HD11	2.31	0.42
46:AB:163:ALA:O	46:AB:164:VAL:C	2.62	0.42
47:AC:70:CYS:SG	47:AC:80:ARG:HD3	2.59	0.42
47:AC:137:GLN:HB3	47:AC:257:MET:HE3	2.02	0.42
68:AC:403:UQ6:H1M1	68:AC:403:UQ6:H71	1.91	0.42
48:AD:159:ASN:CB	48:AD:166:MET:HE2	2.47	0.42
48:AD:189:ASN:CG	48:AD:194:PRO:HG3	2.45	0.42
52:AH:43:LYS:O	52:AH:46:GLU:HB2	2.20	0.42
46:Ab:61:ILE:CG2	46:Ab:220:LEU:HD11	2.49	0.42
46:Ab:218:MET:CE	46:Ab:238:LEU:HD22	2.50	0.42
46:Ab:396:ILE:HG12	46:Ab:406:TYR:HE1	1.85	0.42
47:Ac:171:ASP:CG	47:Ac:172:LYS:N	2.77	0.42
48:Ad:253:LEU:C	48:Ad:253:LEU:HD12	2.44	0.42
48:Ad:264:SER:O	48:Ad:267:ALA:HB3	2.20	0.42
49:Ae:249:ILE:HG22	49:Ae:257:ASN:OD1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Af:95:LEU:O	50:Af:96:LYS:C	2.62	0.42
53:Aj:30:LEU:CD1	54:Ak:34:TRP:HB2	2.47	0.42
1:A:78:ALA:O	1:A:87:MET:SD	2.78	0.42
2:B:141:MET:CE	4:D:115:LEU:HB3	2.37	0.42
4:D:35:ARG:HE	32:g:59:PRO:HD3	1.85	0.42
4:D:37:TRP:CE3	4:D:37:TRP:O	2.73	0.42
5:E:99:LYS:O	5:E:99:LYS:HD3	2.20	0.42
5:E:129:TYR:HA	5:E:188:ASN:ND2	2.31	0.42
5:E:174:GLU:O	5:E:175:CYS:C	2.63	0.42
6:F:261:TRP:CE3	6:F:262:PHE:CD1	3.05	0.42
8:H:107:ALA:HB1	10:J:56:PHE:CD2	2.55	0.42
8:H:201:THR:O	8:H:202:GLU:C	2.62	0.42
10:J:133:VAL:HG12	26:a:41:VAL:CB	2.49	0.42
10:J:165:ILE:O	10:J:169:ILE:HG12	2.20	0.42
11:K:4:THR:HA	11:K:7:ASN:ND2	2.35	0.42
12:L:117:PHE:HZ	12:L:242:PRO:HG2	1.85	0.42
12:L:286:LEU:HG	12:L:290:ILE:HD11	2.01	0.42
12:L:365:ILE:O	35:j:50:LEU:HD21	2.19	0.42
13:M:181:PHE:CZ	41:p:86:TYR:HD1	2.38	0.42
13:M:258:ALA:O	13:M:259:TYR:C	2.62	0.42
13:M:388:TRP:CD1	38:m:109:ARG:HD2	2.55	0.42
14:N:108:LEU:HD22	14:N:191:LEU:HD22	2.02	0.42
14:N:148:LEU:N	14:N:148:LEU:CD1	2.83	0.42
14:N:202:LEU:HD11	30:e:3:PHE:CE1	2.55	0.42
14:N:215:MET:SD	14:N:244:ILE:CD1	3.08	0.42
14:N:308:ASN:C	15:O:319:ILE:HG23	2.44	0.42
15:O:48:LYS:O	15:O:52:LYS:HE3	2.20	0.42
16:P:262:THR:HG22	16:P:263:PHE:N	2.35	0.42
19:S:79:LEU:HA	19:S:82:LEU:CG	2.46	0.42
20:U:128:PHE:HZ	20:U:148:ILE:CD1	2.33	0.42
21:V:20:PRO:HG3	21:V:65:VAL:HG22	2.02	0.42
23:X:131:VAL:HG22	27:b:56:PRO:HB2	2.02	0.42
23:X:132:LYS:CB	27:b:59:ASP:HB3	2.48	0.42
23:X:147:ARG:HH12	30:e:39:GLU:HA	1.85	0.42
29:d:24:PRO:HD2	29:d:73:TYR:CE2	2.55	0.42
33:h:55:PHE:HE1	33:h:57:VAL:HA	1.85	0.42
35:j:99:ILE:HA	40:o:108:LEU:CD2	2.50	0.42
37:l:159:LYS:HE3	37:l:161:TYR:HE1	1.85	0.42
37:l:184:TYR:HD1	40:o:35:LYS:C	2.27	0.42
38:m:8:PRO:HD3	38:m:14:LEU:HD13	2.02	0.42
45:AA:79:SER:HB3	45:AA:201:VAL:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:10:LEU:CA	47:Ac:198:LEU:HD21	2.49	0.42
47:AC:119:LEU:CD2	47:AC:192:LEU:HB2	2.50	0.42
47:AC:130:GLY:HA3	67:AC:401:HEM:C2D	2.55	0.42
47:AC:169:SER:O	47:AC:170:VAL:C	2.62	0.42
48:AD:249:TYR:O	48:AD:250:THR:C	2.63	0.42
49:AE:93:ARG:O	49:AE:94:ALA:C	2.62	0.42
50:AF:35:ASP:HB3	50:AF:91:LEU:HB3	2.01	0.42
50:AF:50:ARG:O	50:AF:51:LEU:C	2.63	0.42
51:AG:46:ILE:C	51:AG:48:ARG:H	2.28	0.42
52:AH:28:LEU:O	52:AH:32:ARG:HG3	2.20	0.42
45:Aa:119:HIS:ND1	46:Ab:298:HIS:HA	2.35	0.42
45:Aa:186:TYR:OH	49:Ae:80:HIS:HB2	2.19	0.42
45:Aa:397:ASN:N	45:Aa:397:ASN:HD22	2.18	0.42
46:Ab:64:PHE:CZ	46:Ab:394:SER:HA	2.55	0.42
49:Ae:159:ILE:HG21	49:Ae:178:HIS:CB	2.50	0.42
1:A:75:LEU:O	1:A:76:PRO:C	2.60	0.41
6:F:196:PHE:CD1	44:s:91:ARG:NE	2.87	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:555:ILE:HD13	7:G:560:LEU:HD11	2.01	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
9:I:144:ARG:NH2	17:Q:112:MET:O	2.53	0.41
55:K:101:3PE:H361	55:K:101:3PE:H392	1.68	0.41
12:L:293:LEU:O	12:L:425:ARG:HD2	2.20	0.41
12:L:489:THR:O	12:L:492:ILE:HG13	2.20	0.41
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.01	0.41
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.50	0.41
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.50	0.41
21:V:13:GLY:O	21:V:14:LEU:C	2.63	0.41
22:W:130:ASP:HB2	22:W:131:PRO:HD2	2.02	0.41
23:X:42:GLU:O	23:X:135:ARG:NH2	2.53	0.41
62:a:101:CDL:HB32	43:r:8:ILE:HG13	2.01	0.41
30:e:33:CYS:O	30:e:34:HIS:C	2.62	0.41
30:e:44:ALA:HA	30:e:47:ILE:CG1	2.49	0.41
37:l:59:VAL:O	37:l:59:VAL:HG12	2.20	0.41
45:AA:74:TRP:CZ3	45:AA:232:ALA:HB3	2.54	0.41
45:AA:410:CYS:O	45:AA:413:ILE:N	2.52	0.41
47:AC:120:LEU:O	47:AC:121:PHE:C	2.62	0.41
48:AD:248:ILE:HG22	48:AD:263:MET:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:148:ALA:O	45:Aa:152:GLN:HG2	2.20	0.41
46:Ab:147:ARG:HD2	46:Ab:150:GLU:OE2	2.20	0.41
47:Ac:169:SER:O	47:Ac:170:VAL:C	2.62	0.41
47:Ac:284:ILE:HG21	47:Ac:289:GLY:HA3	2.02	0.41
48:Ad:95:PRO:HG2	52:Ah:85:PHE:HB2	2.02	0.41
48:Ad:118:LYS:HA	48:Ad:122:SER:HB2	2.01	0.41
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG23	2.01	0.41
1:A:79:ILE:CD1	8:H:155:LEU:CD2	2.88	0.41
2:B:110:PRO:O	9:I:83:THR:HG22	2.21	0.41
4:D:128:THR:HG22	4:D:131:GLN:CD	2.45	0.41
4:D:184:ILE:HG23	4:D:203:MET:HB3	2.00	0.41
5:E:78:VAL:HG23	5:E:79:LEU:H	1.84	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
7:G:403:VAL:HG13	7:G:476:LEU:CD1	2.50	0.41
10:J:20:ALA:C	10:J:22:LYS:N	2.77	0.41
10:J:43:VAL:HG13	11:K:49:LEU:CD1	2.50	0.41
10:J:136:GLU:O	10:J:137:GLY:C	2.62	0.41
12:L:58:ASN:HA	12:L:58:ASN:HD22	1.65	0.41
12:L:355:ASP:O	12:L:359:MET:HG3	2.20	0.41
12:L:407:TRP:CE3	12:L:410:LEU:HD21	2.55	0.41
13:M:319:HIS:HA	13:M:322:THR:CG2	2.44	0.41
55:M:502:3PE:H371	55:M:502:3PE:H342	1.82	0.41
14:N:22:SER:HB2	30:e:6:ILE:HG22	2.02	0.41
14:N:285:MET:HE1	14:N:288:LEU:HD22	2.03	0.41
15:O:70:LYS:O	15:O:71:ASN:C	2.62	0.41
15:O:267:THR:O	15:O:271:GLU:HG3	2.19	0.41
16:P:110:ALA:HB1	16:P:148:ILE:HD12	2.02	0.41
18:R:79:CYS:O	18:R:88:HIS:CE1	2.73	0.41
20:U:118:ILE:HA	36:k:51:TRP:CH2	2.55	0.41
21:V:114:TRP:O	21:V:114:TRP:CE3	2.72	0.41
23:X:40:ASN:OD1	23:X:63:VAL:HG22	2.19	0.41
26:a:34:LYS:O	26:a:35:GLU:C	2.63	0.41
28:c:57:TYR:CD2	29:d:70:PHE:CZ	3.08	0.41
31:f:8:ARG:O	31:f:9:GLU:HB2	2.20	0.41
32:g:140:PHE:HB3	41:p:75:THR:CG2	2.50	0.41
34:i:20:ARG:HH11	34:i:20:ARG:HG3	1.84	0.41
55:m:202:3PE:H351	55:m:202:3PE:H321	1.75	0.41
39:n:56:ASP:O	39:n:59:ARG:N	2.53	0.41
39:n:114:MET:HG3	39:n:115:TYR:CD2	2.55	0.41
42:q:20:LEU:HD23	42:q:20:LEU:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:53:LEU:HD21	45:AA:243:LEU:CD1	2.50	0.41
45:AA:453:CYS:HB3	45:AA:468:TYR:OH	2.20	0.41
46:AB:346:ALA:O	46:AB:347:ALA:C	2.62	0.41
48:AD:106:ASP:O	48:AD:110:ILE:HG13	2.21	0.41
48:AD:242:ILE:HG12	48:AD:244:MET:N	2.31	0.41
45:Aa:174:GLU:C	45:Aa:176:ASP:H	2.27	0.41
46:Ab:126:ILE:H	46:Ab:126:ILE:CD1	2.26	0.41
55:Ac:403:3PE:H321	62:Ag:101:CDL:C12	2.50	0.41
48:Ad:123:SER:O	48:Ad:178:PRO:CB	2.68	0.41
48:Ad:292:MET:HE3	48:Ad:292:MET:HB3	1.95	0.41
48:Ad:318:LYS:CD	49:Ae:86:PRO:HB2	2.49	0.41
49:Ae:173:PRO:O	49:Ae:214:ILE:HA	2.20	0.41
49:Ae:195:LEU:CD1	49:Ae:248:ARG:HD2	2.50	0.41
53:Aj:23:LEU:HB2	54:Ak:27:VAL:HG22	2.02	0.41
54:Ak:12:GLU:HA	54:Ak:15:ARG:HD3	2.02	0.41
2:B:179:ARG:NH2	3:C:204:THR:OG1	2.53	0.41
3:C:87:ILE:HG21	3:C:95:THR:HG21	2.02	0.41
3:C:114:THR:OG1	4:D:421:ARG:NH1	2.53	0.41
3:C:127:ILE:HD11	3:C:175:VAL:HG21	2.02	0.41
4:D:140:ASP:OD1	4:D:457:VAL:HG11	2.20	0.41
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.20	0.41
4:D:181:LEU:HD22	4:D:214:TYR:OH	2.21	0.41
5:E:155:LEU:CD1	5:E:204:ILE:HD13	2.50	0.41
6:F:94:PRO:CG	6:F:97:LEU:HD12	2.45	0.41
6:F:262:PHE:HA	6:F:265:PHE:CD2	2.56	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:330:LEU:HD12	7:G:544:MET:CE	2.50	0.41
7:G:652:ASN:HA	7:G:655:ARG:CZ	2.51	0.41
8:H:43:TYR:CD1	26:a:4:GLU:HG2	2.54	0.41
8:H:102:ILE:HG12	8:H:162:LEU:HD23	2.02	0.41
12:L:249:SER:HB2	12:L:340:PHE:CD2	2.55	0.41
12:L:434:LYS:HG3	36:k:59:TYR:CE1	2.55	0.41
12:L:437:PHE:HB2	12:L:438:PRO:CD	2.49	0.41
12:L:532:ILE:HG21	37:l:133:LEU:HD22	2.02	0.41
14:N:218:ALA:CB	14:N:240:MET:SD	3.08	0.41
15:O:76:GLU:HG3	15:O:266:PRO:HG2	2.00	0.41
15:O:146:ALA:CB	15:O:159:LEU:HD21	2.50	0.41
15:O:179:ILE:CD1	15:O:184:VAL:HG22	2.50	0.41
15:O:354:LEU:HD12	15:O:354:LEU:HA	1.95	0.41
16:P:225:ALA:HB3	16:P:291:TYR:CE2	2.55	0.41
16:P:332:LEU:HA	16:P:333:PRO:HD3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:69:GLU:C	17:Q:72:ILE:HG22	2.45	0.41
18:R:40:GLU:HA	18:R:45:ARG:NH1	2.35	0.41
20:T:90:TYR:CD2	20:T:93:ILE:HG12	2.56	0.41
20:T:112:SER:O	20:T:116:VAL:HG23	2.20	0.41
21:V:114:TRP:O	21:V:116:ILE:N	2.52	0.41
22:W:69:MET:O	22:W:70:PHE:C	2.60	0.41
24:Y:10:SER:O	24:Y:11:TYR:C	2.62	0.41
25:Z:116:TRP:CZ2	25:Z:119:PRO:HD3	2.55	0.41
27:b:72:ASP:HB3	27:b:74:LEU:HD12	2.02	0.41
33:h:90:ASN:HD21	62:h:201:CDL:PA1	2.43	0.41
34:i:83:HIS:HD2	41:p:37:TYR:CE2	2.37	0.41
38:m:49:LEU:HA	39:n:133:TRP:HH2	1.84	0.41
40:o:59:CYS:SG	40:o:91:GLU:HG2	2.61	0.41
42:q:25:ARG:HB3	42:q:29:ARG:NH1	2.28	0.41
42:q:75:TRP:CE3	42:q:75:TRP:HA	2.55	0.41
45:AA:230:VAL:HG21	45:AA:417:LEU:HB3	2.00	0.41
46:AB:166:PHE:CE1	46:AB:171:THR:HG22	2.56	0.41
47:AC:153:ILE:HB	47:AC:157:GLY:HA2	2.01	0.41
48:AD:157:GLY:CA	48:AD:167:ARG:HB3	2.24	0.41
48:AD:159:ASN:HB3	48:AD:166:MET:CE	2.48	0.41
48:AD:214:LEU:HG	48:AD:242:ILE:HD12	2.01	0.41
50:AF:54:ASP:OD1	50:AF:55:LEU:N	2.52	0.41
45:Aa:92:PHE:HD2	45:Aa:216:LEU:HD21	1.85	0.41
45:Aa:192:PHE:HD1	45:Aa:269:ARG:O	2.04	0.41
45:Aa:204:PRO:O	45:Aa:205:SER:C	2.63	0.41
46:Ab:92:LYS:HB2	46:Ab:143:ALA:HB1	2.02	0.41
46:Ab:212:HIS:NE2	46:Ab:246:LEU:HD23	2.21	0.41
48:Ad:181:ASN:C	48:Ad:183:GLU:N	2.76	0.41
48:Ad:294:LEU:CB	53:Aj:36:PHE:HZ	2.31	0.41
49:Ae:147:LEU:HD12	49:Ae:147:LEU:O	2.20	0.41
52:Ah:51:CYS:SG	52:Ah:69:LEU:HB2	2.60	0.41
1:A:8:PHE:HB2	55:H:401:3PE:H2D1	2.01	0.41
4:D:181:LEU:HD11	4:D:210:MET:HB3	2.02	0.41
5:E:73:HIS:ND1	17:Q:166:TRP:CE2	2.88	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.41
7:G:82:ILE:HD13	7:G:100:TRP:CZ3	2.55	0.41
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.41
7:G:308:ARG:HG3	7:G:581:ASP:HA	2.01	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:35:LYS:HE2	9:I:83:THR:OG1	2.20	0.41
8:H:102:ILE:HG12	8:H:162:LEU:CD2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:135:ALA:HB2	8:H:201:THR:HB	2.02	0.41
8:H:211:PHE:C	8:H:213:VAL:H	2.27	0.41
9:I:78:PHE:HB3	43:r:8:ILE:CG2	2.50	0.41
10:J:133:VAL:CG1	26:a:41:VAL:CG2	2.98	0.41
11:K:1:MET:O	11:K:2:PRO:C	2.62	0.41
11:K:73:VAL:CG2	14:N:38:LEU:HD22	2.50	0.41
62:L:704:CDL:HA62	33:h:68:LEU:CD1	2.42	0.41
13:M:85:LYS:O	13:M:85:LYS:HG2	2.21	0.41
13:M:127:ILE:HD11	14:N:256:PRO:HG2	1.96	0.41
13:M:270:ILE:HD12	13:M:395:LEU:HD22	2.02	0.41
13:M:394:ILE:HG21	55:m:202:3PE:H2C2	2.01	0.41
14:N:25:ASN:HB3	30:e:15:ASP:OD1	2.19	0.41
14:N:317:GLN:HG2	15:O:301:LYS:HB3	2.01	0.41
15:O:59:VAL:HG22	15:O:157:VAL:HG21	2.02	0.41
15:O:66:ILE:HD11	15:O:218:ILE:HG12	1.97	0.41
15:O:179:ILE:HD12	15:O:184:VAL:HG22	2.02	0.41
18:R:84:GLY:O	18:R:85:ALA:CB	2.65	0.41
22:W:53:MET:O	22:W:54:GLN:C	2.62	0.41
23:X:16:GLU:O	23:X:64:ASN:ND2	2.53	0.41
23:X:44:MET:HG3	27:b:53:TYR:CE2	2.56	0.41
24:Y:83:ARG:O	24:Y:84:GLU:HB3	2.20	0.41
26:a:43:TYR:O	26:a:47:LEU:HD13	2.20	0.41
27:b:72:ASP:HB3	27:b:74:LEU:CD1	2.50	0.41
28:c:55:TRP:CE2	29:d:66:THR:HG22	2.55	0.41
31:f:36:ALA:O	31:f:37:PHE:C	2.61	0.41
32:g:71:PHE:CE2	32:g:73:GLY:HA2	2.55	0.41
35:j:44:TYR:CD2	35:j:45:ARG:HG3	2.56	0.41
38:m:42:ARG:O	38:m:43:LEU:C	2.62	0.41
45:AA:172:MET:HA	45:AA:175:ASN:CG	2.44	0.41
46:AB:173:ILE:CG2	46:AB:174:ILE:N	2.83	0.41
46:AB:293:LEU:HB3	46:AB:309:LEU:CG	2.48	0.41
47:AC:54:HIS:O	47:AC:65:SER:HB2	2.20	0.41
47:AC:135:TRP:CE2	47:AC:259:ALA:HB3	2.54	0.41
48:AD:216:THR:O	52:AH:32:ARG:NH2	2.53	0.41
48:AD:245:ALA:O	48:AD:247:PRO:HD3	2.20	0.41
48:AD:259:THR:O	48:AD:260:PRO:C	2.60	0.41
49:AE:127:TYR:CG	53:AJ:32:PHE:HD1	2.37	0.41
49:AE:164:ASN:HB3	49:AE:226:ALA:CB	2.49	0.41
52:AH:65:CYS:O	52:AH:66:THR:C	2.63	0.41
45:Aa:342:GLN:HE21	45:Aa:357:HIS:CB	2.31	0.41
46:Ab:234:ALA:C	46:Ab:236:GLN:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:312:SER:OG	46:Ab:357:GLN:NE2	2.40	0.41
47:Ac:96:LEU:HD23	55:Ac:403:3PE:H292	2.01	0.41
47:Ac:153:ILE:HB	47:Ac:157:GLY:HA2	2.01	0.41
47:Ac:193:ALA:HB3	68:Ac:405:UQ6:H202	2.01	0.41
48:Ad:291:LYS:HD3	71:Ad:402:3PH:H31	2.01	0.41
48:Ad:317:ARG:HD2	48:Ad:319:LEU:HD21	2.02	0.41
71:Ad:402:3PH:C36	49:Ae:128:ALA:HB1	2.49	0.41
52:Ah:39:GLU:CG	52:Ah:40:LYS:H	2.31	0.41
49:Ai:71:ASN:C	49:Ai:73:PRO:HD2	2.45	0.41
3:C:72:VAL:HG22	3:C:87:ILE:HG22	2.01	0.41
5:E:198:LYS:HA	5:E:201:GLU:HB3	2.02	0.41
6:F:132:ARG:HE	6:F:133:HIS:HE2	1.67	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
10:J:29:GLY:O	10:J:33:ILE:HG13	2.21	0.41
10:J:130:ASP:CB	25:Z:79:LYS:HE2	2.50	0.41
11:K:1:MET:HB3	11:K:2:PRO:HD3	2.02	0.41
12:L:142:ILE:HG12	13:M:370:PRO:HB2	2.01	0.41
12:L:253:VAL:HB	12:L:310:LEU:CD1	2.50	0.41
12:L:365:ILE:CD1	12:L:366:MET:HG3	2.24	0.41
13:M:47:GLU:O	13:M:48:ASN:C	2.64	0.41
13:M:142:ARG:HG3	13:M:143:LEU:N	2.36	0.41
13:M:178:ILE:O	13:M:179:LEU:C	2.60	0.41
13:M:270:ILE:HD11	13:M:395:LEU:HA	2.03	0.41
14:N:159:ILE:HB	14:N:278:MET:HE1	2.01	0.41
14:N:168:GLY:HA3	14:N:181:TYR:CE1	2.56	0.41
14:N:324:LEU:CD1	29:d:64:PHE:HZ	2.32	0.41
14:N:338:PRO:HB3	62:X:201:CDL:H712	2.02	0.41
15:O:164:TYR:CE1	15:O:201:PRO:HD3	2.56	0.41
15:O:261:TRP:H	15:O:261:TRP:HE3	1.68	0.41
15:O:355:LYS:HE2	28:c:37:ALA:O	2.21	0.41
16:P:147:ASN:N	16:P:147:ASN:ND2	2.69	0.41
17:Q:78:ARG:O	17:Q:80:PHE:CD1	2.74	0.41
17:Q:126:LEU:CD1	17:Q:137:PHE:HE2	2.33	0.41
17:Q:160:TYR:CE2	17:Q:164:PHE:CE2	3.09	0.41
21:V:5:LEU:O	21:V:6:LYS:C	2.64	0.41
21:V:47:TYR:O	21:V:50:GLN:HB3	2.20	0.41
21:V:81:ILE:O	21:V:84:ALA:N	2.53	0.41
23:X:69:ASN:O	23:X:70:PHE:C	2.63	0.41
28:c:69:TYR:O	28:c:73:ASN:ND2	2.54	0.41
30:e:96:PRO:HB2	30:e:102:GLU:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:63:ASN:CG	39:n:106:TYR:HE1	2.29	0.41
33:h:133:TYR:OH	41:p:87:GLU:HA	2.21	0.41
34:i:22:TRP:CD2	39:n:172:THR:CG2	3.00	0.41
37:l:184:TYR:HD1	40:o:36:GLU:N	2.17	0.41
38:m:127:ILE:O	41:p:139:TYR:HE2	2.04	0.41
40:o:8:ARG:HH21	40:o:9:TYR:HE1	1.68	0.41
40:o:53:LEU:HD23	40:o:56:ARG:NE	2.34	0.41
41:p:71:VAL:HB	41:p:72:PRO:CD	2.50	0.41
45:AA:356:ALA:HB3	45:AA:372:LEU:CD2	2.50	0.41
46:AB:163:ALA:HB1	49:AI:43:LEU:HD23	2.01	0.41
46:AB:168:ASN:N	46:AB:168:ASN:OD1	2.54	0.41
47:AC:47:THR:HB	47:AC:83:HIS:HB2	2.02	0.41
68:AC:403:UQ6:H162	68:AC:403:UQ6:H121	1.80	0.41
48:AD:214:LEU:HG	48:AD:242:ILE:CD1	2.51	0.41
51:AG:45:ARG:O	51:AG:46:ILE:C	2.62	0.41
45:Aa:53:LEU:HD21	45:Aa:243:LEU:CD1	2.50	0.41
45:Aa:152:GLN:NE2	45:Aa:250:LEU:HA	2.35	0.41
46:Ab:39:GLU:O	46:Ab:50:ALA:HA	2.21	0.41
46:Ab:109:LYS:CG	46:Ab:124:GLU:HB3	2.44	0.41
48:Ad:170:LYS:O	48:Ad:173:ASP:HB3	2.20	0.41
48:Ad:306:MET:HE2	48:Ad:306:MET:HB3	1.70	0.41
49:Ae:218:THR:HG21	49:Ae:256:LEU:HB2	2.01	0.41
49:Ae:241:SER:HA	49:Ae:251:LYS:O	2.21	0.41
50:Af:86:GLU:O	50:Af:87:ASP:C	2.60	0.41
3:C:202:PRO:O	3:C:203:LEU:C	2.62	0.41
4:D:240:LEU:HG	4:D:244:ILE:HD11	2.02	0.41
4:D:253:LEU:HD23	4:D:254:ARG:HH22	1.86	0.41
4:D:312:ASP:OD1	4:D:313:GLN:HG3	2.20	0.41
4:D:381:HIS:HE1	9:I:161:ALA:O	2.03	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
6:F:64:LYS:HE3	6:F:67:GLU:OE1	2.21	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
8:H:248:TYR:O	8:H:249:ILE:C	2.62	0.41
8:H:257:THR:O	8:H:260:MET:HB3	2.20	0.41
9:I:36:TYR:HB3	43:r:104:TRP:HE3	1.85	0.41
12:L:202:MET:HE3	12:L:265:PRO:CB	2.50	0.41
12:L:231:PRO:O	12:L:234:PRO:HD2	2.20	0.41
55:L:703:3PE:H322	55:L:703:3PE:H351	1.84	0.41
13:M:247:SER:OG	13:M:304:GLN:NE2	2.53	0.41
13:M:250:LEU:HD12	13:M:250:LEU:C	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:301:ILE:HG22	13:M:301:ILE:O	2.19	0.41
14:N:233:LEU:CD2	14:N:241:LEU:HD12	2.27	0.41
15:O:117:PHE:CZ	15:O:173:MET:HE3	2.54	0.41
15:O:200:PRO:HG3	15:O:282:PRO:CD	2.47	0.41
15:O:263:ALA:C	15:O:265:ASP:N	2.77	0.41
15:O:295:ARG:HH12	15:O:299:GLN:CB	2.33	0.41
15:O:353:TRP:HB2	29:d:58:LEU:HD12	2.02	0.41
17:Q:85:ASN:C	17:Q:87:MET:N	2.77	0.41
17:Q:160:TYR:CE2	17:Q:164:PHE:CZ	3.09	0.41
18:R:72:VAL:HG12	18:R:73:GLU:H	1.85	0.41
20:U:87:LEU:C	20:U:89:LEU:N	2.78	0.41
23:X:31:HIS:CB	23:X:70:PHE:HZ	2.31	0.41
23:X:75:LYS:O	23:X:79:ALA:HB2	2.20	0.41
27:b:32:MET:N	27:b:33:PRO:CD	2.84	0.41
30:e:49:GLY:O	30:e:52:ALA:N	2.53	0.41
33:h:59:PRO:HD3	39:n:99:VAL:HG11	2.03	0.41
62:h:201:CDL:H171	55:i:201:3PE:H372	2.02	0.41
35:j:52:ARG:HG2	35:j:56:ILE:HD12	2.02	0.41
36:k:20:MET:HE2	36:k:20:MET:HB3	1.98	0.41
37:l:151:PRO:HD2	40:o:9:TYR:CZ	2.55	0.41
37:l:184:TYR:CD1	40:o:36:GLU:CA	3.03	0.41
38:m:124:LYS:O	38:m:126:ASN:N	2.53	0.41
41:p:73:ASP:OD1	41:p:73:ASP:N	2.54	0.41
43:r:4:ALA:O	43:r:5:THR:C	2.63	0.41
45:AA:92:PHE:HD1	45:AA:168:ILE:HD12	1.86	0.41
46:AB:100:THR:CG2	49:AI:70:LEU:HD11	2.50	0.41
46:AB:173:ILE:HG23	46:AB:174:ILE:N	2.34	0.41
46:AB:272:VAL:HA	46:AB:337:GLY:HA3	2.02	0.41
46:AB:313:VAL:HG11	46:AB:321:PHE:CD1	2.54	0.41
47:AC:100:ARG:HH12	67:AC:402:HEM:HBD1	1.86	0.41
48:AD:146:LYS:HD2	48:AD:149:ALA:HB3	2.01	0.41
48:AD:281:GLU:N	48:AD:281:GLU:OE1	2.53	0.41
51:AG:24:GLN:O	51:AG:25:ARG:C	2.62	0.41
51:AG:40:ARG:NH2	51:AG:41:ARG:HB2	2.35	0.41
45:Aa:450:TYR:HD2	53:Aj:16:ARG:HH11	1.69	0.41
46:Ab:171:THR:HA	49:Ai:64:LEU:CD2	2.47	0.41
48:Ad:158:PRO:HB2	48:Ad:164:MET:CB	2.47	0.41
48:Ad:223:THR:OG1	52:Ah:55:VAL:HG11	2.21	0.41
2:B:98:ALA:HB2	2:B:135:GLY:HA3	2.01	0.41
4:D:50:ALA:C	4:D:51:VAL:HG13	2.45	0.41
4:D:67:ASN:HB2	15:O:193:LEU:HD22	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:ILE:O	4:D:72:LEU:C	2.62	0.41
4:D:386:THR:HG22	9:I:118:LEU:CD1	2.50	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.02	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.20	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:51:GLN:HE22	17:Q:158:LYS:HB2	1.85	0.41
7:G:136:GLU:HA	17:Q:88:GLN:HE21	1.85	0.41
7:G:193:ASP:OD1	7:G:193:ASP:N	2.53	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:475:VAL:HG22	7:G:514:ASN:OD1	2.20	0.41
7:G:671:LEU:HD12	19:S:42:VAL:HG23	2.02	0.41
8:H:69:SER:O	8:H:73:ILE:HB	2.21	0.41
10:J:60:LEU:O	10:J:64:LEU:HB2	2.20	0.41
10:J:124:LEU:O	10:J:125:MET:C	2.62	0.41
12:L:211:ILE:N	12:L:212:PRO:CD	2.82	0.41
12:L:368:PHE:HB3	12:L:445:GLU:OE1	2.20	0.41
13:M:7:PRO:HG3	31:f:20:PHE:CA	2.50	0.41
13:M:22:LYS:HE3	13:M:26:ASN:HD21	1.86	0.41
14:N:272:LYS:HE3	33:h:154:GLN:HG2	2.02	0.41
15:O:42:ALA:O	15:O:45:LEU:O	2.39	0.41
15:O:150:LEU:O	15:O:154:GLY:HA2	2.20	0.41
15:O:287:ASP:HB3	15:O:290:THR:HG23	2.02	0.41
16:P:128:ASN:HD21	16:P:149:PRO:HB3	1.84	0.41
22:W:53:MET:O	22:W:103:ARG:HG2	2.20	0.41
22:W:93:LEU:HA	22:W:93:LEU:HD23	1.77	0.41
23:X:21:SER:O	23:X:24:VAL:HG22	2.21	0.41
23:X:49:GLU:OE1	27:b:58:ARG:NH2	2.54	0.41
23:X:89:LEU:HD21	23:X:95:GLN:HB3	2.02	0.41
25:Z:23:ARG:CG	25:Z:25:LEU:HD13	2.51	0.41
25:Z:126:GLY:C	25:Z:128:ARG:H	2.28	0.41
27:b:74:LEU:HD12	27:b:74:LEU:N	2.35	0.41
30:e:32:ARG:O	30:e:33:CYS:CB	2.69	0.41
30:e:101:ARG:C	30:e:104:PRO:HD3	2.46	0.41
34:i:74:HIS:O	34:i:78:PRO:HG2	2.20	0.41
37:l:122:THR:HG22	37:l:124:VAL:H	1.85	0.41
39:n:164:PRO:HA	39:n:165:PRO:HD3	1.94	0.41
41:p:91:GLN:O	41:p:91:GLN:HG2	2.21	0.41
45:AA:341:PHE:CE2	45:AA:371:PHE:HE2	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:463:GLU:OE2	51:AG:6:GLY:N	2.54	0.41
46:AB:225:VAL:HG22	46:AB:229:VAL:HG21	2.02	0.41
46:AB:312:SER:HA	46:AB:315:LYS:HE3	2.02	0.41
48:AD:129:TYR:CD2	48:AD:198:SER:HB2	2.55	0.41
48:AD:179:TYR:CE1	48:AD:188:ALA:HB3	2.55	0.41
48:AD:183:GLU:H	48:AD:183:GLU:CD	2.27	0.41
46:Ab:36:GLN:OE1	46:Ab:36:GLN:N	2.53	0.41
47:Ac:119:LEU:HB3	67:Ac:402:HEM:CBB	2.51	0.41
47:Ac:364:ILE:O	47:Ac:368:ILE:HG13	2.21	0.41
48:Ad:186:ARG:HA	48:Ad:191:GLY:C	2.46	0.41
48:Ad:292:MET:HA	71:Ad:402:3PH:C33	2.44	0.41
49:Ae:235:TYR:CZ	49:Ae:240:GLY:HA2	2.55	0.41
52:Ah:31:VAL:O	52:Ah:34:HIS:HB3	2.21	0.41
53:Aj:21:PHE:O	53:Aj:24:THR:HG22	2.20	0.41
1:A:34:ALA:HB1	8:H:63:PRO:HA	2.02	0.41
1:A:52:SER:O	1:A:53:MET:C	2.62	0.41
2:B:110:PRO:HA	8:H:34:ARG:HB3	2.02	0.41
58:B:304:PC1:C38	8:H:57:MET:HE2	2.50	0.41
3:C:116:VAL:HG21	4:D:412:VAL:HG21	2.02	0.41
3:C:151:PRO:HG2	22:W:23:ILE:HG23	2.03	0.41
3:C:152:ILE:HD11	3:C:177:PHE:CD2	2.51	0.41
4:D:128:THR:N	4:D:131:GLN:HG2	2.36	0.41
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.56	0.41
4:D:207:ARG:HA	4:D:210:MET:HE3	2.03	0.41
4:D:410:TYR:HB3	4:D:423:LYS:HB3	2.03	0.41
5:E:77:ALA:C	5:E:80:PRO:HD2	2.46	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.41
6:F:174:ARG:CB	44:s:87:LEU:HD11	2.49	0.41
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:379:CYS:SG	56:F:502:SF4:S2	3.19	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.20	0.41
9:I:135:ARG:O	9:I:135:ARG:CG	2.69	0.41
10:J:33:ILE:HG12	10:J:64:LEU:HD23	2.02	0.41
10:J:101:PHE:HD2	10:J:102:LEU:HD22	1.86	0.41
10:J:116:LEU:HD11	30:e:73:MET:HG3	2.02	0.41
12:L:258:PHE:O	12:L:261:VAL:HG22	2.20	0.41
12:L:570:HIS:O	12:L:573:MET:N	2.54	0.41
12:L:571:THR:O	12:L:574:THR:HG22	2.20	0.41
13:M:4:ILE:CD1	13:M:41:LEU:HD21	2.51	0.41
13:M:218:LYS:HE3	13:M:218:LYS:HB3	1.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:THR:HG22	14:N:84:TRP:N	2.35	0.41
14:N:175:MET:O	14:N:176:ARG:C	2.63	0.41
15:O:262:GLU:O	15:O:265:ASP:HB3	2.21	0.41
15:O:343:TYR:HB3	29:d:52:PRO:HD3	2.03	0.41
19:S:16:LEU:HD21	19:S:19:ILE:CD1	2.50	0.41
20:T:122:MET:HG3	20:T:144:ILE:HG21	2.02	0.41
21:V:51:ILE:H	21:V:51:ILE:HG13	1.77	0.41
23:X:28:ALA:HB3	23:X:71:PHE:HE1	1.86	0.41
29:d:101:PHE:CZ	33:h:159:LEU:HD22	2.55	0.41
37:l:63:GLU:O	37:l:64:PRO:C	2.63	0.41
38:m:50:GLN:O	38:m:50:GLN:HG2	2.20	0.41
41:p:40:VAL:O	41:p:44:PRO:HG2	2.21	0.41
45:AA:109:LEU:HD21	45:AA:120:LEU:CD2	2.51	0.41
45:AA:115:SER:O	45:AA:116:ILE:C	2.64	0.41
45:AA:139:ASP:O	45:AA:143:VAL:HG23	2.20	0.41
45:AA:152:GLN:HE22	45:AA:250:LEU:HA	1.85	0.41
45:AA:275:ILE:HD11	49:AE:85:VAL:HG22	2.03	0.41
45:AA:397:ASN:N	45:AA:397:ASN:HD22	2.18	0.41
46:AB:407:MET:HE1	46:AB:415:GLN:CD	2.45	0.41
47:AC:140:PHE:CE2	47:AC:261:PRO:HA	2.56	0.41
47:AC:253:PRO:CB	48:AD:202:ARG:O	2.68	0.41
47:AC:256:TYR:OH	48:AD:202:ARG:NH1	2.54	0.41
47:AC:272:TRP:HA	47:AC:275:LEU:HD12	2.02	0.41
48:AD:127:MET:O	48:AD:175:PHE:HB2	2.20	0.41
48:AD:146:LYS:HB2	48:AD:171:LEU:HD21	2.03	0.41
50:AF:110:LYS:CA	54:Ak:10:TYR:HE1	2.34	0.41
49:AI:71:ASN:C	49:AI:73:PRO:HD2	2.45	0.41
45:Aa:341:PHE:O	45:Aa:341:PHE:CG	2.74	0.41
45:Aa:404:ASP:O	45:Aa:408:PRO:HG2	2.21	0.41
46:Ab:43:LEU:HB2	46:Ab:45:ASN:OD1	2.21	0.41
47:Ac:240:MET:HB3	48:Ad:292:MET:HG3	2.03	0.41
47:Ac:294:LEU:C	47:Ac:294:LEU:HD23	2.46	0.41
48:Ad:215:LEU:HD11	69:Ad:401:HEC:CMB	2.51	0.41
49:Ae:142:ALA:CB	49:Ae:147:LEU:CD2	2.82	0.41
52:Ah:35:CYS:O	52:Ah:38:LEU:HD13	2.21	0.41
52:Ah:42:VAL:C	52:Ah:45:ARG:H	2.29	0.41
1:A:7:ILE:O	1:A:11:ILE:HG13	2.20	0.41
1:A:73:LEU:O	8:H:160:TYR:OH	2.36	0.41
2:B:137:LEU:HD21	2:B:145:LEU:HD23	2.02	0.41
2:B:146:ARG:NH1	2:B:149:TYR:HD2	2.18	0.41
3:C:184:ARG:HH22	4:D:112:HIS:HE2	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:211:PHE:O	4:D:214:TYR:N	2.53	0.41
4:D:420:TYR:CD2	21:V:114:TRP:HH2	2.38	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:199:ARG:HD3	44:s:80:PHE:CD2	2.55	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
8:H:17:MET:HG2	8:H:228:TYR:CB	2.50	0.41
8:H:91:MET:C	8:H:93:HIS:N	2.77	0.41
8:H:179:TRP:HE1	25:Z:43:LEU:HB2	1.86	0.41
8:H:277:TYR:HA	8:H:278:PRO:HD2	1.95	0.41
9:I:50:MET:HG2	25:Z:33:TYR:OH	2.21	0.41
9:I:117:LYS:HA	9:I:130:ILE:HD11	2.03	0.41
55:I:301:3PE:H3F1	55:I:301:3PE:H3C1	1.96	0.41
10:J:5:ILE:O	10:J:6:PHE:C	2.63	0.41
10:J:86:TRP:CE3	10:J:89:LEU:HD12	2.56	0.41
11:K:6:PHE:O	11:K:7:ASN:C	2.63	0.41
12:L:61:TYR:HA	34:i:98:VAL:O	2.21	0.41
12:L:210:LEU:O	12:L:211:ILE:C	2.62	0.41
12:L:321:GLN:NE2	12:L:324:LEU:HD13	2.36	0.41
12:L:357:ARG:CZ	39:n:78:GLN:O	2.69	0.41
55:L:701:3PE:H382	40:o:78:LEU:CD1	2.51	0.41
13:M:160:LEU:O	13:M:164:LEU:HD13	2.21	0.41
13:M:164:LEU:HB3	13:M:174:LEU:HD11	2.03	0.41
13:M:175:ASN:ND2	33:h:143:GLU:HG2	2.31	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.03	0.41
13:M:303:ILE:HG13	13:M:385:LEU:HD23	2.02	0.41
13:M:412:ILE:HG21	37:l:115:ASN:ND2	2.35	0.41
14:N:125:HIS:CE1	14:N:129:ILE:HD11	2.56	0.41
14:N:191:LEU:HG	14:N:191:LEU:O	2.21	0.41
14:N:224:SER:HB2	14:N:229:SER:HB2	2.01	0.41
14:N:331:ILE:HD12	14:N:335:MET:HE3	2.03	0.41
15:O:71:ASN:OD1	15:O:71:ASN:N	2.54	0.41
15:O:90:GLY:H	15:O:93:TYR:HB2	1.86	0.41
15:O:96:THR:O	28:c:31:VAL:HG21	2.21	0.41
15:O:105:ASP:OD1	15:O:106:ILE:N	2.54	0.41
15:O:263:ALA:C	15:O:265:ASP:H	2.29	0.41
15:O:268:LYS:HA	15:O:271:GLU:OE1	2.21	0.41
16:P:113:LYS:O	16:P:114:ASP:CB	2.69	0.41
16:P:170:LEU:HG	16:P:171:ASN:N	2.36	0.41
16:P:237:LYS:HE2	16:P:322:ILE:O	2.20	0.41
16:P:286:ARG:NH1	16:P:358:THR:HG22	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:357:ARG:NH2	16:P:364:SER:HB3	2.36	0.41
17:Q:86:ASN:OD1	17:Q:86:ASN:O	2.39	0.41
20:U:83:VAL:HG13	20:U:122:MET:SD	2.61	0.41
23:X:48:TRP:HH2	33:h:185:ALA:C	2.29	0.41
23:X:130:LYS:HD2	27:b:59:ASP:CG	2.45	0.41
24:Y:51:THR:HG23	24:Y:52:LEU:N	2.35	0.41
26:a:41:VAL:O	26:a:42:GLN:C	2.64	0.41
30:e:65:GLU:OE2	30:e:71:LYS:N	2.54	0.41
34:i:29:SER:O	34:i:32:GLU:HB2	2.21	0.41
34:i:92:THR:O	41:p:5:TRP:CD1	2.74	0.41
35:j:102:ASP:O	35:j:103:ASP:HB2	2.21	0.41
36:k:81:PHE:O	36:k:85:VAL:HG23	2.21	0.41
37:l:44:THR:HG23	37:l:46:GLU:HG2	2.03	0.41
37:l:80:ASN:HB3	37:l:112:TYR:OH	2.20	0.41
37:l:110:ASP:HB2	38:m:72:ARG:HH12	1.85	0.41
37:l:122:THR:CG2	37:l:129:MET:HE1	2.45	0.41
39:n:41:ALA:C	39:n:43:LEU:N	2.78	0.41
39:n:94:TYR:HB3	39:n:178:PRO:HD2	2.03	0.41
39:n:139:GLN:O	39:n:140:LEU:C	2.64	0.41
39:n:157:ALA:O	39:n:158:ARG:HB2	2.21	0.41
39:n:165:PRO:O	39:n:166:LEU:C	2.64	0.41
40:o:28:ASP:O	40:o:29:LEU:C	2.62	0.41
40:o:71:ARG:NH1	40:o:72:ASP:OD1	2.54	0.41
45:AA:249:HIS:O	45:AA:250:LEU:CB	2.64	0.41
45:AA:298:ASN:OD1	45:AA:299:PRO:HD2	2.21	0.41
46:AB:85:LEU:CD2	49:AI:68:VAL:HG11	2.49	0.41
47:AC:198:LEU:HD11	47:Ac:9:PRO:O	2.20	0.41
47:AC:284:ILE:HG21	47:AC:289:GLY:HA3	2.02	0.41
48:AD:133:ARG:NH2	48:AD:174:TYR:OH	2.54	0.41
48:AD:183:GLU:OE2	48:Ad:160:ASP:HB3	2.20	0.41
48:AD:317:ARG:HD2	48:AD:319:LEU:HD21	2.02	0.41
49:AE:115:TYR:O	49:AE:116:LEU:C	2.62	0.41
49:AE:127:TYR:HB2	53:AJ:32:PHE:CD1	2.56	0.41
49:AE:162:GLY:N	49:AE:178:HIS:O	2.54	0.41
49:AE:231:PHE:CD2	49:AE:250:ARG:NH1	2.88	0.41
51:AG:69:GLN:HE21	51:AG:72:ARG:CZ	2.34	0.41
49:AI:71:ASN:OD1	49:AI:71:ASN:O	2.38	0.41
45:Aa:49:GLN:CD	45:Aa:239:HIS:CD2	2.99	0.41
45:Aa:62:GLU:HB2	45:Aa:413:ILE:HD11	2.02	0.41
45:Aa:72:GLY:HA2	45:Aa:132:LEU:HA	2.03	0.41
45:Aa:74:TRP:CZ3	45:Aa:410:CYS:SG	3.13	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:95:HIS:HB3	45:Aa:164:GLU:OE1	2.21	0.41
45:Aa:298:ASN:OD1	45:Aa:299:PRO:HD2	2.20	0.41
46:Ab:38:LEU:HD22	46:Ab:38:LEU:N	2.35	0.41
46:Ab:60:ARG:HG2	46:Ab:393:LEU:HD13	2.02	0.41
46:Ab:92:LYS:HG2	46:Ab:145:GLU:HG2	2.03	0.41
46:Ab:123:VAL:HG22	46:Ab:133:LEU:HD13	2.03	0.41
46:Ab:227:HIS:CD2	46:Ab:231:LYS:HD3	2.55	0.41
46:Ab:272:VAL:HA	46:Ab:337:GLY:HA3	2.02	0.41
47:Ac:124:MET:HG2	47:Ac:274:PHE:HE1	1.85	0.41
47:Ac:208:PRO:HB2	47:Ac:316:MET:HE3	2.02	0.41
47:Ac:296:LEU:O	47:Ac:297:SER:C	2.64	0.41
48:Ad:114:PHE:CE1	48:Ad:175:PHE:CE2	3.01	0.41
49:Ae:130:LYS:HZ2	53:Aj:33:GLU:CD	2.25	0.41
49:Ae:179:ARG:HH21	49:Ae:205:VAL:HG21	1.86	0.41
49:Ae:180:THR:O	49:Ae:181:LYS:C	2.63	0.41
49:Ae:214:ILE:HB	49:Ae:259:GLU:HB3	2.03	0.41
3:C:134:LEU:HD12	3:C:134:LEU:H	1.86	0.41
3:C:202:PRO:HD3	17:Q:121:LEU:HD21	2.02	0.41
4:D:220:ALA:HB2	9:I:98:ARG:NH2	2.32	0.41
6:F:109:ARG:HH21	6:F:239:PRO:CD	2.34	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
6:F:427:LEU:HB2	60:F:501:FMN:C7M	2.51	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH1	2.48	0.41
7:G:557:ARG:HG3	7:G:579:MET:HB2	2.03	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.83	0.41
8:H:130:PHE:CE1	8:H:134:ARG:HD2	2.56	0.41
9:I:76:TYR:HE1	9:I:79:ARG:CZ	2.34	0.41
9:I:96:ARG:NH1	9:I:208:ASP:OD1	2.50	0.41
10:J:6:PHE:O	10:J:9:SER:N	2.54	0.41
12:L:3:ILE:HG22	12:L:49:LEU:CD2	2.51	0.41
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.56	0.41
13:M:248:ILE:HG13	13:M:249:ILE:H	1.85	0.41
13:M:329:LEU:HD23	13:M:437:MET:CE	2.49	0.41
13:M:422:HIS:HD2	39:n:102:TRP:CD1	2.39	0.41
15:O:117:PHE:CE1	15:O:128:SER:CB	2.96	0.41
15:O:246:LEU:HD23	15:O:246:LEU:C	2.46	0.41
16:P:227:PRO:HB3	16:P:291:TYR:CZ	2.56	0.41
20:U:133:ILE:CG2	20:U:134:ASP:N	2.84	0.41
23:X:23:ALA:HB2	23:X:95:GLN:NE2	2.35	0.41
24:Y:5:LYS:C	24:Y:7:PHE:N	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:9:LEU:O	26:a:10:ALA:C	2.64	0.41
62:a:101:CDL:C52	42:q:3:LEU:HD13	2.49	0.41
29:d:25:LYS:HE3	29:d:27:ASN:OD1	2.21	0.41
30:e:49:GLY:HA2	30:e:52:ALA:HB3	2.02	0.41
34:i:111:LEU:HD21	41:p:19:ALA:CB	2.51	0.41
35:j:81:LEU:O	35:j:81:LEU:HD23	2.20	0.41
35:j:98:GLY:O	40:o:30:GLY:HA3	2.20	0.41
36:k:57:TRP:HA	36:k:60:MET:HB3	2.02	0.41
38:m:59:HIS:O	38:m:60:ILE:C	2.64	0.41
45:AA:66:HIS:CD2	46:AB:387:GLU:O	2.73	0.41
45:AA:127:GLU:OE2	45:AA:348:TYR:HB3	2.21	0.41
45:AA:404:ASP:O	45:AA:408:PRO:HG2	2.21	0.41
46:AB:168:ASN:HB2	46:AB:170:GLN:OE1	2.21	0.41
47:AC:44:GLN:HB3	67:AC:401:HEM:C2C	2.56	0.41
47:AC:294:LEU:HD23	47:AC:294:LEU:C	2.46	0.41
48:AD:189:ASN:O	48:AD:192:ALA:N	2.54	0.41
48:AD:237:PHE:CE1	48:AD:242:ILE:HA	2.56	0.41
49:AE:132:VAL:O	49:AE:136:PHE:CB	2.69	0.41
50:AF:34:ARG:C	50:AF:36:ASP:N	2.77	0.41
51:AG:43:ARG:HA	51:AG:46:ILE:HG22	2.02	0.41
46:Ab:91:THR:O	46:Ab:93:GLY:N	2.55	0.41
46:Ab:142:THR:CG2	46:Ab:238:LEU:HD23	2.51	0.41
47:Ac:100:ARG:N	55:Ac:403:3PE:H252	2.36	0.41
47:Ac:372:ILE:O	47:Ac:376:MET:HG2	2.21	0.41
49:Ae:172:LYS:HD3	49:Ae:216:VAL:CG2	2.51	0.41
51:Ag:26:ALA:C	51:Ag:28:PRO:HD3	2.46	0.41
1:A:56:PHE:O	1:A:57:LEU:C	2.63	0.40
1:A:104:TYR:CE2	10:J:167:ILE:CD1	3.03	0.40
2:B:108:ALA:CA	2:B:114:MET:HE3	2.50	0.40
2:B:137:LEU:CD2	2:B:145:LEU:HD23	2.51	0.40
3:C:155:ILE:O	3:C:158:VAL:N	2.54	0.40
3:C:223:VAL:HG23	3:C:225:LEU:HD11	1.93	0.40
4:D:132:ALA:O	4:D:133:LEU:C	2.64	0.40
4:D:151:TYR:O	4:D:152:SER:C	2.63	0.40
6:F:313:ASN:O	6:F:358:ASP:HA	2.21	0.40
6:F:427:LEU:HB2	60:F:501:FMN:HM73	2.03	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
8:H:245:PRO:HG2	8:H:255:TYR:CZ	2.55	0.40
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.21	0.40
9:I:154:TYR:CD1	9:I:154:TYR:N	2.90	0.40
10:J:66:VAL:O	10:J:69:TYR:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:84:SER:C	10:J:86:TRP:N	2.78	0.40
12:L:22:SER:HA	12:L:27:ILE:CG2	2.52	0.40
12:L:68:TRP:CE3	12:L:76:LEU:CD2	3.04	0.40
12:L:324:LEU:HB3	12:L:395:ILE:CD1	2.51	0.40
12:L:554:ASP:OD2	13:M:213:HIS:HE1	2.04	0.40
13:M:6:LEU:O	13:M:7:PRO:C	2.60	0.40
13:M:177:MET:HB3	13:M:177:MET:HE3	1.70	0.40
13:M:350:MET:HE3	13:M:350:MET:HB2	1.80	0.40
14:N:139:LEU:HD23	14:N:139:LEU:HA	1.86	0.40
14:N:146:TYR:CG	14:N:147:PRO:N	2.88	0.40
14:N:211:LEU:CD2	14:N:333:SER:HB2	2.45	0.40
15:O:104:LEU:HD23	15:O:104:LEU:HA	1.90	0.40
16:P:88:VAL:HG12	16:P:92:MET:HE2	2.03	0.40
16:P:141:PHE:CD1	16:P:145:PHE:HE2	2.39	0.40
16:P:302:GLY:HA2	16:P:305:PHE:CD2	2.54	0.40
16:P:335:LEU:O	16:P:339:GLY:N	2.54	0.40
20:U:113:LEU:HD11	39:n:20:TYR:CG	2.56	0.40
20:U:128:PHE:CZ	20:U:148:ILE:CD1	3.04	0.40
28:c:57:TYR:CD2	29:d:70:PHE:HZ	2.39	0.40
29:d:45:ASP:O	29:d:46:ASN:C	2.62	0.40
31:f:43:LEU:HD13	41:p:69:ARG:O	2.21	0.40
31:f:56:TRP:CD1	33:h:134:GLU:OE1	2.73	0.40
33:h:87:THR:O	33:h:91:ILE:HG13	2.21	0.40
34:i:69:LEU:HD23	34:i:69:LEU:N	2.36	0.40
37:l:159:LYS:HE3	37:l:161:TYR:CE1	2.56	0.40
39:n:148:GLY:O	39:n:149:ILE:C	2.63	0.40
41:p:43:TRP:HB3	41:p:44:PRO:HD3	2.03	0.40
47:AC:50:PHE:HZ	49:AE:136:PHE:CZ	2.38	0.40
47:AC:148:ASN:O	47:AC:149:LEU:C	2.63	0.40
47:AC:276:PHE:CG	47:AC:277:ALA:N	2.88	0.40
48:AD:155:GLN:CD	48:AD:164:MET:O	2.64	0.40
48:AD:275:ARG:HH21	48:AD:282:HIS:HD2	1.69	0.40
52:AH:80:VAL:O	52:AH:84:LEU:N	2.55	0.40
45:Aa:48:THR:HG21	45:Aa:423:ARG:CB	2.51	0.40
46:Ab:233:VAL:C	46:Ab:236:GLN:HG2	2.46	0.40
47:Ac:71:ARG:NH1	48:Ad:130:VAL:HG22	2.37	0.40
48:Ad:170:LYS:HD2	49:Ae:151:LYS:HG3	2.02	0.40
49:Ae:184:ILE:CG2	49:Ae:208:PRO:HB3	2.50	0.40
49:Ae:216:VAL:HG13	49:Ae:221:GLY:HA2	2.03	0.40
53:Aj:11:TYR:CZ	53:Aj:16:ARG:HB2	2.57	0.40
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:THR:HA	4:D:99:LEU:O	2.20	0.40
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.02	0.40
5:E:233:LEU:H	6:F:37:ASP:CG	2.29	0.40
6:F:39:ASP:HA	6:F:261:TRP:CZ2	2.56	0.40
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:50:LEU:HB2	7:G:91:ALA:O	2.21	0.40
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.40
7:G:377:ALA:O	7:G:380:ASP:HB2	2.20	0.40
8:H:84:SER:C	8:H:86:TRP:N	2.75	0.40
8:H:87:VAL:CG2	8:H:88:PRO:HD3	2.49	0.40
8:H:142:TYR:O	8:H:146:MET:HG3	2.22	0.40
8:H:184:MET:CG	8:H:293:PHE:HD2	2.23	0.40
10:J:32:LEU:O	10:J:33:ILE:C	2.64	0.40
12:L:14:LEU:CD2	34:i:74:HIS:O	2.69	0.40
12:L:52:LEU:O	12:L:53:MET:C	2.62	0.40
12:L:400:ASN:HD22	12:L:409:LEU:HD11	1.85	0.40
55:L:701:3PE:H381	35:j:71:TRP:CH2	2.56	0.40
13:M:53:SER:O	13:M:54:ASN:C	2.63	0.40
13:M:158:ILE:CG2	14:N:283:ALA:HB1	2.50	0.40
13:M:263:LEU:HD21	38:m:105:PHE:HD2	1.86	0.40
13:M:313:THR:HG21	13:M:456:GLY:CA	2.47	0.40
13:M:394:ILE:O	13:M:398:ILE:HG13	2.22	0.40
14:N:109:ALA:O	14:N:112:HIS:ND1	2.52	0.40
14:N:215:MET:HE3	14:N:215:MET:HB3	1.96	0.40
17:Q:112:MET:CE	42:q:126:PRO:HB3	2.51	0.40
19:S:18:GLU:OE2	19:S:68:ARG:NE	2.50	0.40
20:T:105:MET:HE3	20:T:139:MET:HE2	2.03	0.40
23:X:60:GLY:C	25:Z:81:ARG:NH2	2.79	0.40
27:b:66:VAL:HG13	27:b:66:VAL:O	2.20	0.40
32:g:115:TRP:CD1	41:p:65:HIS:CE1	3.10	0.40
62:h:201:CDL:H131	55:i:201:3PE:H321	2.03	0.40
35:j:47:PHE:O	35:j:48:PRO:C	2.62	0.40
40:o:52:THR:O	40:o:53:LEU:C	2.62	0.40
42:q:43:LYS:O	42:q:44:TYR:CB	2.70	0.40
45:AA:184:PHE:O	45:AA:188:HIS:ND1	2.44	0.40
47:AC:145:VAL:O	49:Ae:220:LEU:HD22	2.21	0.40
49:AE:168:LYS:NZ	49:AE:171:GLY:HA2	2.36	0.40
52:AH:38:LEU:O	52:AH:42:VAL:N	2.42	0.40
45:Aa:111:LYS:HG3	46:Ab:305:THR:HG21	2.04	0.40
45:Aa:310:ILE:HG21	45:Aa:379:LEU:CD2	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:78:GLY:O	46:Ab:79:THR:C	2.61	0.40
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG21	2.03	0.40
50:Af:101:GLU:O	50:Af:105:ARG:HG3	2.21	0.40
1:A:91:ALA:O	1:A:92:PHE:C	2.64	0.40
3:C:208:GLU:HG3	3:C:221:GLU:HG3	2.00	0.40
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.51	0.40
4:D:275:ILE:HG22	4:D:450:ILE:HD11	2.02	0.40
5:E:107:PRO:O	5:E:108:PRO:C	2.64	0.40
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.40
6:F:128:ARG:HA	6:F:131:MET:CE	2.51	0.40
7:G:161:GLU:OE2	18:R:96:ASP:HB3	2.22	0.40
7:G:381:LEU:HD21	19:S:41:TYR:CZ	2.56	0.40
7:G:403:VAL:O	7:G:476:LEU:HD12	2.21	0.40
7:G:557:ARG:HD3	42:q:144:TYR:CE2	2.56	0.40
7:G:611:THR:HG23	17:Q:104:ARG:O	2.20	0.40
8:H:24:GLU:OE1	8:H:228:TYR:CE2	2.74	0.40
8:H:65:THR:HG22	8:H:67:SER:N	2.37	0.40
8:H:130:PHE:CZ	8:H:134:ARG:HD2	2.56	0.40
8:H:142:TYR:CE2	8:H:289:LEU:HD12	2.57	0.40
8:H:146:MET:CG	8:H:188:SER:HB2	2.52	0.40
8:H:314:VAL:HG23	8:H:314:VAL:O	2.22	0.40
9:I:63:TRP:HZ3	55:I:301:3PE:H322	1.85	0.40
9:I:78:PHE:HA	26:a:2:TRP:CD1	2.56	0.40
10:J:52:GLY:O	10:J:53:LEU:C	2.62	0.40
12:L:210:LEU:HD12	12:L:270:ASN:HD21	1.86	0.40
12:L:399:ILE:HG22	12:L:409:LEU:CD1	2.52	0.40
62:L:704:CDL:H372	33:h:75:LEU:HD13	2.04	0.40
13:M:197:LEU:O	13:M:201:MET:HB2	2.21	0.40
14:N:59:TYR:O	14:N:63:GLN:HG2	2.21	0.40
14:N:89:GLN:HG2	30:e:60:PHE:CD2	2.55	0.40
14:N:106:LEU:HD21	14:N:138:PRO:HB2	2.03	0.40
15:O:117:PHE:HE1	15:O:173:MET:HE1	1.80	0.40
15:O:168:VAL:CG1	15:O:241:TYR:CE1	2.97	0.40
15:O:170:LEU:CD2	15:O:184:VAL:HG13	2.51	0.40
15:O:176:GLN:CG	15:O:177:GLY:H	2.23	0.40
15:O:235:GLN:HE21	15:O:239:ASN:ND2	2.19	0.40
15:O:351:TRP:CH2	28:c:41:TRP:CH2	3.06	0.40
16:P:83:PRO:C	16:P:108:TRP:CD1	3.00	0.40
17:Q:69:GLU:HG2	17:Q:73:LYS:HG3	2.03	0.40
17:Q:71:HIS:NE2	17:Q:120:PRO:HD2	2.36	0.40
23:X:148:PRO:HG3	30:e:47:ILE:HD13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:115:MET:HE3	55:Y:201:3PE:H261	2.01	0.40
25:Z:10:MET:O	25:Z:11:PRO:C	2.63	0.40
29:d:107:LYS:HB3	29:d:111:GLU:HB3	2.04	0.40
31:f:53:GLU:C	31:f:54:VAL:HG13	2.46	0.40
32:g:112:MET:HE3	32:g:115:TRP:CE3	2.56	0.40
35:j:71:TRP:HZ3	35:j:72:ARG:NH2	2.19	0.40
37:l:129:MET:HE3	37:l:129:MET:HB2	1.89	0.40
38:m:124:LYS:HG2	38:m:125:PHE:CD2	2.57	0.40
41:p:45:VAL:O	41:p:46:THR:C	2.64	0.40
43:r:7:VAL:HG13	43:r:8:ILE:N	2.37	0.40
45:AA:453:CYS:CB	45:AA:472:ARG:HH12	2.34	0.40
46:AB:167:GLN:NE2	49:AI:43:LEU:HB3	2.36	0.40
46:AB:339:TYR:HD2	49:AI:59:ALA:HB1	1.85	0.40
46:AB:453:LEU:O	46:AB:453:LEU:HD23	2.21	0.40
47:AC:122:ALA:CB	47:AC:189:ILE:HG12	2.52	0.40
50:AF:78:LYS:HA	50:AF:81:TRP:CD2	2.57	0.40
45:Aa:91:TYR:CE1	45:Aa:95:HIS:HE1	2.39	0.40
45:Aa:152:GLN:O	45:Aa:153:ASN:CB	2.69	0.40
45:Aa:152:GLN:HE22	45:Aa:250:LEU:HA	1.86	0.40
45:Aa:387:GLU:O	45:Aa:388:VAL:C	2.64	0.40
46:Ab:65:VAL:HG11	46:Ab:213:PHE:CD2	2.56	0.40
48:Ad:118:LYS:HZ2	48:Ad:148:LEU:HB3	1.86	0.40
48:Ad:118:LYS:NZ	48:Ad:148:LEU:HD22	2.36	0.40
49:Ae:180:THR:OG1	49:Ae:183:GLU:HG3	2.22	0.40
51:Ag:28:PRO:O	51:Ag:29:SER:C	2.64	0.40
52:Ah:43:LYS:HA	52:Ah:46:GLU:OE2	2.21	0.40
1:A:88:MET:HE3	1:A:88:MET:HB2	1.80	0.40
1:A:92:PHE:HA	8:H:302:MET:HE2	2.04	0.40
2:B:96:GLY:O	2:B:97:LEU:C	2.63	0.40
2:B:175:TYR:CZ	4:D:117:HIS:HE1	2.39	0.40
3:C:118:VAL:CG1	3:C:120:THR:HG22	2.45	0.40
3:C:164:TRP:CZ2	4:D:111:PRO:HG2	2.57	0.40
4:D:112:HIS:HE1	22:W:100:TRP:NE1	2.18	0.40
4:D:305:THR:OG1	4:D:306:GLN:N	2.54	0.40
6:F:196:PHE:CE1	44:s:91:ARG:CD	2.89	0.40
7:G:49:VAL:HG11	7:G:80:VAL:HG21	2.02	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.10	0.40
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.40
7:G:546:PHE:CD1	7:G:546:PHE:N	2.89	0.40
12:L:59:MET:HE2	12:L:59:MET:HB3	1.89	0.40
12:L:67:HIS:HD2	12:L:76:LEU:O	2.05	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:172:ILE:HG22	13:M:405:MET:HE1	2.04	0.40
12:L:348:HIS:HD2	20:U:69:SER:CB	2.34	0.40
55:L:702:3PE:H221	55:L:702:3PE:H2	1.84	0.40
13:M:131:ILE:HD12	55:N:401:3PE:H362	2.02	0.40
13:M:259:TYR:HB2	13:M:260:PRO:HD3	2.03	0.40
13:M:435:THR:HG23	13:M:436:LEU:N	2.36	0.40
14:N:132:THR:HB	14:N:209:ILE:HG12	2.03	0.40
15:O:74:ALA:HB1	15:O:85:HIS:CD2	2.56	0.40
16:P:132:ARG:NH2	64:P:401:NDP:O2X	2.53	0.40
16:P:175:LYS:HE2	16:P:175:LYS:HB3	1.89	0.40
22:W:58:THR:O	22:W:59:VAL:C	2.62	0.40
23:X:49:GLU:HG3	23:X:50:GLU:N	2.36	0.40
23:X:141:PRO:O	23:X:142:TYR:CB	2.69	0.40
25:Z:10:MET:HE2	25:Z:10:MET:HB2	1.59	0.40
27:b:25:VAL:O	27:b:26:TRP:C	2.62	0.40
27:b:80:TRP:HE3	27:b:84:LEU:HD13	1.87	0.40
30:e:69:ARG:CD	30:e:72:THR:HG21	2.50	0.40
31:f:37:PHE:HZ	41:p:83:LEU:HD13	1.86	0.40
33:h:148:GLU:O	33:h:152:LYS:HG3	2.21	0.40
34:i:89:HIS:NE2	55:i:201:3PE:H221	2.37	0.40
34:i:99:SER:O	34:i:100:SER:C	2.64	0.40
34:i:125:ASP:OD1	34:i:127:HIS:HB2	2.21	0.40
42:q:66:THR:O	42:q:67:GLU:HG3	2.21	0.40
43:r:58:ASP:OD1	43:r:58:ASP:O	2.39	0.40
45:AA:100:GLY:HA2	45:AA:104:ARG:O	2.21	0.40
45:AA:174:GLU:C	45:AA:176:ASP:H	2.27	0.40
45:AA:383:ALA:O	45:AA:384:THR:C	2.64	0.40
46:AB:38:LEU:HD13	46:AB:52:LEU:HB2	2.02	0.40
47:AC:9:PRO:HG3	47:Ac:202:GLU:CD	2.45	0.40
47:AC:100:ARG:HH22	67:AC:402:HEM:HBD1	1.86	0.40
47:AC:220:PHE:CE2	68:AC:403:UQ6:H4M2	2.56	0.40
47:AC:280:ILE:HD13	47:AC:297:SER:HB2	2.02	0.40
47:AC:295:ILE:HG22	47:AC:299:LEU:HD12	2.03	0.40
48:AD:150:GLU:CD	48:AD:150:GLU:O	2.64	0.40
48:AD:154:VAL:C	48:AD:156:ASP:N	2.79	0.40
48:AD:195:PRO:O	48:AD:196:ASP:C	2.64	0.40
48:AD:210:TYR:O	48:AD:211:VAL:C	2.63	0.40
51:AG:35:ILE:O	51:AG:36:PRO:C	2.63	0.40
51:AG:56:VAL:O	51:AG:59:ILE:N	2.54	0.40
53:AJ:23:LEU:HD22	54:AK:23:MET:HG3	2.00	0.40
46:Ab:43:LEU:HD12	46:Ab:47:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:117:GLU:HB2	46:Ab:330:TYR:HD1	1.85	0.40
46:Ab:453:LEU:HD23	46:Ab:453:LEU:O	2.21	0.40
47:Ac:283:SER:OG	47:Ac:284:ILE:HD12	2.22	0.40
48:Ad:121:CYS:O	48:Ad:124:CYS:N	2.52	0.40
48:Ad:189:ASN:CG	69:Ad:401:HEC:HMD3	2.47	0.40
52:Ah:47:ARG:O	52:Ah:50:LEU:HB2	2.22	0.40
52:Ah:72:PHE:O	52:Ah:73:LEU:C	2.63	0.40
1:A:30:TYR:O	1:A:31:SER:HB2	2.20	0.40
3:C:236:SER:HA	3:C:237:PRO:HD3	1.84	0.40
4:D:113:ILE:HG23	4:D:432:LEU:HD21	2.03	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.37	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.57	0.40
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.56	0.40
8:H:30:TYR:HB3	9:I:77:LEU:HA	2.03	0.40
9:I:192:ASN:OD1	9:I:193:ASN:N	2.54	0.40
11:K:82:SER:HA	11:K:86:GLY:H	1.85	0.40
12:L:277:MET:HG3	12:L:318:GLY:HA3	2.04	0.40
12:L:371:SER:O	12:L:374:VAL:HG12	2.21	0.40
12:L:466:PHE:CD1	12:L:470:TYR:HE2	2.39	0.40
55:L:705:3PE:H3A2	13:M:155:ILE:HD13	2.03	0.40
13:M:5:ILE:CG1	13:M:6:LEU:N	2.85	0.40
13:M:186:LEU:CB	13:M:253:LEU:HD13	2.52	0.40
13:M:449:THR:OG1	55:M:502:3PE:H281	2.22	0.40
14:N:264:TRP:CZ2	23:X:168:PHE:CG	3.09	0.40
14:N:307:THR:CA	15:O:319:ILE:HG12	2.52	0.40
16:P:64:PHE:CE2	16:P:242:VAL:HG22	2.56	0.40
17:Q:55:VAL:HG11	22:W:79:PRO:HD2	2.03	0.40
19:S:35:ASP:HA	19:S:38:VAL:HG22	2.03	0.40
19:S:62:GLN:HA	19:S:63:PRO:HD3	1.98	0.40
20:T:111:ASP:O	20:T:112:SER:C	2.64	0.40
20:U:87:LEU:C	20:U:89:LEU:H	2.29	0.40
23:X:60:GLY:C	25:Z:81:ARG:HH22	2.30	0.40
24:Y:64:THR:O	24:Y:68:ILE:HG23	2.20	0.40
29:d:99:GLU:HG2	29:d:100:ASP:OD1	2.22	0.40
30:e:87:MET:HG2	30:e:92:TYR:O	2.21	0.40
34:i:120:MET:SD	34:i:123:PHE:CZ	3.15	0.40
37:l:160:GLN:OE1	40:o:37:ARG:NH2	2.54	0.40
40:o:3:ALA:O	40:o:6:THR:N	2.55	0.40
43:r:18:GLN:O	43:r:20:LEU:HG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:86:ASN:OD1	45:AA:86:ASN:N	2.54	0.40
45:AA:361:ASP:OD1	45:AA:361:ASP:N	2.55	0.40
47:AC:296:LEU:O	47:AC:297:SER:C	2.64	0.40
48:AD:137:GLY:N	48:AD:140:TYR:O	2.51	0.40
48:AD:239:GLY:C	48:AD:241:ALA:N	2.78	0.40
49:AE:236:CYS:HA	49:AE:237:PRO:HD2	1.91	0.40
50:AF:29:LYS:HA	50:AF:81:TRP:CD1	2.57	0.40
52:AH:47:ARG:NH1	52:AH:47:ARG:HB2	2.36	0.40
45:Aa:120:LEU:CD2	46:Ab:299:ILE:HG23	2.51	0.40
46:Ab:297:PRO:CB	46:Ab:304:ASN:OD1	2.69	0.40
46:Ab:303:ASN:O	46:Ab:304:ASN:C	2.63	0.40
46:Ab:426:LYS:HA	46:Ab:429:LYS:NZ	2.36	0.40
47:Ac:97:HIS:CE1	47:Ac:100:ARG:NH2	2.90	0.40
47:Ac:100:ARG:HH12	67:Ac:402:HEM:CBD	2.35	0.40
48:Ad:129:TYR:HD2	48:Ad:198:SER:CB	2.35	0.40
48:Ad:199:TYR:HA	48:Ad:278:SER:OG	2.21	0.40
48:Ad:228:ARG:O	48:Ad:231:LEU:HB2	2.20	0.40
48:Ad:255:TYR:CD2	48:Ad:261:ALA:HB2	2.56	0.40
48:Ad:266:VAL:O	48:Ad:270:VAL:HG12	2.21	0.40
50:Af:36:ASP:OD1	50:Af:90:TYR:OH	2.38	0.40
51:Ag:47:LEU:HD21	55:Ag:103:3PE:H3H2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
2	B	153/224 (68%)	141 (92%)	11 (7%)	1 (1%)	18	54
3	C	196/263 (74%)	189 (96%)	7 (4%)	0	100	100
4	D	423/463 (91%)	398 (94%)	24 (6%)	1 (0%)	43	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	208/248 (84%)	194 (93%)	14 (7%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	635 (93%)	50 (7%)	0	100	100
8	H	313/318 (98%)	281 (90%)	31 (10%)	1 (0%)	36	71
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	J	157/172 (91%)	148 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	573 (95%)	31 (5%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
16	P	337/377 (89%)	309 (92%)	28 (8%)	0	100	100
17	Q	114/175 (65%)	100 (88%)	14 (12%)	0	100	100
18	R	81/116 (70%)	72 (89%)	9 (11%)	0	100	100
19	S	81/99 (82%)	74 (91%)	7 (9%)	0	100	100
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
20	U	87/156 (56%)	81 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	167/172 (97%)	148 (89%)	19 (11%)	0	100	100
24	Y	137/143 (96%)	132 (96%)	5 (4%)	0	100	100
25	Z	136/144 (94%)	129 (95%)	5 (4%)	2 (2%)	8	38
26	a	65/70 (93%)	59 (91%)	6 (9%)	0	100	100
27	b	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	i	91/128 (71%)	81 (89%)	10 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	71/104 (68%)	68 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	176/179 (98%)	165 (94%)	10 (6%)	1 (1%)	21	58
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
41	p	170/176 (97%)	153 (90%)	17 (10%)	0	100	100
42	q	119/145 (82%)	110 (92%)	9 (8%)	0	100	100
43	r	78/113 (69%)	75 (96%)	3 (4%)	0	100	100
44	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
45	AA	389/480 (81%)	372 (96%)	17 (4%)	0	100	100
45	Aa	386/480 (80%)	369 (96%)	17 (4%)	0	100	100
46	AB	416/453 (92%)	408 (98%)	8 (2%)	0	100	100
46	Ab	416/453 (92%)	396 (95%)	20 (5%)	0	100	100
47	AC	371/381 (97%)	361 (97%)	10 (3%)	0	100	100
47	Ac	371/381 (97%)	366 (99%)	5 (1%)	0	100	100
48	AD	234/325 (72%)	213 (91%)	21 (9%)	0	100	100
48	Ad	237/325 (73%)	224 (94%)	12 (5%)	1 (0%)	30	66
49	AE	101/274 (37%)	95 (94%)	6 (6%)	0	100	100
49	AI	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
49	Ae	184/274 (67%)	168 (91%)	15 (8%)	1 (0%)	24	62
49	Ai	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
50	AF	95/111 (86%)	94 (99%)	1 (1%)	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
51	Ag	72/82 (88%)	72 (100%)	0	0	100	100
52	AH	62/89 (70%)	61 (98%)	1 (2%)	0	100	100
52	Ah	58/89 (65%)	55 (95%)	3 (5%)	0	100	100
53	AJ	19/64 (30%)	19 (100%)	0	0	100	100
53	Aj	41/64 (64%)	40 (98%)	1 (2%)	0	100	100
54	AK	15/56 (27%)	15 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Ak	36/56 (64%)	34 (94%)	2 (6%)	0	100	100
All	All	11672/14392 (81%)	11022 (94%)	641 (6%)	9 (0%)	49	82

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	324	GLY
8	H	196	ALA
14	N	109	ALA
25	Z	129	THR
2	B	195	PRO
25	Z	18	PRO
39	n	156	PRO
49	Ae	160	PRO
48	Ad	194	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	89/104 (86%)	88 (99%)	1 (1%)	65	73
2	B	131/185 (71%)	129 (98%)	2 (2%)	57	70
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	368/395 (93%)	366 (100%)	2 (0%)	81	81
5	E	182/206 (88%)	180 (99%)	2 (1%)	65	73
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	84
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	279/280 (100%)	277 (99%)	2 (1%)	76	78
9	I	146/178 (82%)	146 (100%)	0	100	100
10	J	129/137 (94%)	126 (98%)	3 (2%)	44	64
11	K	87/88 (99%)	87 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	85
14	N	307/308 (100%)	305 (99%)	2 (1%)	76	78
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	296/325 (91%)	295 (100%)	1 (0%)	86	84
17	Q	103/153 (67%)	101 (98%)	2 (2%)	50	66
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	82/135 (61%)	82 (100%)	0	100	100
21	V	100/102 (98%)	98 (98%)	2 (2%)	48	65
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	119/123 (97%)	119 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	92 (99%)	1 (1%)	65	73
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	90/120 (75%)	89 (99%)	1 (1%)	65	73
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	80
40	o	112/121 (93%)	112 (100%)	0	100	100
41	p	156/158 (99%)	156 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	76/96 (79%)	75 (99%)	1 (1%)	61	71
44	s	23/95 (24%)	23 (100%)	0	100	100
45	AA	333/398 (84%)	332 (100%)	1 (0%)	86	84
45	Aa	332/398 (83%)	332 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	327 (100%)	1 (0%)	86	84
47	AC	325/333 (98%)	323 (99%)	2 (1%)	78	80
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	201/260 (77%)	201 (100%)	0	100	100
48	Ad	204/260 (78%)	201 (98%)	3 (2%)	57	70
49	AE	86/224 (38%)	86 (100%)	0	100	100
49	AI	21/224 (9%)	20 (95%)	1 (5%)	23	45
49	Ae	158/224 (70%)	156 (99%)	2 (1%)	61	71
49	Ai	21/224 (9%)	20 (95%)	1 (5%)	23	45
50	AF	89/99 (90%)	89 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	67/74 (90%)	67 (100%)	0	100	100
52	AH	61/83 (74%)	60 (98%)	1 (2%)	55	69
52	Ah	59/83 (71%)	59 (100%)	0	100	100
53	AJ	16/55 (29%)	16 (100%)	0	100	100
53	Aj	34/55 (62%)	34 (100%)	0	100	100
54	AK	10/46 (22%)	10 (100%)	0	100	100
54	Ak	29/46 (63%)	29 (100%)	0	100	100
All	All	10260/12260 (84%)	10218 (100%)	42 (0%)	81	82

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
2	B	82	ILE
2	B	177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	94	VAL
4	D	127	LYS
5	E	99	LYS
5	E	200	ILE
6	F	137	LYS
7	G	271	MET
8	H	87	VAL
8	H	144	VAL
10	J	3	ASN
10	J	60	LEU
10	J	65	VAL
12	L	3	ILE
12	L	69	VAL
13	M	218	LYS
14	N	148	LEU
14	N	159	ILE
16	P	318	LYS
17	Q	125	VAL
17	Q	135	ILE
19	S	48	HIS
21	V	51	ILE
21	V	93	LYS
30	e	91	LYS
34	i	72	VAL
39	n	98	LYS
43	r	91	GLU
45	AA	387	GLU
47	AC	51	LEU
47	AC	294	LEU
52	AH	42	VAL
49	AI	45	VAL
46	Ab	168	ASN
47	Ac	294	LEU
48	Ad	201	VAL
48	Ad	225	VAL
48	Ad	252	VAL
49	Ae	135	GLN
49	Ae	152	ILE
49	Ai	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (244) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	207	GLN
2	B	209	GLN
3	C	88	HIS
3	C	102	HIS
3	C	130	ASN
3	C	163	ASN
3	C	195	HIS
4	D	36	GLN
4	D	79	ASN
4	D	92	HIS
4	D	117	HIS
4	D	147	ASN
4	D	149	GLN
4	D	168	GLN
4	D	182	ASN
4	D	234	GLN
4	D	270	ASN
4	D	285	ASN
4	D	313	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	245	GLN
6	F	116	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	51	GLN
7	G	74	ASN
7	G	101	ASN
7	G	140	GLN
7	G	205	GLN
7	G	384	ASN
7	G	388	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	571	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	572	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	124	ASN
8	H	171	HIS
8	H	284	GLN
8	H	287	HIS
8	H	292	ASN
9	I	180	HIS
11	K	7	ASN
12	L	2	ASN
12	L	25	ASN
12	L	58	ASN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	170	GLN
12	L	192	ASN
12	L	194	ASN
12	L	199	GLN
12	L	209	ASN
12	L	264	HIS
12	L	269	ASN
12	L	296	ASN
12	L	321	GLN
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	ASN
12	L	505	ASN
12	L	579	ASN
12	L	605	ASN
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN
13	M	138	ASN
13	M	170	HIS
13	M	175	ASN
13	M	213	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	374	ASN
13	M	415	GLN
14	N	120	GLN
14	N	134	GLN
14	N	273	ASN
14	N	289	ASN
14	N	310	ASN
15	O	80	GLN
15	O	155	GLN
15	O	175	ASN
15	O	225	HIS
15	O	239	ASN
15	O	286	GLN
15	O	292	HIS
15	O	306	ASN
15	O	323	GLN
16	P	79	GLN
16	P	128	ASN
16	P	251	ASN
16	P	285	HIS
17	Q	86	ASN
17	Q	88	GLN
19	S	22	HIS
19	S	48	HIS
19	S	81	ASN
19	S	92	GLN
20	T	103	HIS
20	U	101	ASN
21	V	50	GLN
21	V	110	ASN
22	W	54	GLN
22	W	61	GLN
22	W	102	GLN
22	W	105	HIS
22	W	129	HIS
23	X	64	ASN
23	X	99	HIS
24	Y	19	GLN
24	Y	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Y	91	ASN
25	Z	24	ASN
25	Z	90	ASN
25	Z	137	ASN
27	b	46	ASN
28	c	62	HIS
29	d	59	HIS
31	f	13	HIS
33	h	109	HIS
33	h	154	GLN
33	h	170	GLN
33	h	181	HIS
33	h	189	ASN
34	i	83	HIS
34	i	127	HIS
34	i	128	HIS
35	j	83	HIS
36	k	39	GLN
36	k	66	ASN
37	l	83	GLN
37	l	91	GLN
37	l	106	HIS
37	l	115	ASN
37	l	154	GLN
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	13	GLN
39	n	14	GLN
39	n	26	HIS
39	n	33	HIS
39	n	53	ASN
39	n	62	GLN
39	n	74	ASN
39	n	139	GLN
40	o	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	17	HIS
42	q	91	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	q	135	HIS
43	r	18	GLN
43	r	21	GLN
43	r	29	GLN
44	s	76	ASN
45	AA	103	ASN
45	AA	119	HIS
45	AA	152	GLN
45	AA	173	GLN
45	AA	240	GLN
45	AA	249	HIS
45	AA	301	ASN
45	AA	305	GLN
45	AA	342	GLN
45	AA	345	ASN
45	AA	397	ASN
45	AA	402	HIS
46	AB	280	ASN
46	AB	284	ASN
46	AB	298	HIS
46	AB	357	GLN
46	AB	365	ASN
46	AB	415	GLN
46	AB	443	ASN
47	AC	8	HIS
47	AC	32	ASN
47	AC	312	GLN
48	AD	189	ASN
48	AD	240	GLN
49	AE	135	GLN
49	AE	227	ASN
49	AE	242	HIS
50	AF	39	HIS
50	AF	74	GLN
51	AG	7	ASN
51	AG	24	GLN
51	AG	37	ASN
51	AG	69	GLN
52	AH	37	GLN
52	AH	82	HIS
49	AI	71	ASN
45	Aa	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	Aa	95	HIS
45	Aa	173	GLN
45	Aa	207	ASN
45	Aa	240	GLN
45	Aa	247	GLN
45	Aa	286	HIS
45	Aa	342	GLN
45	Aa	397	ASN
45	Aa	402	HIS
46	Ab	211	ASN
46	Ab	212	HIS
46	Ab	284	ASN
46	Ab	304	ASN
46	Ab	357	GLN
46	Ab	365	ASN
46	Ab	415	GLN
46	Ab	443	ASN
47	Ac	32	ASN
47	Ac	221	HIS
47	Ac	312	GLN
48	Ad	115	GLN
48	Ad	189	ASN
48	Ad	284	HIS
48	Ad	309	HIS
49	Ae	131	ASN
49	Ae	164	ASN
49	Ae	200	HIS
49	Ae	219	HIS
49	Ae	239	HIS
50	Af	80	GLN
51	Ag	69	GLN
52	Ah	82	HIS
54	Ak	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 1 is monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
56	SF4	F	502	6	0,12,12	-	-	-		
58	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.11	3 (7%)
64	NDP	P	401	-	49,52,52	1.20	6 (12%)	66,80,80	1.67	12 (18%)
66	EHZ	W	201	-	27,31,37	1.73	5 (18%)	37,41,47	1.55	5 (13%)
55	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.10	4 (8%)
55	3PE	N	401	-	50,50,50	0.91	2 (4%)	53,55,55	1.06	4 (7%)
69	HEC	Ad	401	48	50,50,50	1.71	5 (10%)	68,82,82	1.35	7 (10%)
56	SF4	I	303	9	0,12,12	-	-	-		
67	HEM	Ac	402	47	50,50,50	1.60	8 (16%)	66,82,82	1.91	15 (22%)
61	UQ9	H	400	-	35,35,58	0.80	2 (5%)	42,45,73	0.47	0
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.13	4 (7%)
62	CDL	X	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.27	7 (9%)
55	3PE	Y	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.17	5 (11%)
55	3PE	H	401	-	47,47,50	0.93	2 (4%)	50,52,55	1.11	3 (6%)
55	3PE	i	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.05	2 (4%)
55	3PE	m	203	-	40,40,50	1.00	2 (5%)	43,45,55	1.12	3 (6%)
59	FES	E	301	5	0,4,4	-	-	-		
68	UQ6	Ac	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.51	6 (18%)
63	ADP	O	401	-	27,29,29	1.32	4 (14%)	42,45,45	2.01	11 (26%)
62	CDL	Ag	102	-	55,55,99	1.21	4 (7%)	61,67,111	1.24	6 (9%)
55	3PE	m	202	-	50,50,50	0.91	2 (4%)	53,55,55	1.14	4 (7%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
57	UQ1	B	302	-	18,18,18	1.96	2 (11%)	22,25,25	1.25	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.19	6 (12%)
67	HEM	Ac	401	47	50,50,50	1.31	8 (16%)	66,82,82	1.69	15 (22%)
56	SF4	G	801	7	0,12,12	-	-	-	-	-
62	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
55	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.14	3 (7%)
56	SF4	B	301	2	0,12,12	-	-	-	-	-
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.15	4 (7%)
55	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.14	3 (8%)
69	HEC	AD	401	48	50,50,50	2.80	25 (50%)	68,82,82	2.45	26 (38%)
62	CDL	L	704	-	77,77,99	1.01	4 (5%)	83,89,111	1.13	6 (7%)
55	3PE	I	301	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	2 (3%)
55	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.20	3 (7%)
59	FES	G	803	7	0,4,4	-	-	-	-	-
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.20	6 (9%)
67	HEM	AC	401	47	50,50,50	1.55	6 (12%)	66,82,82	1.78	12 (18%)
67	HEM	AC	402	47	50,50,50	1.59	8 (16%)	66,82,82	1.80	17 (25%)
55	3PE	L	705	-	37,37,50	1.03	2 (5%)	40,42,55	1.13	3 (7%)
68	UQ6	AC	403	-	28,28,43	2.47	6 (21%)	33,37,55	1.67	10 (30%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.26	4 (10%)
55	3PE	A	201	-	41,41,50	1.01	2 (4%)	44,46,55	1.09	2 (4%)
55	3PE	Aa	501	-	22,22,50	1.36	2 (9%)	25,27,55	1.20	3 (12%)
55	3PE	L	703	-	39,39,50	1.02	2 (5%)	42,44,55	1.15	3 (7%)
56	SF4	I	302	9	0,12,12	-	-	-	-	-
58	PC1	B	304	-	42,42,53	1.04	2 (4%)	48,50,61	1.01	3 (6%)
66	EHZ	n	201	-	27,31,37	1.87	7 (25%)	37,41,47	1.58	6 (16%)
56	SF4	G	802	7	0,12,12	-	-	-	-	-
70	U10	Ac	404	-	23,23,63	1.25	3 (13%)	28,31,79	2.09	7 (25%)
55	3PE	m	201	-	46,46,50	0.96	2 (4%)	49,51,55	1.11	3 (6%)
55	3PE	Ag	103	-	37,37,50	1.06	2 (5%)	40,42,55	1.20	3 (7%)
55	3PE	d	201	-	30,30,50	1.14	2 (6%)	33,35,55	1.31	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	B	303	-	-	13/38/38/57	-
56	SF4	F	502	6	-	-	0/6/5/5
64	NDP	P	401	-	-	6/34/77/77	0/5/5/5
66	EHZ	W	201	-	-	12/39/39/45	-
55	3PE	K	101	-	-	17/49/49/54	-
55	3PE	N	401	-	-	11/54/54/54	-
56	SF4	I	303	9	-	-	0/6/5/5
67	HEM	Ac	402	47	-	7/14/54/54	-
61	UQ9	H	400	-	-	16/30/54/81	0/1/1/1
55	3PE	L	702	-	-	13/52/52/54	-
62	CDL	X	201	-	-	25/77/77/110	-
55	3PE	Y	201	-	-	10/44/44/54	-
55	3PE	H	401	-	-	13/51/51/54	-
55	3PE	i	201	-	-	16/43/43/54	-
55	3PE	m	203	-	-	7/44/44/54	-
68	UQ6	Ac	405	-	-	5/21/21/39	0/1/1/1
59	FES	E	301	5	-	-	0/1/1/1
63	ADP	O	401	-	-	2/16/32/32	0/3/3/3
62	CDL	Ag	102	-	-	18/66/66/110	-
55	3PE	m	202	-	-	8/54/54/54	-
62	CDL	h	201	-	-	23/80/80/110	-
57	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
67	HEM	Ac	401	47	-	9/14/54/54	-
56	SF4	G	801	7	-	-	0/6/5/5
62	CDL	Ag	101	-	-	11/52/52/110	-
55	3PE	L	701	-	-	5/43/43/54	-
56	SF4	B	301	2	-	-	0/6/5/5
55	3PE	M	502	-	-	13/54/54/54	-
69	HEC	AD	401	48	1/1/3/7	8/14/54/54	-
69	HEC	Ad	401	48	1/1/3/7	0/14/54/54	-
55	3PE	Ac	403	-	-	2/38/38/54	-
55	3PE	I	301	-	-	17/54/54/54	-
55	3PE	M	501	-	-	14/40/40/54	-
62	CDL	L	704	-	-	28/88/88/110	-
62	CDL	a	101	-	-	18/67/67/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	HEM	AC	401	47	-	9/14/54/54	-
67	HEM	AC	402	47	-	6/14/54/54	-
55	3PE	L	705	-	-	14/41/41/54	-
68	UQ6	AC	403	-	-	3/21/21/39	0/1/1/1
71	3PH	Ad	402	-	-	9/37/37/49	-
59	FES	G	803	7	-	-	0/1/1/1
55	3PE	A	201	-	-	12/45/45/54	-
55	3PE	Aa	501	-	-	5/26/26/54	-
55	3PE	L	703	-	-	7/43/43/54	-
58	PC1	B	304	-	-	14/46/46/57	-
66	EHZ	n	201	-	-	13/39/39/45	-
56	SF4	I	302	9	-	-	0/6/5/5
56	SF4	G	802	7	-	-	0/6/5/5
70	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
55	3PE	m	201	-	-	10/50/50/54	-
55	3PE	Ag	103	-	-	8/41/41/54	-
55	3PE	d	201	-	-	8/34/34/54	-

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	Ad	401	HEC	C3D-C2D	7.94	1.53	1.36
57	B	302	UQ1	C6-C5	7.34	1.48	1.35
68	AC	403	UQ6	C5-C4	5.98	1.49	1.39
68	Ac	405	UQ6	C5-C6	5.97	1.49	1.40
68	Ac	405	UQ6	C2-C3	5.90	1.49	1.39
68	AC	403	UQ6	C2-C3	5.86	1.48	1.39
68	Ac	405	UQ6	C5-C4	5.82	1.48	1.39
68	AC	403	UQ6	C5-C6	5.79	1.48	1.40
67	AC	401	HEM	FE-NB	5.47	2.11	1.94
66	n	201	EHZ	C15-N2	5.24	1.45	1.33
67	AC	402	HEM	FE-NB	5.17	2.10	1.94
66	W	201	EHZ	C15-N2	5.16	1.44	1.33
66	n	201	EHZ	C12-N1	5.13	1.45	1.33
68	Ac	405	UQ6	C6-C1	5.12	1.49	1.40
68	AC	403	UQ6	C6-C1	5.05	1.48	1.40
66	W	201	EHZ	C12-N1	5.03	1.44	1.33
69	AD	401	HEC	C2A-C3A	4.97	1.47	1.36
67	Ac	402	HEM	FE-NB	4.94	2.10	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	AD	401	HEC	C3B-C2B	4.91	1.47	1.36
69	AD	401	HEC	FE-ND	4.89	2.10	1.94
69	AD	401	HEC	FE-NB	4.89	2.10	1.94
60	F	501	FMN	C9A-C5A	4.84	1.49	1.41
69	AD	401	HEC	CHA-C1A	4.79	1.47	1.38
69	AD	401	HEC	C3D-C2D	4.75	1.46	1.36
68	Ac	405	UQ6	C4-C3	4.64	1.49	1.39
69	AD	401	HEC	CHC-C4B	4.62	1.47	1.38
69	AD	401	HEC	CHB-C4A	4.59	1.47	1.38
68	AC	403	UQ6	C4-C3	4.59	1.49	1.39
69	AD	401	HEC	FE-NA	4.50	2.10	1.95
69	AD	401	HEC	FE-NC	4.46	2.10	1.95
69	AD	401	HEC	CHD-C1D	4.36	1.47	1.38
62	a	101	CDL	OA8-CA7	4.31	1.45	1.33
67	Ac	402	HEM	FE-NC	4.28	2.09	1.95
55	A	201	3PE	O31-C31	4.28	1.45	1.33
68	Ac	405	UQ6	C2-C1	4.27	1.49	1.40
62	X	201	CDL	OB8-CB7	4.27	1.45	1.33
62	Ag	101	CDL	OA8-CA7	4.26	1.45	1.33
62	Ag	101	CDL	OB8-CB7	4.25	1.45	1.33
55	K	101	3PE	O31-C31	4.24	1.45	1.33
55	m	202	3PE	O31-C31	4.23	1.45	1.33
55	N	401	3PE	O31-C31	4.23	1.45	1.33
55	m	201	3PE	O31-C31	4.22	1.45	1.33
55	m	201	3PE	O21-C21	4.21	1.46	1.34
55	i	201	3PE	O31-C31	4.21	1.45	1.33
62	X	201	CDL	OA8-CA7	4.20	1.45	1.33
58	B	303	PC1	O31-C31	4.20	1.45	1.33
55	Aa	501	3PE	O31-C31	4.20	1.45	1.33
55	M	501	3PE	O21-C21	4.20	1.46	1.34
63	O	401	ADP	C5-C4	4.20	1.46	1.39
55	M	501	3PE	O31-C31	4.19	1.45	1.33
55	L	703	3PE	O31-C31	4.19	1.45	1.33
68	AC	403	UQ6	C2-C1	4.18	1.48	1.40
62	L	704	CDL	OB8-CB7	4.18	1.45	1.33
55	L	701	3PE	O31-C31	4.17	1.45	1.33
55	Y	201	3PE	O21-C21	4.17	1.46	1.34
55	m	203	3PE	O31-C31	4.17	1.45	1.33
55	Ag	103	3PE	O31-C31	4.17	1.45	1.33
58	B	304	PC1	O31-C31	4.16	1.45	1.33
55	Ag	103	3PE	O21-C21	4.16	1.46	1.34
62	a	101	CDL	OB8-CB7	4.16	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B	304	PC1	O21-C21	4.16	1.46	1.34
55	I	301	3PE	O31-C31	4.15	1.45	1.33
55	L	705	3PE	O31-C31	4.15	1.45	1.33
62	Ag	102	CDL	OB8-CB7	4.14	1.45	1.33
55	Y	201	3PE	O31-C31	4.13	1.45	1.33
55	M	502	3PE	O31-C31	4.13	1.45	1.33
55	L	701	3PE	O21-C21	4.13	1.45	1.34
62	h	201	CDL	OA8-CA7	4.13	1.45	1.33
64	P	401	NDP	C5A-C4A	4.12	1.46	1.39
55	H	401	3PE	O31-C31	4.12	1.45	1.33
62	Ag	102	CDL	OA8-CA7	4.12	1.45	1.33
62	h	201	CDL	OB8-CB7	4.11	1.45	1.33
55	Ac	403	3PE	O31-C31	4.11	1.45	1.33
62	L	704	CDL	OB6-CB5	4.11	1.45	1.34
55	i	201	3PE	O21-C21	4.11	1.45	1.34
71	Ad	402	3PH	O21-C21	4.08	1.45	1.34
55	I	301	3PE	O21-C21	4.08	1.45	1.34
62	h	201	CDL	OB6-CB5	4.07	1.45	1.34
55	H	401	3PE	O21-C21	4.06	1.45	1.34
55	A	201	3PE	O21-C21	4.06	1.45	1.34
55	d	201	3PE	O31-C31	4.05	1.45	1.33
62	a	101	CDL	OA6-CA5	4.04	1.45	1.34
62	Ag	101	CDL	OA6-CA5	4.03	1.45	1.34
62	h	201	CDL	OA6-CA5	4.03	1.45	1.34
55	L	702	3PE	O31-C31	4.03	1.45	1.33
62	Ag	102	CDL	OA6-CA5	4.02	1.45	1.34
55	Aa	501	3PE	O21-C21	4.01	1.45	1.34
62	Ag	102	CDL	OB6-CB5	3.99	1.45	1.34
62	L	704	CDL	OA8-CA7	3.99	1.45	1.33
55	m	202	3PE	O21-C21	3.98	1.45	1.34
62	X	201	CDL	OB6-CB5	3.97	1.45	1.34
55	L	703	3PE	O21-C21	3.97	1.45	1.34
71	Ad	402	3PH	O31-C31	3.97	1.44	1.33
55	K	101	3PE	O21-C21	3.96	1.45	1.34
55	d	201	3PE	O21-C21	3.96	1.45	1.34
55	L	702	3PE	O21-C21	3.95	1.45	1.34
58	B	303	PC1	O21-C21	3.94	1.45	1.34
62	X	201	CDL	OA6-CA5	3.93	1.45	1.34
55	N	401	3PE	O21-C21	3.93	1.45	1.34
67	AC	402	HEM	FE-NC	3.93	2.08	1.95
62	a	101	CDL	OB6-CB5	3.93	1.45	1.34
55	m	203	3PE	O21-C21	3.92	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Ac	403	3PE	O21-C21	3.92	1.45	1.34
62	Ag	101	CDL	OB6-CB5	3.91	1.45	1.34
55	M	502	3PE	O21-C21	3.91	1.45	1.34
55	L	705	3PE	O21-C21	3.88	1.45	1.34
69	AD	401	HEC	CHC-C1C	3.85	1.48	1.39
67	AC	402	HEM	C4D-ND	-3.83	1.33	1.40
67	AC	401	HEM	C1B-NB	-3.81	1.33	1.40
62	L	704	CDL	OA6-CA5	3.81	1.45	1.34
69	AD	401	HEC	CHA-C4D	3.69	1.47	1.39
69	Ad	401	HEC	FE-ND	3.68	2.06	1.94
67	Ac	401	HEM	C4D-ND	-3.67	1.34	1.40
69	Ad	401	HEC	FE-NB	3.61	2.06	1.94
69	AD	401	HEC	CHD-C4C	3.53	1.47	1.39
67	Ac	402	HEM	C4D-ND	-3.52	1.34	1.40
67	AC	402	HEM	C1B-NB	-3.37	1.34	1.40
67	Ac	402	HEM	C1B-NB	-3.35	1.34	1.40
67	AC	401	HEM	FE-NC	3.27	2.06	1.95
64	P	401	NDP	C6N-C5N	3.25	1.39	1.33
67	AC	401	HEM	C4D-ND	-3.18	1.34	1.40
69	AD	401	HEC	C3C-C2C	3.16	1.47	1.38
69	AD	401	HEC	C1D-ND	-3.13	1.34	1.40
60	F	501	FMN	C8-C7	3.11	1.48	1.40
69	AD	401	HEC	CHB-C1B	3.10	1.46	1.39
57	B	302	UQ1	C3-C2	3.09	1.48	1.36
67	Ac	401	HEM	C1B-NB	-3.05	1.35	1.40
69	AD	401	HEC	C4B-NB	-2.98	1.35	1.40
70	Ac	404	U10	C4-C3	2.94	1.48	1.36
70	Ac	404	U10	C6-C5	-2.91	1.38	1.46
69	Ad	401	HEC	FE-NA	2.90	2.04	1.95
60	F	501	FMN	C4-N3	-2.76	1.33	1.38
67	Ac	402	HEM	C1D-ND	-2.76	1.33	1.38
67	AC	401	HEM	C1C-C2C	-2.67	1.40	1.45
61	H	400	UQ9	C3-C2	-2.66	1.41	1.48
69	Ad	401	HEC	FE-NC	2.63	2.04	1.95
63	O	401	ADP	C5-C6	2.61	1.48	1.41
66	n	201	EHZ	P1-O7	2.60	1.64	1.54
69	AD	401	HEC	C1C-C2C	2.58	1.49	1.43
70	Ac	404	U10	C3-C2	-2.56	1.41	1.48
67	Ac	401	HEM	C1C-C2C	-2.55	1.40	1.45
61	H	400	UQ9	C4-C5	-2.53	1.41	1.48
67	AC	402	HEM	FE-ND	-2.53	1.87	1.94
67	Ac	402	HEM	C1C-C2C	-2.50	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Ac	401	HEM	C1D-ND	-2.46	1.33	1.38
66	n	201	EHZ	O4-C15	-2.45	1.18	1.23
66	n	201	EHZ	C9-S1	2.45	1.82	1.76
66	W	201	EHZ	O4-C15	-2.44	1.18	1.23
64	P	401	NDP	C5A-N7A	-2.43	1.34	1.39
64	P	401	NDP	C5A-C6A	2.43	1.47	1.41
69	AD	401	HEC	C4C-NC	-2.40	1.35	1.39
69	AD	401	HEC	C4A-NA	-2.38	1.35	1.39
60	F	501	FMN	C5A-N5	-2.38	1.34	1.39
66	W	201	EHZ	O3-C12	-2.37	1.18	1.23
67	Ac	402	HEM	C1A-C2A	-2.37	1.39	1.44
64	P	401	NDP	C8A-N7A	2.36	1.36	1.31
67	Ac	401	HEM	FE-NB	2.35	2.02	1.94
63	O	401	ADP	C8-N7	2.32	1.36	1.31
69	AD	401	HEC	C1A-NA	-2.31	1.35	1.39
67	Ac	401	HEM	FE-ND	2.31	2.02	1.94
67	AC	402	HEM	C1C-C2C	-2.30	1.40	1.45
66	n	201	EHZ	P1-OP3	-2.30	1.46	1.54
67	Ac	401	HEM	C3C-C4C	-2.28	1.42	1.46
66	n	201	EHZ	O3-C12	-2.28	1.18	1.23
69	AD	401	HEC	C4D-C3D	2.28	1.49	1.45
67	AC	401	HEM	C3C-C4C	-2.28	1.42	1.46
69	AD	401	HEC	C4B-C3B	2.24	1.48	1.45
66	W	201	EHZ	C9-S1	2.23	1.81	1.76
63	O	401	ADP	C5-N7	-2.23	1.34	1.39
67	Ac	402	HEM	FE-ND	-2.18	1.88	1.94
67	AC	402	HEM	C1D-ND	-2.16	1.34	1.38
67	AC	402	HEM	C3C-C4C	-2.14	1.42	1.46
69	AD	401	HEC	C1A-C2A	2.13	1.49	1.45
67	Ac	401	HEM	C4B-NB	-2.08	1.34	1.38
64	P	401	NDP	C4A-N9A	-2.07	1.33	1.37
60	F	501	FMN	C4A-N5	2.06	1.34	1.30

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Ac	404	U10	C6-C1-C2	7.78	125.33	119.18
69	Ad	401	HEC	C1D-ND-C4D	6.34	111.63	105.07
69	AD	401	HEC	C1B-C2B-C3B	-6.22	100.42	106.96
69	AD	401	HEC	C2B-C1B-NB	6.13	117.22	109.88
67	Ac	402	HEM	CHC-C4B-NB	6.08	131.03	124.42
66	W	201	EHZ	C8-C9-S1	6.03	121.09	113.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	O	401	ADP	C5-C4-N3	-6.03	118.88	126.75
64	P	401	NDP	C5A-C4A-N3A	-6.01	118.91	126.75
67	AC	402	HEM	CHC-C4B-NB	5.76	130.67	124.42
67	AC	401	HEM	CHC-C4B-NB	5.12	129.98	124.42
66	n	201	EHZ	C8-C9-S1	5.01	119.83	113.63
69	AD	401	HEC	C1C-C2C-C3C	-4.91	101.08	106.83
67	AC	401	HEM	CHD-C4C-NC	4.84	129.68	124.44
67	AC	402	HEM	CHD-C1D-ND	4.80	129.63	124.42
63	O	401	ADP	N3-C4-N9	4.79	134.97	127.08
69	AD	401	HEC	C2A-C1A-NA	4.78	114.97	110.32
69	AD	401	HEC	C2D-C1D-ND	4.77	115.50	109.84
69	AD	401	HEC	C3D-C4D-ND	4.76	114.96	110.36
64	P	401	NDP	N3A-C4A-N9A	4.71	134.85	127.08
67	Ac	401	HEM	CHC-C4B-NB	4.71	129.53	124.42
55	m	201	3PE	O21-C21-C22	4.69	121.62	111.50
55	Ag	103	3PE	O21-C21-C22	4.69	121.61	111.50
55	M	501	3PE	O21-C21-C22	4.65	121.52	111.50
55	m	202	3PE	O21-C21-C22	4.44	121.07	111.50
62	h	201	CDL	OB6-CB5-C51	4.43	121.06	111.50
67	Ac	402	HEM	C4C-NC-C1C	4.42	109.67	105.35
62	X	201	CDL	OB6-CB5-C51	4.35	120.88	111.50
67	Ac	401	HEM	CHD-C4C-NC	4.34	129.14	124.44
55	M	502	3PE	O21-C21-C22	4.28	120.72	111.50
62	L	704	CDL	OA6-CA5-C11	4.27	120.69	111.50
67	Ac	402	HEM	C1B-NB-C4B	4.22	109.43	105.07
62	X	201	CDL	OA6-CA5-C11	4.22	120.60	111.50
62	a	101	CDL	OA6-CA5-C11	4.21	120.58	111.50
67	Ac	402	HEM	CHB-C1B-NB	4.17	129.52	124.37
55	Y	201	3PE	O21-C21-C22	4.16	120.46	111.50
69	AD	401	HEC	CHB-C1B-C2B	-4.16	118.49	124.98
68	AC	403	UQ6	C10-C9-C11	4.14	122.23	115.27
70	Ac	404	U10	C1-C6-C5	-4.13	115.69	119.58
55	K	101	3PE	O21-C21-C22	4.12	120.38	111.50
55	I	301	3PE	O21-C21-C22	4.10	120.34	111.50
62	Ag	101	CDL	OB6-CB5-C51	4.10	120.33	111.50
55	L	703	3PE	O21-C21-C22	4.05	120.22	111.50
55	H	401	3PE	O21-C21-C22	4.05	120.22	111.50
64	P	401	NDP	PN-O3-PA	-4.05	118.94	132.83
71	Ad	402	3PH	O21-C21-C22	4.03	120.19	111.50
67	Ac	401	HEM	CHB-C1B-NB	4.01	129.32	124.37
55	L	702	3PE	O21-C21-C22	4.00	120.13	111.50
67	AC	401	HEM	C1B-NB-C4B	4.00	109.20	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Ag	102	CDL	OB6-CB5-C51	3.97	120.06	111.50
62	h	201	CDL	OA6-CA5-C11	3.96	120.04	111.50
68	Ac	405	UQ6	C7-C8-C9	-3.96	121.10	127.24
62	Ag	102	CDL	OA6-CA5-C11	3.96	120.03	111.50
58	B	304	PC1	O21-C21-C22	3.96	120.03	111.50
63	O	401	ADP	C2-N3-C4	3.95	121.08	111.75
67	AC	401	HEM	CHB-C1B-NB	3.94	129.24	124.37
55	A	201	3PE	O21-C21-C22	3.92	119.96	111.50
55	d	201	3PE	O21-C21-C22	3.92	119.94	111.50
69	AD	401	HEC	C1D-C2D-C3D	-3.91	102.84	106.96
55	L	701	3PE	O21-C21-C22	3.88	119.86	111.50
67	AC	401	HEM	C4C-NC-C1C	3.85	109.12	105.35
67	Ac	402	HEM	CHD-C4C-NC	3.83	128.58	124.44
64	P	401	NDP	C2A-N3A-C4A	3.81	120.75	111.75
55	N	401	3PE	O21-C21-C22	3.78	119.64	111.50
55	i	201	3PE	O21-C21-C22	3.77	119.62	111.50
62	L	704	CDL	OB6-CB5-C51	3.77	119.62	111.50
67	AC	402	HEM	C1B-NB-C4B	3.75	108.94	105.07
55	L	705	3PE	O21-C21-C22	3.71	119.50	111.50
68	AC	403	UQ6	C7-C8-C9	-3.68	121.53	127.24
58	B	303	PC1	O21-C21-C22	3.67	119.42	111.50
55	Ac	403	3PE	O21-C21-C22	3.67	119.42	111.50
55	m	203	3PE	O21-C21-C22	3.63	119.33	111.50
67	AC	402	HEM	CHB-C1B-NB	3.60	128.82	124.37
69	AD	401	HEC	C2C-C1C-NC	3.59	115.54	110.08
69	AD	401	HEC	CBC-CAC-C3C	3.59	122.32	112.43
68	AC	403	UQ6	C6-C7-C8	-3.55	106.55	112.17
67	Ac	402	HEM	CHA-C4D-ND	3.54	128.75	124.37
62	a	101	CDL	OB6-CB5-C51	3.53	119.11	111.50
63	O	401	ADP	PA-O3A-PB	-3.52	120.75	132.83
69	AD	401	HEC	C3C-C4C-NC	3.46	114.01	110.15
62	Ag	101	CDL	OB8-CB7-C71	3.45	120.42	111.38
63	O	401	ADP	N3-C2-N1	-3.37	123.34	128.60
69	AD	401	HEC	CBB-CAB-C3B	3.33	121.60	112.43
67	Ac	401	HEM	C4D-ND-C1D	3.32	108.51	105.07
68	Ac	405	UQ6	C12-C13-C14	-3.31	119.68	127.66
62	Ag	101	CDL	OA6-CA5-C11	3.31	120.03	110.80
67	Ac	402	HEM	CHD-C1D-ND	3.27	127.97	124.42
70	Ac	404	U10	C4-C3-C2	-3.25	114.30	120.68
69	AD	401	HEC	C3A-C4A-NA	3.22	115.63	109.69
55	Aa	501	3PE	O21-C21-C22	3.22	119.78	110.80
63	O	401	ADP	C4-C5-N7	-3.21	106.70	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	P	401	NDP	N3A-C2A-N1A	-3.19	123.61	128.60
69	AD	401	HEC	C1A-C2A-C3A	-3.17	102.99	107.13
67	Ac	401	HEM	C1B-NB-C4B	3.17	108.35	105.07
67	AC	402	HEM	CHA-C4D-ND	3.16	128.27	124.37
55	M	502	3PE	C2-O21-C21	-3.15	110.04	117.79
64	P	401	NDP	C4A-C5A-N7A	-3.12	106.81	110.62
69	AD	401	HEC	CAD-C3D-C4D	3.11	130.09	124.66
67	AC	402	HEM	CHD-C4C-NC	3.10	127.79	124.44
55	d	201	3PE	O31-C31-C32	3.09	121.60	111.91
66	n	201	EHZ	C10-S1-C9	3.08	111.46	101.87
55	m	202	3PE	C2-O21-C21	-3.08	110.22	117.79
62	Ag	101	CDL	CB4-OB6-CB5	-3.07	110.22	117.79
55	d	201	3PE	C2-O21-C21	-3.07	110.24	117.79
62	X	201	CDL	CA4-OA6-CA5	-3.06	110.26	117.79
67	AC	402	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
69	AD	401	HEC	C4A-C3A-C2A	-3.05	102.49	106.94
55	m	203	3PE	C2-O21-C21	-3.02	110.35	117.79
55	M	502	3PE	O31-C31-C32	3.00	121.32	111.91
71	Ad	402	3PH	O31-C31-C32	2.98	121.27	111.91
63	O	401	ADP	C4-N9-C8	2.92	108.89	105.73
55	K	101	3PE	C2-O21-C21	-2.90	110.64	117.79
55	H	401	3PE	O31-C31-C32	2.88	120.94	111.91
55	Y	201	3PE	O31-C31-C32	2.87	120.93	111.91
67	Ac	401	HEM	CHD-C1D-ND	2.86	127.53	124.42
67	Ac	402	HEM	CHD-C1D-C2D	-2.85	120.52	124.98
63	O	401	ADP	C5-N7-C8	2.84	107.54	103.51
55	m	202	3PE	O31-C31-C32	2.84	120.81	111.91
55	i	201	3PE	O31-C31-C32	2.84	120.81	111.91
62	Ag	102	CDL	CA4-OA6-CA5	-2.84	110.81	117.79
64	P	401	NDP	C4A-N9A-C8A	2.83	108.79	105.73
57	B	302	UQ1	CM5-C5-C6	-2.82	119.80	124.40
58	B	303	PC1	O31-C31-C32	2.81	120.73	111.91
69	AD	401	HEC	CMB-C2B-C3B	2.81	133.74	126.12
69	AD	401	HEC	C4D-C3D-C2D	-2.80	102.81	106.90
62	h	201	CDL	OB8-CB7-C71	2.80	120.70	111.91
69	AD	401	HEC	CAD-CBD-CGD	-2.80	107.58	113.60
62	a	101	CDL	OA8-CA7-C31	2.80	120.68	111.91
55	m	201	3PE	O31-C31-C32	2.79	120.67	111.91
55	N	401	3PE	C2-O21-C21	-2.78	110.95	117.79
67	AC	402	HEM	CBD-CAD-C3D	-2.77	104.94	112.63
68	Ac	405	UQ6	C15-C14-C16	2.77	119.92	115.27
67	Ac	402	HEM	CMA-C3A-C4A	2.75	129.55	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	L	704	CDL	CA4-OA6-CA5	-2.75	111.03	117.79
67	Ac	402	HEM	CHA-C4D-C3D	-2.73	120.21	125.33
68	Ac	405	UQ6	C10-C9-C11	2.69	119.79	115.27
62	X	201	CDL	OB8-CB7-C71	2.69	120.34	111.91
62	Ag	102	CDL	CB4-OB6-CB5	-2.67	111.21	117.79
62	L	704	CDL	OB8-CB7-C71	2.67	120.30	111.91
64	P	401	NDP	C5A-N7A-C8A	2.67	107.30	103.51
55	m	203	3PE	O31-C31-C32	2.66	120.27	111.91
55	A	201	3PE	O31-C31-C32	2.65	120.23	111.91
55	L	702	3PE	O31-C31-C32	2.65	120.23	111.91
55	K	101	3PE	O31-C31-C32	2.65	120.22	111.91
62	L	704	CDL	OA8-CA7-C31	2.65	120.22	111.91
58	B	303	PC1	C2-O21-C21	-2.64	111.29	117.79
67	Ac	402	HEM	CHA-C1A-NA	2.62	128.68	123.85
55	L	703	3PE	O31-C31-C32	2.62	120.13	111.91
66	W	201	EHZ	C10-S1-C9	2.62	110.03	101.87
55	L	701	3PE	O31-C31-C32	2.62	120.12	111.91
55	Ag	103	3PE	O31-C31-C32	2.61	120.10	111.91
62	h	201	CDL	CA4-OA6-CA5	-2.60	111.38	117.79
67	AC	402	HEM	C4C-NC-C1C	2.59	107.89	105.35
70	Ac	404	U10	C7-C6-C5	2.59	121.60	118.48
68	AC	403	UQ6	C12-C13-C14	-2.59	121.42	127.66
68	AC	403	UQ6	C15-C14-C16	2.59	119.62	115.27
55	N	401	3PE	O31-C31-C32	2.59	120.03	111.91
62	X	201	CDL	OA8-CA7-C31	2.58	120.00	111.91
67	AC	401	HEM	O2A-CGA-CBA	2.58	122.31	114.03
67	AC	401	HEM	O2D-CGD-CBD	2.57	122.30	114.03
55	L	703	3PE	C2-O21-C21	-2.57	111.47	117.79
69	Ad	401	HEC	CAA-CBA-CGA	-2.56	108.09	113.60
67	Ac	401	HEM	CHA-C1A-NA	2.56	128.56	123.85
67	Ac	401	HEM	CHA-C4D-ND	2.55	127.52	124.37
70	Ac	404	U10	O4-C4-C5	-2.54	107.96	116.56
69	AD	401	HEC	CAA-C2A-C1A	2.54	129.68	124.89
67	AC	401	HEM	CHA-C1A-NA	2.53	128.50	123.85
62	Ag	102	CDL	OA8-CA7-C31	2.53	119.84	111.91
55	Ac	403	3PE	O31-C31-C32	2.52	119.83	111.91
67	Ac	402	HEM	C1A-CHA-C4D	-2.50	120.40	126.34
55	I	301	3PE	O31-C31-C32	2.50	119.76	111.91
60	F	501	FMN	C4A-C10-N1	-2.50	118.92	124.73
67	AC	402	HEM	CBA-CAA-C2A	-2.50	105.68	112.63
55	Y	201	3PE	C2-O21-C21	-2.49	111.67	117.79
62	h	201	CDL	OA8-CA7-C31	2.48	119.70	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	F	501	FMN	O4-C4-C4A	-2.48	120.02	126.60
66	n	201	EHZ	OP3-P1-O9	-2.48	100.97	110.68
66	W	201	EHZ	C13-C12-N1	2.48	120.59	116.42
62	h	201	CDL	CB4-OB6-CB5	-2.47	111.70	117.79
62	Ag	101	CDL	OA8-CA7-C31	2.47	119.65	111.91
62	Ag	101	CDL	CA4-OA6-CA5	-2.46	111.73	117.79
67	AC	401	HEM	CHD-C1D-ND	2.46	127.09	124.42
68	AC	403	UQ6	C17-C18-C19	-2.45	119.36	127.75
62	a	101	CDL	OB8-CB7-C71	2.45	119.60	111.91
55	Aa	501	3PE	O31-C31-C32	2.45	119.60	111.91
55	L	702	3PE	C2-O21-C21	-2.45	111.77	117.79
66	W	201	EHZ	C14-N2-C15	-2.44	118.24	122.59
67	Ac	401	HEM	C4B-C3B-C2B	-2.44	105.18	107.11
55	L	705	3PE	C2-O21-C21	-2.43	111.80	117.79
69	AD	401	HEC	CMD-C2D-C1D	2.42	128.73	125.04
69	AD	401	HEC	C3B-C4B-NB	2.42	112.86	110.17
55	Ag	103	3PE	C2-O21-C21	-2.42	111.84	117.79
55	M	501	3PE	C2-O21-C21	-2.41	111.86	117.79
57	B	302	UQ1	C11-C9-C10	2.41	119.92	114.60
55	Ac	403	3PE	C2-O21-C21	-2.40	111.88	117.79
68	Ac	405	UQ6	C21-C19-C20	2.39	119.88	114.60
68	AC	403	UQ6	C21-C19-C20	2.37	119.84	114.60
58	B	304	PC1	O31-C31-C32	2.36	119.33	111.91
63	O	401	ADP	N9-C8-N7	-2.34	110.72	113.91
66	W	201	EHZ	O2-C9-S1	-2.34	119.58	122.61
64	P	401	NDP	C2B-C1B-N9A	-2.32	109.62	113.53
60	F	501	FMN	C4-C4A-N5	2.31	121.53	118.23
55	L	705	3PE	O31-C31-C32	2.31	119.17	111.91
67	Ac	401	HEM	C4A-NA-C1A	2.31	107.61	105.35
63	O	401	ADP	O4'-C1'-N9	2.31	112.60	108.06
66	n	201	EHZ	C10-C11-N1	-2.30	107.58	112.42
55	K	101	3PE	O21-C21-O22	-2.29	118.17	123.70
63	O	401	ADP	C6-C5-N7	2.29	136.28	132.02
69	AD	401	HEC	CMC-C2C-C1C	2.28	128.85	125.37
67	Ac	402	HEM	C4C-C3C-C2C	2.28	108.63	106.75
71	Ad	402	3PH	C2-O21-C21	-2.27	112.19	117.79
67	Ac	402	HEM	CBD-CAD-C3D	-2.26	106.34	112.63
71	Ad	402	3PH	O31-C31-O32	-2.25	117.91	123.59
67	Ac	402	HEM	CHB-C1B-C2B	-2.25	120.47	126.73
55	d	201	3PE	O31-C31-O32	-2.25	117.92	123.59
55	Aa	501	3PE	C2-O21-C21	-2.24	112.27	117.79
64	P	401	NDP	N9A-C8A-N7A	-2.24	110.85	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Ag	101	CDL	OB6-CB5-OB7	-2.23	118.31	123.70
67	AC	402	HEM	C4D-ND-C1D	2.23	107.38	105.07
67	Ac	401	HEM	CHB-C1B-C2B	-2.22	120.56	126.73
68	Ac	405	UQ6	C17-C18-C19	-2.21	120.18	127.75
62	Ag	102	CDL	OB8-CB7-C71	2.21	118.84	111.91
67	Ac	401	HEM	C4C-NC-C1C	2.21	107.51	105.35
55	M	502	3PE	O21-C21-O22	-2.21	118.36	123.70
55	Y	201	3PE	O21-C21-O22	-2.21	118.37	123.70
55	m	202	3PE	O21-C21-O22	-2.21	118.37	123.70
69	AD	401	HEC	CMA-C3A-C4A	2.20	128.59	124.71
67	AC	402	HEM	C4C-CHD-C1D	-2.19	121.33	126.06
55	N	401	3PE	O21-C21-O22	-2.18	118.44	123.70
62	a	101	CDL	CB4-OB6-CB5	-2.16	112.47	117.79
69	Ad	401	HEC	CHA-C4D-ND	2.15	126.76	124.42
67	AC	402	HEM	C4A-NA-C1A	2.15	107.45	105.35
55	M	501	3PE	O31-C31-C32	2.14	118.62	111.91
68	AC	403	UQ6	C4M-O4-C4	2.14	120.64	114.78
66	n	201	EHZ	C5-C6-C7	-2.14	108.69	114.85
67	AC	401	HEM	CHB-C1B-C2B	-2.14	120.79	126.73
58	B	304	PC1	C2-O21-C21	-2.13	112.53	117.79
57	B	302	UQ1	C7-C8-C9	-2.13	120.60	127.26
64	P	401	NDP	C6A-C5A-N7A	2.12	135.98	132.02
62	X	201	CDL	CB6-CB4-CB3	-2.12	106.78	111.79
55	d	201	3PE	O21-C21-O22	-2.12	118.59	123.70
67	AC	401	HEM	C4A-NA-C1A	2.11	107.41	105.35
62	a	101	CDL	CA4-OA6-CA5	-2.10	112.63	117.79
69	Ad	401	HEC	C4A-NA-C1A	2.09	107.40	105.35
67	Ac	401	HEM	C1C-CHC-C4B	-2.09	121.54	126.06
64	P	401	NDP	C3D-C2D-C1D	2.09	105.39	101.43
69	Ad	401	HEC	C2A-C1A-NA	-2.08	108.30	110.32
69	Ad	401	HEC	C3C-C4C-NC	-2.08	107.82	110.15
69	Ad	401	HEC	C4B-NB-C1B	2.07	107.21	105.07
55	L	702	3PE	O21-C21-O22	-2.06	118.71	123.70
69	AD	401	HEC	CMC-C2C-C3C	2.06	130.07	125.61
55	Y	201	3PE	O31-C31-O32	-2.06	118.41	123.59
67	AC	402	HEM	CHA-C1A-NA	2.05	127.63	123.85
62	X	201	CDL	OB6-CB5-OB7	-2.05	118.74	123.70
67	AC	402	HEM	C4A-CHB-C1B	-2.05	121.47	126.34
67	Ac	401	HEM	C4A-CHB-C1B	-2.04	121.50	126.34
60	F	501	FMN	C4A-C10-N10	2.04	119.46	116.48
70	Ac	404	U10	C3M-O3-C3	2.03	123.67	116.47
69	AD	401	HEC	CHD-C1D-C2D	-2.03	121.09	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	302	UQ1	C8-C7-C6	-2.03	106.57	112.05
68	AC	403	UQ6	C10-C9-C8	-2.03	118.47	123.68
60	F	501	FMN	C4A-C4-N3	2.03	118.34	113.19
67	AC	402	HEM	CHB-C1B-C2B	-2.03	121.09	126.73
67	Ac	401	HEM	CAA-CBA-CGA	-2.03	109.24	113.60
60	F	501	FMN	C10-N1-C2	2.02	120.94	116.90
70	Ac	404	U10	O4-C4-C3	2.02	131.26	123.64
55	L	701	3PE	C2-O21-C21	-2.02	112.83	117.79
62	L	704	CDL	OA6-CA5-OA7	-2.01	118.84	123.70
55	m	201	3PE	O21-C21-O22	-2.01	118.84	123.70
68	AC	403	UQ6	C3M-O3-C3	2.01	120.28	114.78
66	n	201	EHZ	C14-C13-C12	-2.00	109.02	112.36
55	H	401	3PE	O21-C21-O22	-2.00	118.86	123.70
67	AC	401	HEM	C4B-C3B-C2B	-2.00	105.53	107.11
67	AC	402	HEM	C2A-C1A-NA	-2.00	107.91	110.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
69	AD	401	HEC	NA
69	Ad	401	HEC	NA

All (475) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	201	3PE	C1-O11-P-O14
55	A	201	3PE	C11-O13-P-O11
55	A	201	3PE	C11-O13-P-O14
55	A	201	3PE	C22-C21-O21-C2
55	H	401	3PE	C1-O11-P-O14
55	H	401	3PE	C11-O13-P-O14
55	H	401	3PE	O22-C21-O21-C2
55	H	401	3PE	C22-C21-O21-C2
55	I	301	3PE	C1-O11-P-O14
55	I	301	3PE	C11-O13-P-O12
55	K	101	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O13
55	L	701	3PE	C2-C1-O11-P
55	L	702	3PE	C1-O11-P-O12
55	L	702	3PE	O22-C21-O21-C2
55	L	702	3PE	C22-C21-O21-C2
55	L	703	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	L	703	3PE	C11-O13-P-O12
55	L	703	3PE	C11-O13-P-O14
55	L	705	3PE	C1-O11-P-O12
55	L	705	3PE	C1-O11-P-O14
55	L	705	3PE	C11-O13-P-O12
55	L	705	3PE	C11-O13-P-O14
55	M	501	3PE	C1-O11-P-O12
55	M	501	3PE	C1-O11-P-O13
55	M	501	3PE	C1-O11-P-O14
55	M	501	3PE	C11-O13-P-O11
55	M	501	3PE	C11-O13-P-O12
55	M	501	3PE	C11-O13-P-O14
55	M	502	3PE	C1-O11-P-O12
55	M	502	3PE	C11-O13-P-O14
55	N	401	3PE	C11-O13-P-O11
55	N	401	3PE	C11-O13-P-O12
55	Y	201	3PE	C1-O11-P-O12
55	d	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C1-O11-P-O12
55	i	201	3PE	C1-O11-P-O13
55	i	201	3PE	C1-O11-P-O14
55	i	201	3PE	C11-O13-P-O12
55	m	201	3PE	C1-O11-P-O14
55	m	201	3PE	C22-C21-O21-C2
55	m	202	3PE	C22-C21-O21-C2
55	m	203	3PE	C1-O11-P-O12
55	m	203	3PE	C1-O11-P-O14
55	m	203	3PE	C22-C21-O21-C2
55	Aa	501	3PE	C22-C21-O21-C2
55	Ag	103	3PE	C1-O11-P-O14
55	Ag	103	3PE	C11-O13-P-O12
55	Ag	103	3PE	C11-O13-P-O14
58	B	303	PC1	C11-O13-P-O14
58	B	303	PC1	C22-C21-O21-C2
58	B	304	PC1	C1-O11-P-O14
58	B	304	PC1	C22-C21-O21-C2
60	F	501	FMN	C5'-O5'-P-O2P
60	F	501	FMN	C5'-O5'-P-O3P
61	H	400	UQ9	C22-C23-C24-C26
61	H	400	UQ9	C22-C23-C24-C25
61	H	400	UQ9	C20-C19-C21-C22
61	H	400	UQ9	C18-C19-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	H	400	UQ9	C15-C14-C16-C17
61	H	400	UQ9	C13-C14-C16-C17
61	H	400	UQ9	C12-C13-C14-C16
61	H	400	UQ9	C12-C13-C14-C15
61	H	400	UQ9	C11-C12-C13-C14
62	L	704	CDL	CA2-OA2-PA1-OA3
62	L	704	CDL	CB2-OB2-PB2-OB4
62	L	704	CDL	CB3-OB5-PB2-OB3
62	L	704	CDL	CB3-OB5-PB2-OB4
62	L	704	CDL	C51-CB5-OB6-CB4
62	X	201	CDL	CA3-OA5-PA1-OA2
62	X	201	CDL	CA3-OA5-PA1-OA3
62	X	201	CDL	CA3-OA5-PA1-OA4
62	X	201	CDL	CB2-OB2-PB2-OB3
62	X	201	CDL	CB2-OB2-PB2-OB5
62	X	201	CDL	CB3-OB5-PB2-OB3
62	X	201	CDL	C51-CB5-OB6-CB4
62	a	101	CDL	CA2-OA2-PA1-OA4
62	a	101	CDL	OA7-CA5-OA6-CA4
62	a	101	CDL	C11-CA5-OA6-CA4
62	a	101	CDL	CB2-OB2-PB2-OB3
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB2-OB2-PB2-OB3
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	Ag	101	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	C1-CB2-OB2-PB2
62	Ag	102	CDL	CB2-OB2-PB2-OB4
62	Ag	102	CDL	CB3-OB5-PB2-OB3
62	Ag	102	CDL	C51-CB5-OB6-CB4
64	P	401	NDP	C5D-O5D-PN-O1N
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	O2-C9-S1-C10
66	W	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C12-C13-C14-N2
66	n	201	EHZ	N2-C15-C16-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
66	n	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C19
66	n	201	EHZ	C15-C16-C17-C20
66	n	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C19
66	n	201	EHZ	O5-C16-C17-C20
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	AC	401	HEM	C2C-C3C-CAC-CBC
67	AC	401	HEM	C4C-C3C-CAC-CBC
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C2C-C3C-CAC-CBC
67	Ac	401	HEM	C2B-C3B-CAB-CBB
67	Ac	401	HEM	C2C-C3C-CAC-CBC
67	Ac	401	HEM	C4C-C3C-CAC-CBC
67	Ac	402	HEM	C2B-C3B-CAB-CBB
68	Ac	405	UQ6	C1-C6-C7-C8
68	Ac	405	UQ6	C13-C14-C16-C17
68	Ac	405	UQ6	C15-C14-C16-C17
70	Ac	404	U10	C7-C8-C9-C10
70	Ac	404	U10	C7-C8-C9-C11
71	Ad	402	3PH	C1-O11-P-O13
71	Ad	402	3PH	O21-C2-C3-O31
70	Ac	404	U10	C12-C13-C14-C15
70	Ac	404	U10	C12-C13-C14-C16
69	AD	401	HEC	C2B-C3B-CAB-CBB
69	AD	401	HEC	C4B-C3B-CAB-CBB
58	B	304	PC1	O32-C31-O31-C3
62	L	704	CDL	OA9-CA7-OA8-CA6
69	AD	401	HEC	C4C-C3C-CAC-CBC
69	AD	401	HEC	C2C-C3C-CAC-CBC
55	A	201	3PE	O22-C21-O21-C2
55	m	202	3PE	O22-C21-O21-C2
55	m	203	3PE	O22-C21-O21-C2
55	Aa	501	3PE	O22-C21-O21-C2
58	B	303	PC1	O22-C21-O21-C2
58	B	304	PC1	O22-C21-O21-C2
62	L	704	CDL	OB7-CB5-OB6-CB4
62	X	201	CDL	OB7-CB5-OB6-CB4
62	h	201	CDL	OB7-CB5-OB6-CB4
62	Ag	102	CDL	OB7-CB5-OB6-CB4
55	K	101	3PE	C32-C31-O31-C3
58	B	304	PC1	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	d	201	3PE	C22-C21-O21-C2
68	AC	403	UQ6	C15-C14-C16-C17
55	I	301	3PE	C32-C31-O31-C3
55	N	401	3PE	C32-C31-O31-C3
62	L	704	CDL	C31-CA7-OA8-CA6
71	Ad	402	3PH	C35-C36-C37-C38
55	m	201	3PE	O22-C21-O21-C2
55	H	401	3PE	O32-C31-O31-C3
55	I	301	3PE	O32-C31-O31-C3
55	N	401	3PE	O32-C31-O31-C3
55	m	203	3PE	O32-C31-O31-C3
62	X	201	CDL	O1-C1-CB2-OB2
55	H	401	3PE	C32-C31-O31-C3
62	a	101	CDL	C31-CA7-OA8-CA6
55	K	101	3PE	O32-C31-O31-C3
55	I	301	3PE	C22-C21-O21-C2
55	L	705	3PE	C22-C21-O21-C2
62	L	704	CDL	C11-CA5-OA6-CA4
55	m	203	3PE	C32-C31-O31-C3
62	h	201	CDL	CA4-CA3-OA5-PA1
62	a	101	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C9-C11-C12-C13
61	H	400	UQ9	C17-C18-C19-C20
55	I	301	3PE	O22-C21-O21-C2
55	L	705	3PE	O22-C21-O21-C2
61	H	400	UQ9	C17-C18-C19-C21
58	B	303	PC1	C11-C12-N-C13
55	i	201	3PE	C32-C31-O31-C3
62	X	201	CDL	C31-CA7-OA8-CA6
71	Ad	402	3PH	C31-C32-C33-C34
55	M	501	3PE	C32-C33-C34-C35
68	AC	403	UQ6	C13-C14-C16-C17
55	m	202	3PE	C32-C31-O31-C3
62	h	201	CDL	C71-CB7-OB8-CB6
62	X	201	CDL	OA9-CA7-OA8-CA6
61	H	400	UQ9	C19-C21-C22-C23
62	L	704	CDL	OA7-CA5-OA6-CA4
55	i	201	3PE	O32-C31-O31-C3
55	m	202	3PE	O32-C31-O31-C3
68	Ac	405	UQ6	C5-C6-C7-C8
55	I	301	3PE	C1-O11-P-O13
55	I	301	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	K	101	3PE	C1-O11-P-O13
55	L	702	3PE	C1-O11-P-O13
55	L	705	3PE	C1-O11-P-O13
55	L	705	3PE	C11-O13-P-O11
55	M	502	3PE	C11-O13-P-O11
55	Y	201	3PE	C1-O11-P-O13
55	Y	201	3PE	C11-O13-P-O11
55	i	201	3PE	C11-O13-P-O11
55	m	203	3PE	C1-O11-P-O13
55	Ag	103	3PE	C1-O11-P-O13
55	Ag	103	3PE	C11-O13-P-O11
58	B	303	PC1	C11-O13-P-O11
58	B	303	PC1	C1-O11-P-O13
62	L	704	CDL	CA2-OA2-PA1-OA5
62	L	704	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA2
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	102	CDL	CB2-OB2-PB2-OB5
62	Ag	102	CDL	CB3-OB5-PB2-OB2
62	X	201	CDL	CA2-C1-CB2-OB2
58	B	303	PC1	C11-C12-N-C14
55	M	502	3PE	C22-C21-O21-C2
55	I	301	3PE	C32-C33-C34-C35
62	h	201	CDL	C18-C19-C20-C21
66	W	201	EHZ	C18-C17-C20-O6
66	W	201	EHZ	C19-C17-C20-O6
55	d	201	3PE	C32-C31-O31-C3
55	M	502	3PE	O22-C21-O21-C2
55	L	703	3PE	C25-C26-C27-C28
62	X	201	CDL	C1-CB2-OB2-PB2
62	h	201	CDL	OB9-CB7-OB8-CB6
55	Aa	501	3PE	C32-C31-O31-C3
55	K	101	3PE	C22-C23-C24-C25
62	X	201	CDL	C71-CB7-OB8-CB6
55	m	201	3PE	C26-C27-C28-C29
55	M	501	3PE	C32-C31-O31-C3
62	Ag	102	CDL	C74-C75-C76-C77
55	d	201	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	Aa	501	3PE	O32-C31-O31-C3
58	B	303	PC1	C11-C12-N-C15
55	m	201	3PE	C32-C31-O31-C3
62	Ag	102	CDL	C31-CA7-OA8-CA6
62	Ag	101	CDL	C51-CB5-OB6-CB4
55	M	502	3PE	C23-C24-C25-C26
62	L	704	CDL	C55-C56-C57-C58
55	m	201	3PE	O32-C31-O31-C3
62	X	201	CDL	OB9-CB7-OB8-CB6
71	Ad	402	3PH	C22-C21-O21-C2
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	AC	402	HEM	C4C-C3C-CAC-CBC
67	Ac	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
55	M	501	3PE	O32-C31-O31-C3
62	Ag	102	CDL	OA9-CA7-OA8-CA6
55	M	502	3PE	C3C-C3D-C3E-C3F
62	Ag	101	CDL	OB7-CB5-OB6-CB4
71	Ad	402	3PH	O22-C21-O21-C2
62	a	101	CDL	C13-C14-C15-C16
55	d	201	3PE	C11-O13-P-O11
58	B	304	PC1	C1-O11-P-O13
62	h	201	CDL	CB3-OB5-PB2-OB2
55	Y	201	3PE	C2-C1-O11-P
62	a	101	CDL	C14-C15-C16-C17
55	K	101	3PE	C33-C34-C35-C36
55	N	401	3PE	C24-C25-C26-C27
66	W	201	EHZ	C3-C4-C5-C6
71	Ad	402	3PH	C1-C2-C3-O31
55	L	702	3PE	C24-C25-C26-C27
66	n	201	EHZ	O4-C15-C16-O5
66	W	201	EHZ	C5-C6-C7-O1
71	Ad	402	3PH	C34-C35-C36-C37
55	L	703	3PE	C32-C31-O31-C3
71	Ad	402	3PH	C36-C37-C38-C39
55	H	401	3PE	C3-C2-O21-C21
62	L	704	CDL	CB6-CB4-OB6-CB5
55	H	401	3PE	C2-C1-O11-P
60	F	501	FMN	C5'-O5'-P-O1P
62	L	704	CDL	OB5-CB3-CB4-OB6
55	I	301	3PE	C3B-C3C-C3D-C3E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	L	702	3PE	C32-C31-O31-C3
62	L	704	CDL	C71-CB7-OB8-CB6
66	W	201	EHZ	C5-C6-C7-C8
55	Ac	403	3PE	C22-C21-O21-C2
55	L	705	3PE	C32-C31-O31-C3
55	Ag	103	3PE	C39-C3A-C3B-C3C
61	H	400	UQ9	C14-C16-C17-C18
55	m	201	3PE	C27-C28-C29-C2A
55	K	101	3PE	C36-C37-C38-C39
55	L	703	3PE	O32-C31-O31-C3
55	i	201	3PE	C22-C21-O21-C2
58	B	303	PC1	C2-C1-O11-P
62	Ag	102	CDL	CB4-CB3-OB5-PB2
67	AC	401	HEM	C2A-CAA-CBA-CGA
67	Ac	401	HEM	C2A-CAA-CBA-CGA
69	AD	401	HEC	C2A-CAA-CBA-CGA
55	A	201	3PE	C1-C2-C3-O31
62	X	201	CDL	CA3-CA4-CA6-OA8
55	H	401	3PE	C2B-C2C-C2D-C2E
55	M	501	3PE	C2-C3-O31-C31
62	h	201	CDL	CB2-OB2-PB2-OB5
62	L	704	CDL	C32-C33-C34-C35
55	K	101	3PE	O11-C1-C2-O21
55	Ac	403	3PE	O22-C21-O21-C2
66	n	201	EHZ	C3-C4-C5-C6
62	L	704	CDL	OB9-CB7-OB8-CB6
62	X	201	CDL	OA6-CA4-CA6-OA8
55	i	201	3PE	O22-C21-O21-C2
55	i	201	3PE	C2-C1-O11-P
62	X	201	CDL	C1-CA2-OA2-PA1
62	h	201	CDL	C14-C15-C16-C17
66	n	201	EHZ	O2-C9-S1-C10
58	B	304	PC1	C38-C39-C3A-C3B
55	L	705	3PE	O32-C31-O31-C3
62	L	704	CDL	C12-C13-C14-C15
55	H	401	3PE	C2C-C2D-C2E-C2F
55	Y	201	3PE	C22-C21-O21-C2
62	X	201	CDL	C11-CA5-OA6-CA4
64	P	401	NDP	C2B-O2B-P2B-O1X
55	Y	201	3PE	C32-C31-O31-C3
55	i	201	3PE	C1-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
66	n	201	EHZ	C8-C9-S1-C10
67	Ac	402	HEM	C2C-C3C-CAC-CBC
62	h	201	CDL	CB4-CB3-OB5-PB2
55	L	702	3PE	O32-C31-O31-C3
55	M	501	3PE	O11-C1-C2-O21
63	O	401	ADP	PA-O3A-PB-O3B
58	B	303	PC1	C31-C32-C33-C34
55	L	702	3PE	C28-C29-C2A-C2B
55	Y	201	3PE	O22-C21-O21-C2
62	X	201	CDL	OA7-CA5-OA6-CA4
64	P	401	NDP	PN-O3-PA-O2A
55	M	502	3PE	C1-O11-P-O13
62	L	704	CDL	CA3-OA5-PA1-OA2
64	P	401	NDP	O4D-C1D-N1N-C6N
55	K	101	3PE	C2-C1-O11-P
62	a	101	CDL	CB4-CB3-OB5-PB2
55	I	301	3PE	C1-O11-P-O12
55	I	301	3PE	C11-O13-P-O14
55	K	101	3PE	C1-O11-P-O12
55	K	101	3PE	C1-O11-P-O14
55	L	701	3PE	C1-O11-P-O12
55	M	502	3PE	C11-O13-P-O12
55	N	401	3PE	C11-O13-P-O14
55	Y	201	3PE	C11-O13-P-O12
55	Y	201	3PE	C11-O13-P-O14
55	i	201	3PE	C11-O13-P-O14
55	Ag	103	3PE	C1-O11-P-O12
58	B	303	PC1	C11-O13-P-O12
58	B	303	PC1	C1-O11-P-O14
58	B	304	PC1	C1-O11-P-O12
62	L	704	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA3-OA5-PA1-OA3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	CB3-OB5-PB2-OB4
55	Y	201	3PE	O32-C31-O31-C3
55	N	401	3PE	C12-C11-O13-P
55	d	201	3PE	C12-C11-O13-P
62	Ag	102	CDL	C51-C52-C53-C54
60	F	501	FMN	N10-C1'-C2'-O2'
55	L	702	3PE	C25-C26-C27-C28
66	W	201	EHZ	C2-C3-C4-C5
58	B	304	PC1	C11-C12-N-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
61	H	400	UQ9	C12-C11-C9-C10
66	W	201	EHZ	O4-C15-C16-O5
62	X	201	CDL	C52-C53-C54-C55
66	n	201	EHZ	C2-C3-C4-C5
55	m	201	3PE	C1-C2-O21-C21
62	X	201	CDL	CB6-CB4-OB6-CB5
55	M	501	3PE	O11-C1-C2-C3
62	L	704	CDL	OB5-CB3-CB4-CB6
55	L	701	3PE	C26-C27-C28-C29
55	A	201	3PE	O21-C2-C3-O31
55	A	201	3PE	C1-O11-P-O13
55	H	401	3PE	C11-O13-P-O11
55	K	101	3PE	C11-O13-P-O11
55	N	401	3PE	C1-O11-P-O13
62	X	201	CDL	CA2-OA2-PA1-OA5
62	X	201	CDL	CB3-OB5-PB2-OB2
62	a	101	CDL	CB3-OB5-PB2-OB2
55	m	202	3PE	C32-C33-C34-C35
55	L	702	3PE	C33-C34-C35-C36
55	N	401	3PE	C34-C35-C36-C37
55	d	201	3PE	C24-C25-C26-C27
55	L	705	3PE	C2-C1-O11-P
62	L	704	CDL	CA4-CA3-OA5-PA1
62	L	704	CDL	C1-CB2-OB2-PB2
62	Ag	101	CDL	C1-CA2-OA2-PA1
62	Ag	102	CDL	C1-CA2-OA2-PA1
55	m	202	3PE	C23-C24-C25-C26
55	N	401	3PE	C28-C29-C2A-C2B
55	M	501	3PE	O13-C11-C12-N
62	L	704	CDL	C34-C35-C36-C37
55	i	201	3PE	C24-C25-C26-C27
67	Ac	402	HEM	C4C-C3C-CAC-CBC
62	a	101	CDL	C71-CB7-OB8-CB6
67	AC	401	HEM	CAA-CBA-CGA-O2A
70	Ac	404	U10	C12-C11-C9-C10
61	H	400	UQ9	C12-C11-C9-C8
67	Ac	402	HEM	CAD-CBD-CGD-O2D
62	Ag	101	CDL	C71-CB7-OB8-CB6
67	AC	402	HEM	CAD-CBD-CGD-O1D
55	i	201	3PE	C2B-C2C-C2D-C2E
55	L	705	3PE	C24-C25-C26-C27
67	AC	401	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
67	Ac	401	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O1D
55	Aa	501	3PE	C1-C2-O21-C21
55	M	502	3PE	C2B-C2C-C2D-C2E
67	Ac	401	HEM	CAD-CBD-CGD-O1D
55	m	201	3PE	C1-O11-P-O13
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	Ac	401	HEM	CAA-CBA-CGA-O2A
58	B	304	PC1	C2-C1-O11-P
55	H	401	3PE	C31-C32-C33-C34
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	Ac	401	HEM	CAA-CBA-CGA-O1A
55	A	201	3PE	C23-C24-C25-C26
55	I	301	3PE	O11-C1-C2-C3
62	Ag	101	CDL	OB9-CB7-OB8-CB6
62	h	201	CDL	C31-CA7-OA8-CA6
67	AC	402	HEM	CAD-CBD-CGD-O2D
62	Ag	102	CDL	C11-C12-C13-C14
70	Ac	404	U10	C12-C11-C9-C8
62	a	101	CDL	OB9-CB7-OB8-CB6
64	P	401	NDP	PN-O3-PA-O1A
62	a	101	CDL	C15-C16-C17-C18
55	A	201	3PE	C39-C3A-C3B-C3C
67	Ac	402	HEM	C2A-CAA-CBA-CGA
62	h	201	CDL	OA9-CA7-OA8-CA6
55	K	101	3PE	C26-C27-C28-C29
55	M	502	3PE	C39-C3A-C3B-C3C
55	K	101	3PE	O11-C1-C2-C3
55	L	705	3PE	C34-C35-C36-C37
62	X	201	CDL	C59-C60-C61-C62
58	B	304	PC1	C11-C12-N-C13
55	N	401	3PE	C23-C24-C25-C26
55	A	201	3PE	C35-C36-C37-C38
69	AD	401	HEC	CAA-CBA-CGA-O2A
55	I	301	3PE	C31-C32-C33-C34
58	B	304	PC1	C3A-C3B-C3C-C3D
55	m	202	3PE	O11-C1-C2-O21
58	B	304	PC1	C11-C12-N-C15
63	O	401	ADP	PA-O3A-PB-O2B
62	Ag	102	CDL	OA6-CA4-CA6-OA8
55	L	702	3PE	C39-C3A-C3B-C3C
55	M	502	3PE	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
64	P	401	NDP	C5D-O5D-PN-O3
62	Ag	102	CDL	C53-C54-C55-C56
68	AC	403	UQ6	C14-C16-C17-C18
55	Ag	103	3PE	O21-C21-C22-C23
55	H	401	3PE	C37-C38-C39-C3A
55	L	705	3PE	C33-C34-C35-C36
62	L	704	CDL	C11-C12-C13-C14
62	Ag	102	CDL	C52-C53-C54-C55
69	AD	401	HEC	CAA-CBA-CGA-O1A
62	a	101	CDL	C18-C19-C20-C21
68	Ac	405	UQ6	C6-C7-C8-C9
55	L	702	3PE	C34-C35-C36-C37
62	L	704	CDL	C77-C78-C79-C80
55	i	201	3PE	O21-C21-C22-C23
55	K	101	3PE	C2A-C2B-C2C-C2D
55	L	701	3PE	C38-C39-C3A-C3B
55	K	101	3PE	C11-O13-P-O14
55	M	502	3PE	C1-O11-P-O14
55	d	201	3PE	C11-O13-P-O14
55	m	201	3PE	C1-O11-P-O12
55	m	202	3PE	C1-O11-P-O14
62	a	101	CDL	CB3-OB5-PB2-OB3
55	A	201	3PE	C25-C26-C27-C28
55	L	702	3PE	C2B-C2C-C2D-C2E
55	I	301	3PE	C12-C11-O13-P
55	M	501	3PE	C12-C11-O13-P
58	B	303	PC1	C33-C34-C35-C36
62	a	101	CDL	C12-C11-CA5-OA7
58	B	304	PC1	C3F-C3G-C3H-C3I
55	I	301	3PE	O31-C31-C32-C33
62	a	101	CDL	C12-C11-CA5-OA6
62	Ag	101	CDL	C72-C71-CB7-OB8
55	i	201	3PE	O22-C21-C22-C23
55	K	101	3PE	C27-C28-C29-C2A
62	h	201	CDL	C72-C71-CB7-OB8
55	I	301	3PE	O32-C31-C32-C33
55	L	703	3PE	C22-C23-C24-C25
69	AD	401	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

51 monomers are involved in 465 short contacts:

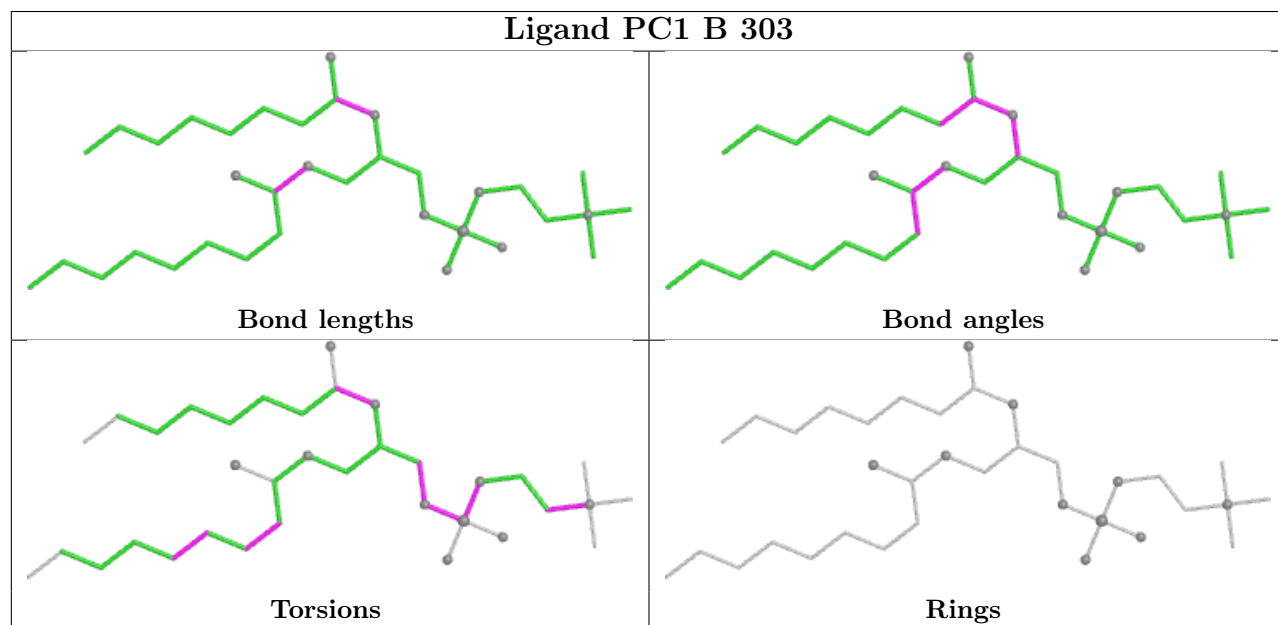
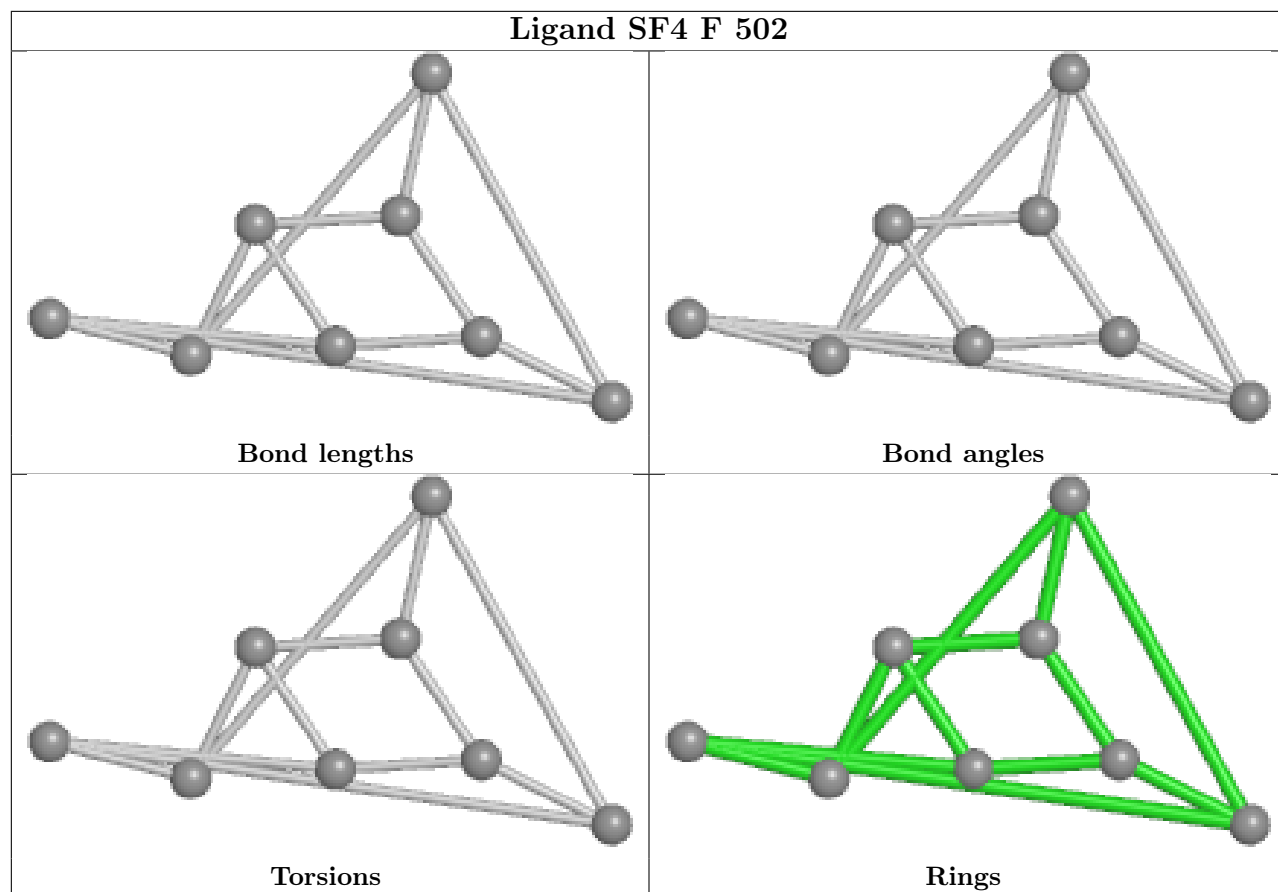
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	F	502	SF4	10	0
58	B	303	PC1	9	0
64	P	401	NDP	7	0
66	W	201	EHZ	3	0
55	K	101	3PE	9	0
55	N	401	3PE	11	0
69	Ad	401	HEC	12	0
56	I	303	SF4	2	0
67	Ac	402	HEM	10	0
61	H	400	UQ9	4	0
55	L	702	3PE	9	0
62	X	201	CDL	9	0
55	Y	201	3PE	8	0
55	H	401	3PE	12	0
55	i	201	3PE	19	0
55	m	203	3PE	4	0
59	E	301	FES	3	0
68	Ac	405	UQ6	15	0
63	O	401	ADP	11	0
62	Ag	102	CDL	4	0
55	m	202	3PE	10	0
62	h	201	CDL	17	0
57	B	302	UQ1	11	0
60	F	501	FMN	3	0
67	Ac	401	HEM	1	0
62	Ag	101	CDL	5	0
55	L	701	3PE	8	0
56	B	301	SF4	6	0
55	M	502	3PE	5	0
55	Ac	403	3PE	7	0
69	AD	401	HEC	18	0
62	L	704	CDL	16	0
55	I	301	3PE	8	0
55	M	501	3PE	3	0
59	G	803	FES	4	0
62	a	101	CDL	12	0
67	AC	401	HEM	18	0
67	AC	402	HEM	9	0
55	L	705	3PE	5	0
68	AC	403	UQ6	11	0
71	Ad	402	3PH	39	0
55	A	201	3PE	8	0
55	Aa	501	3PE	3	0

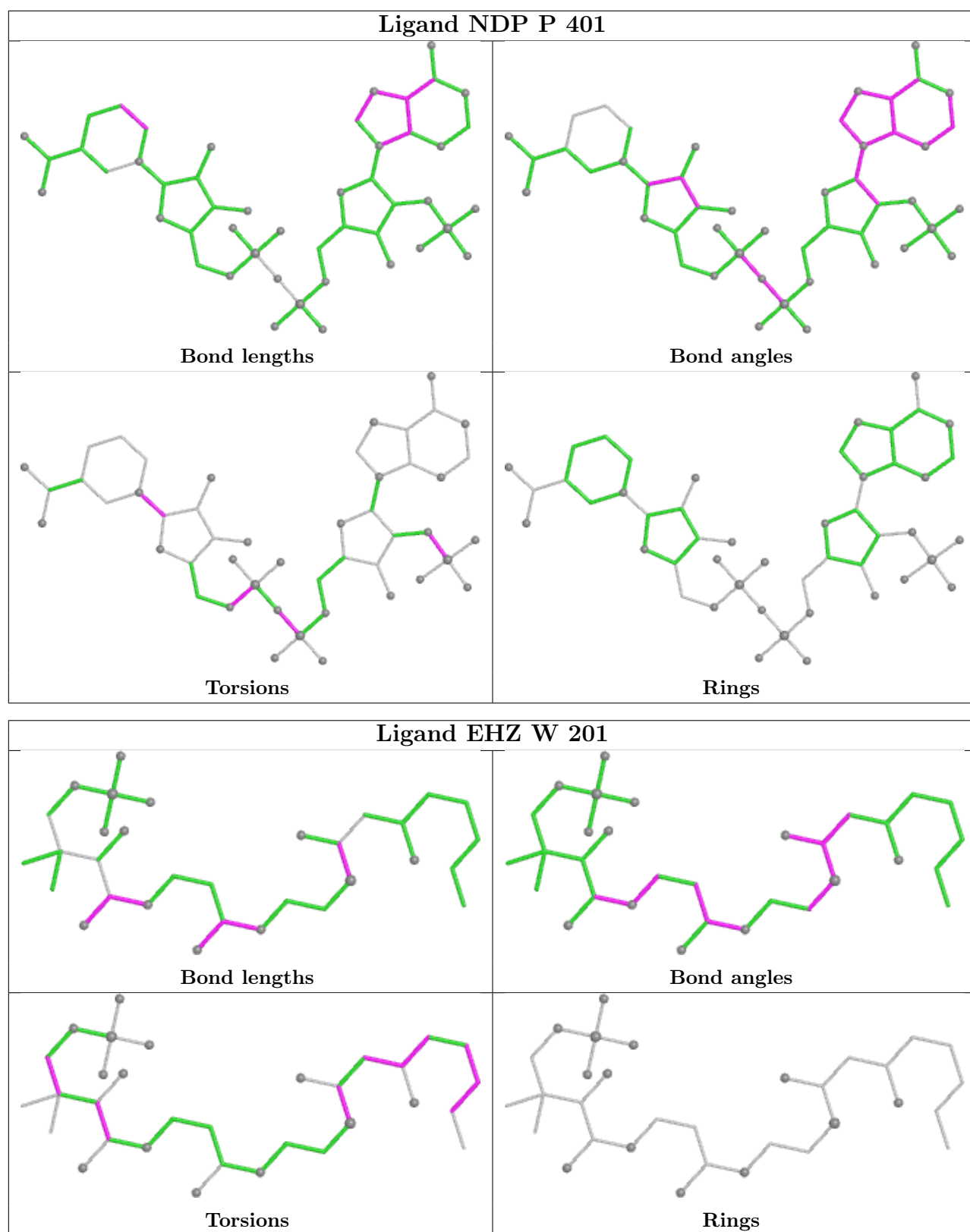
Continued on next page...

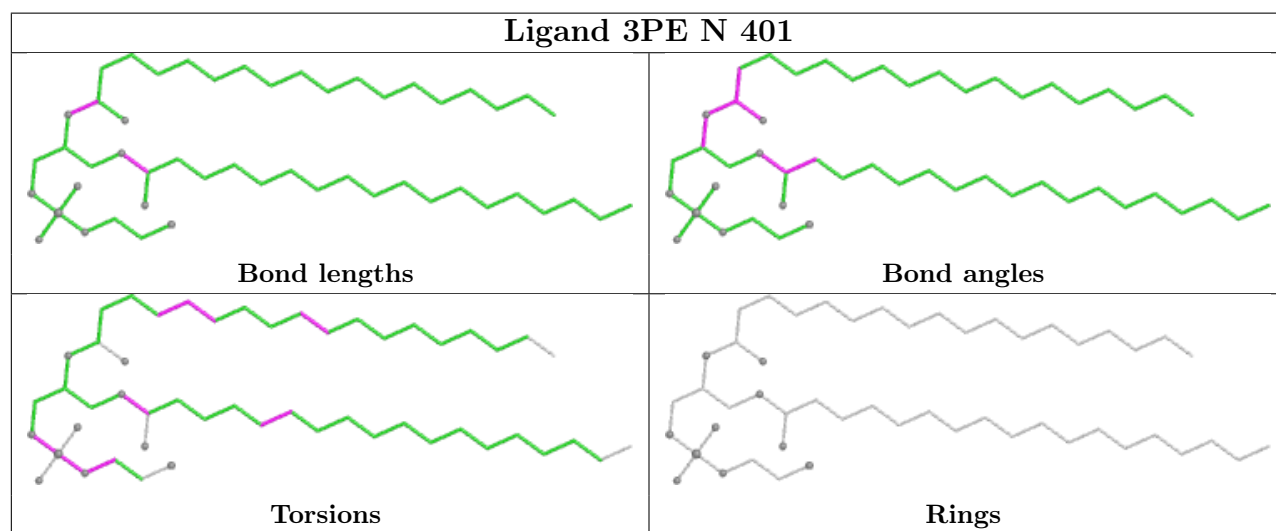
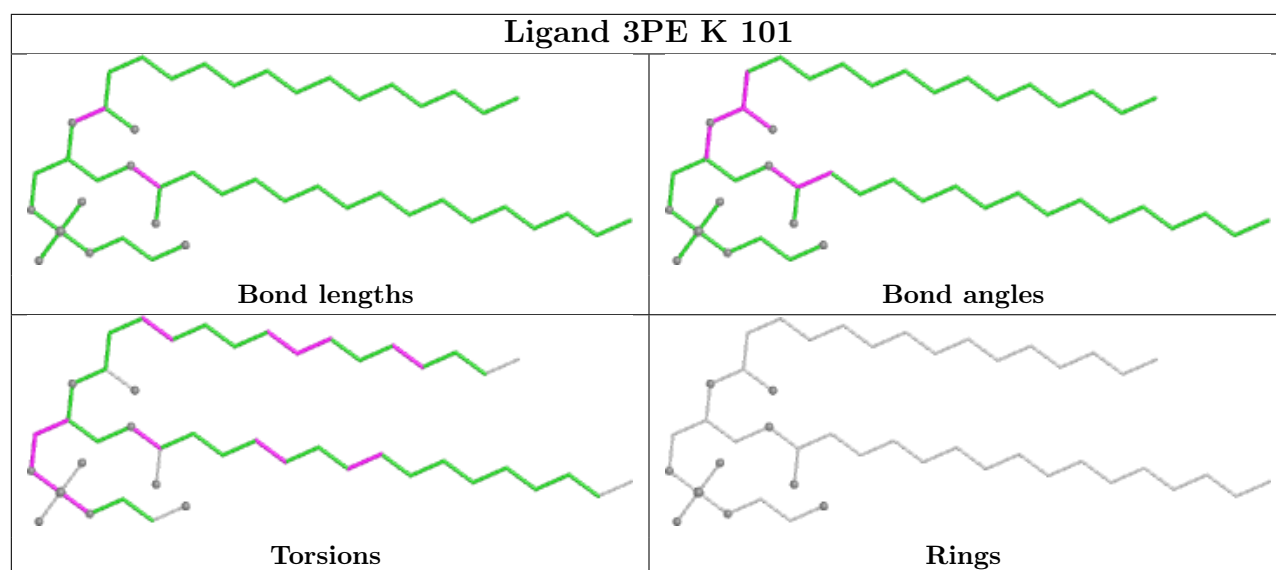
Continued from previous page...

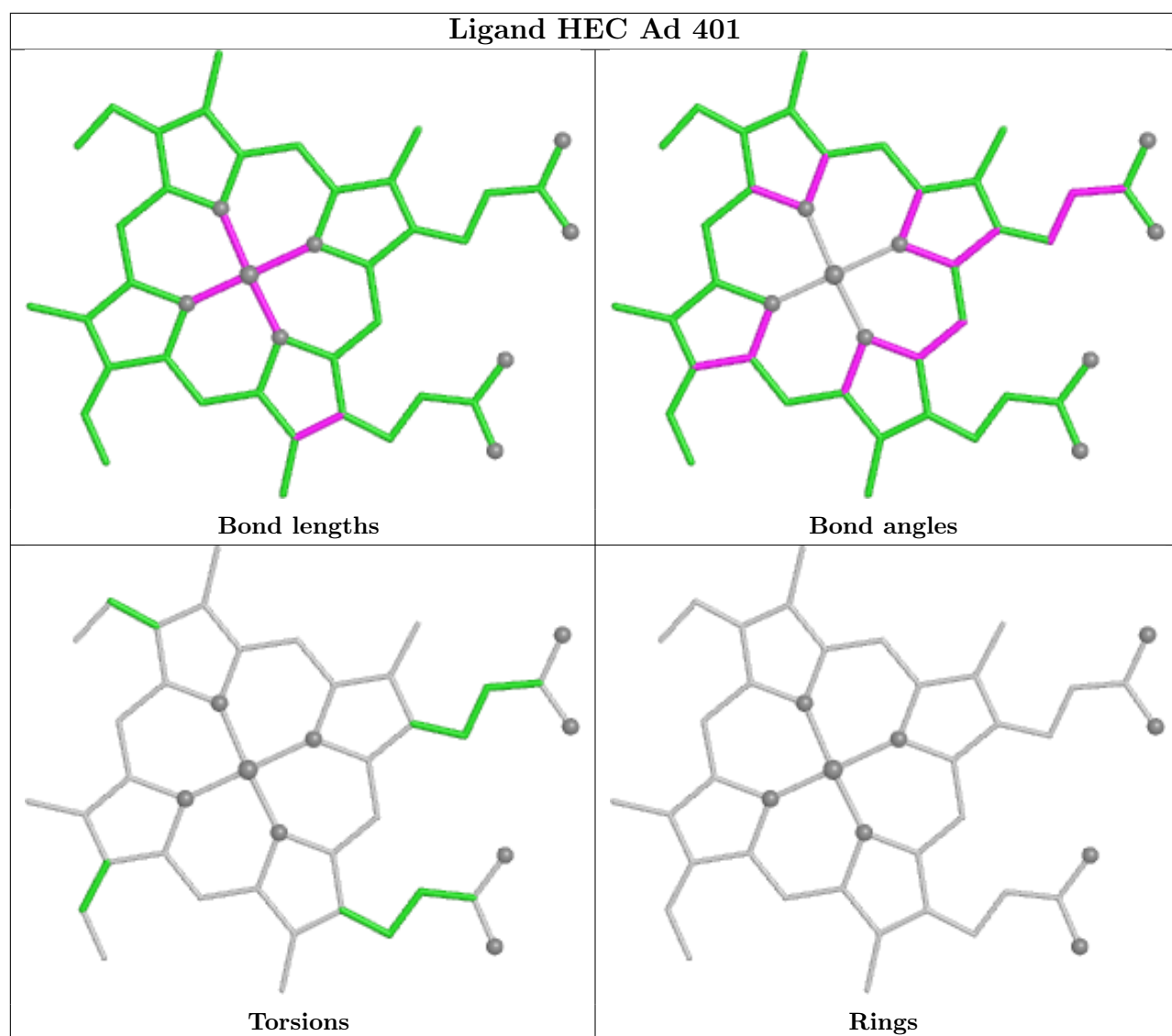
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	L	703	3PE	6	0
56	I	302	SF4	7	0
58	B	304	PC1	14	0
56	G	802	SF4	8	0
70	Ac	404	U10	20	0
55	m	201	3PE	12	0
55	Ag	103	3PE	9	0
55	d	201	3PE	8	0

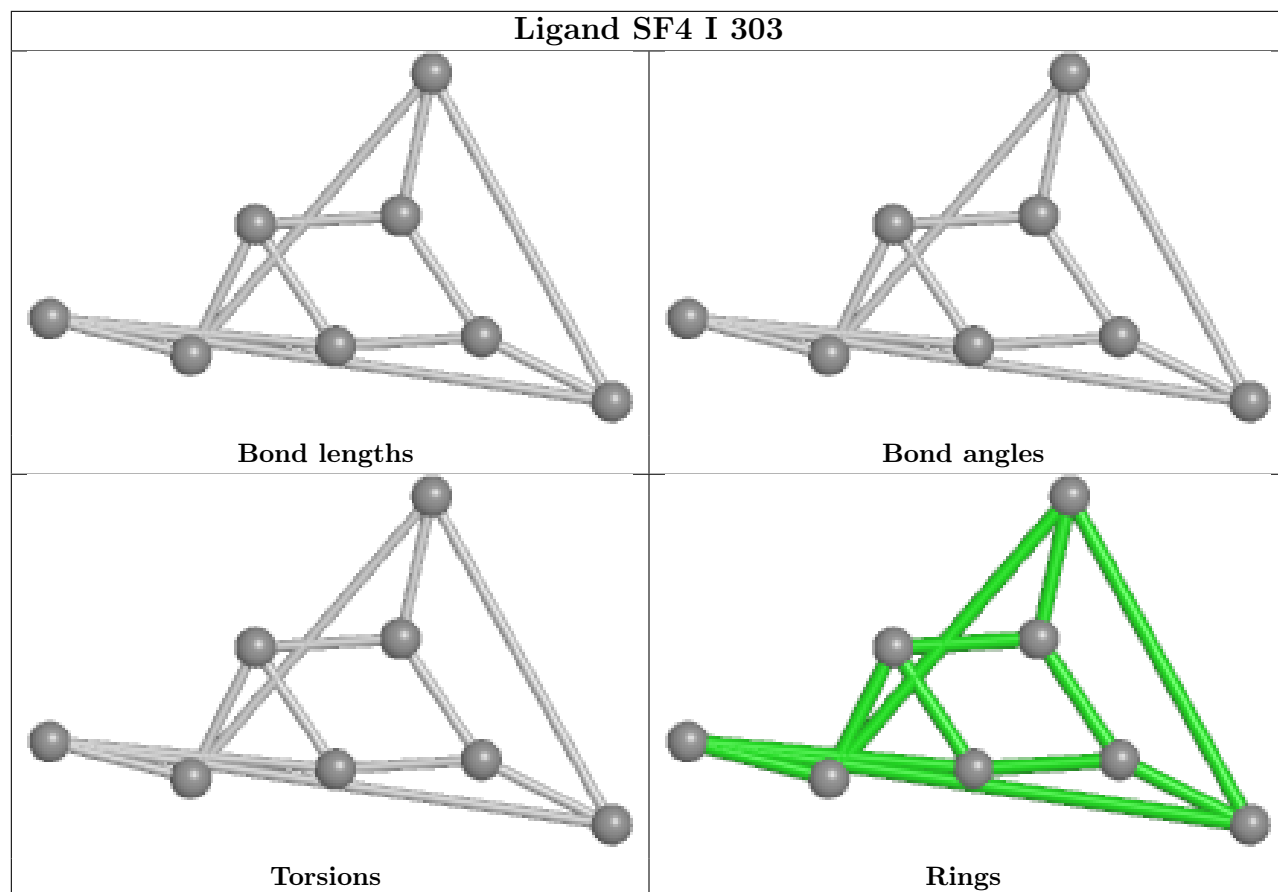
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



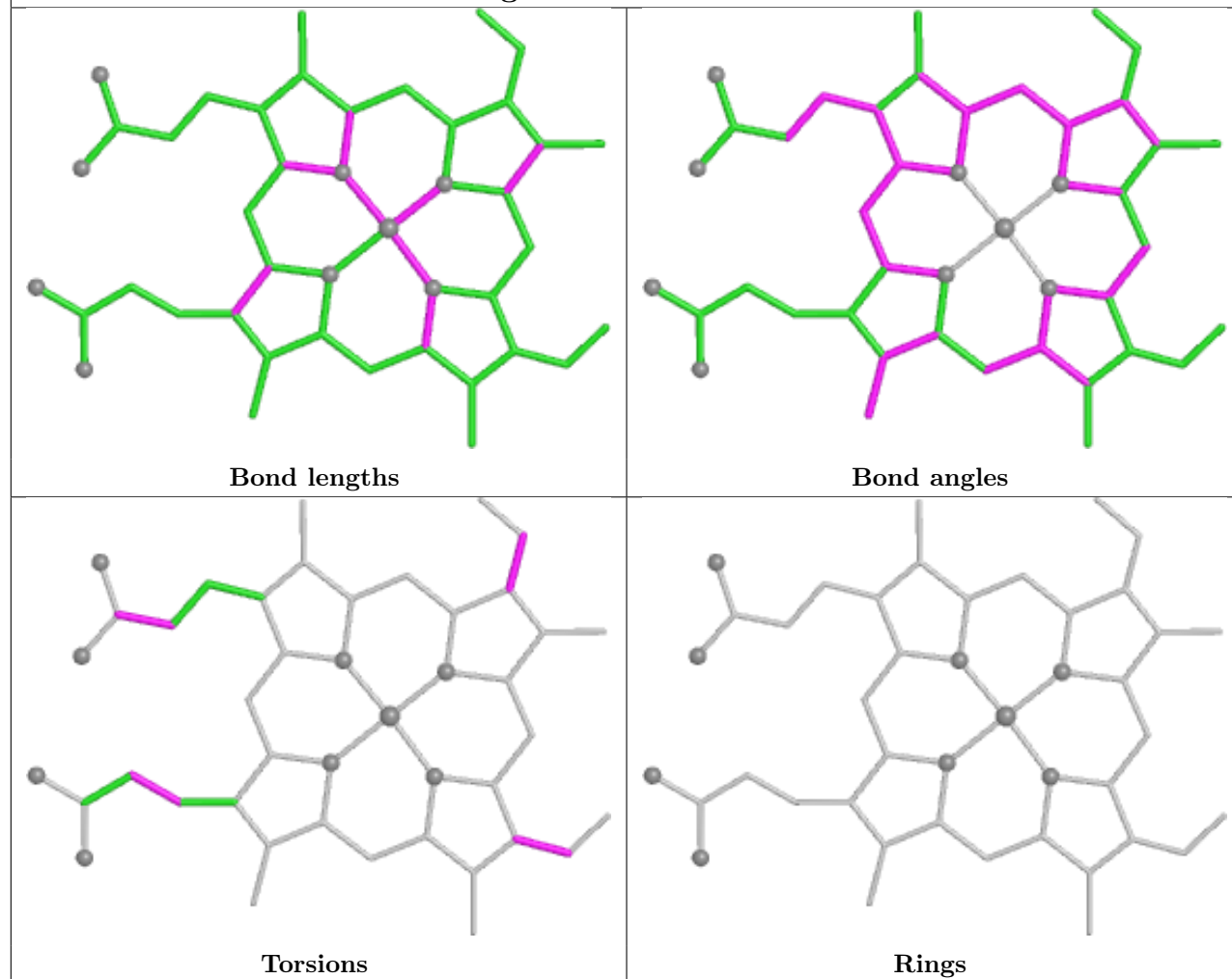




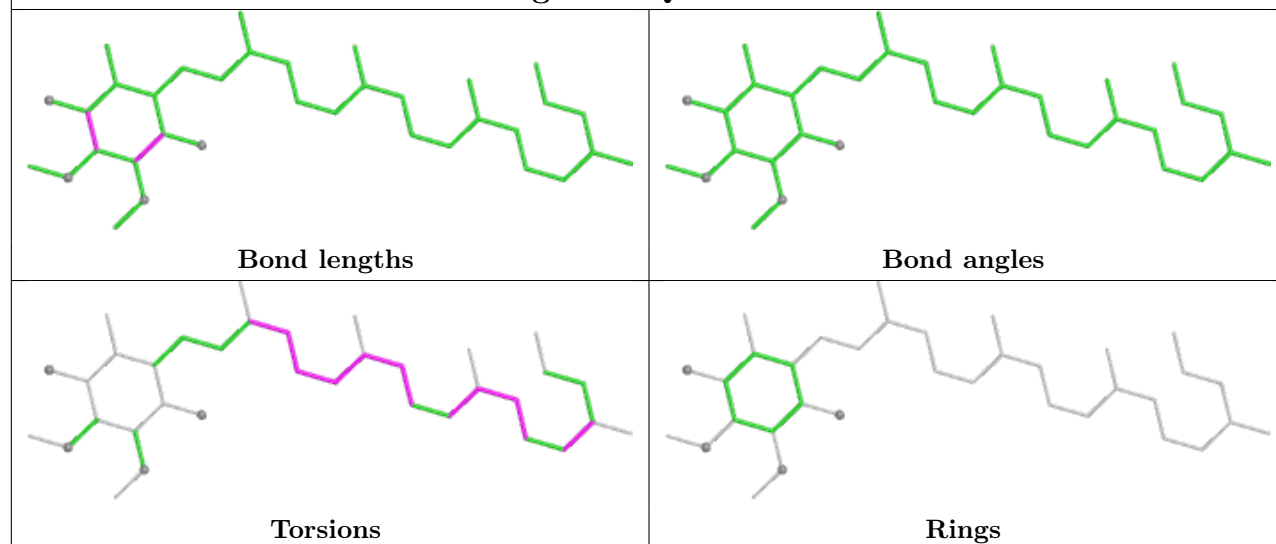


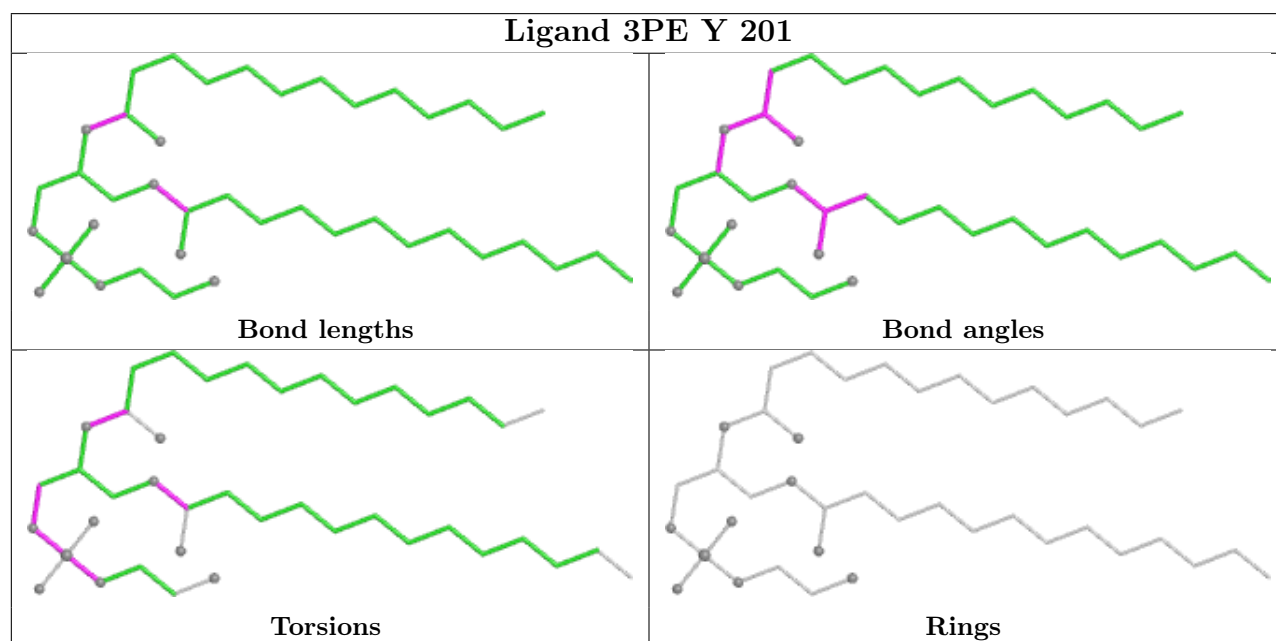
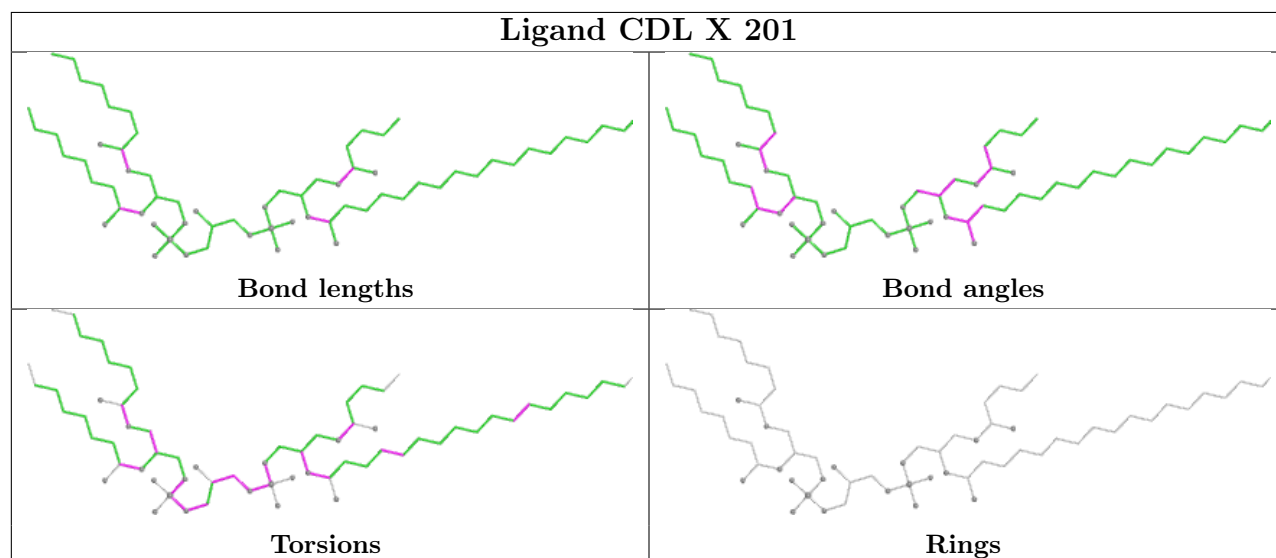
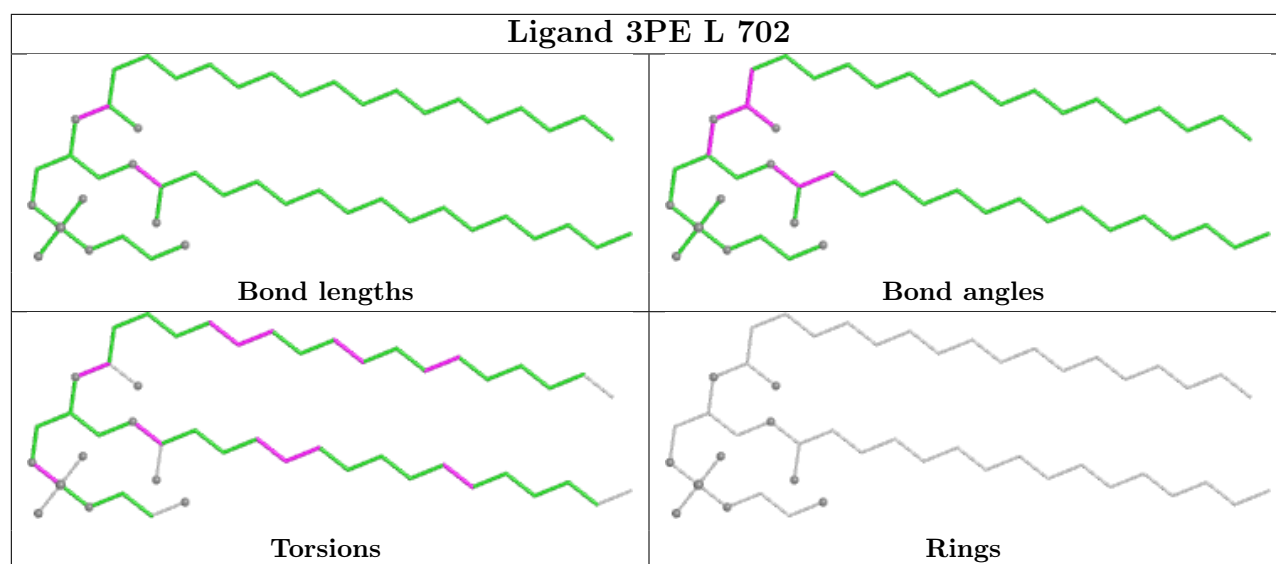


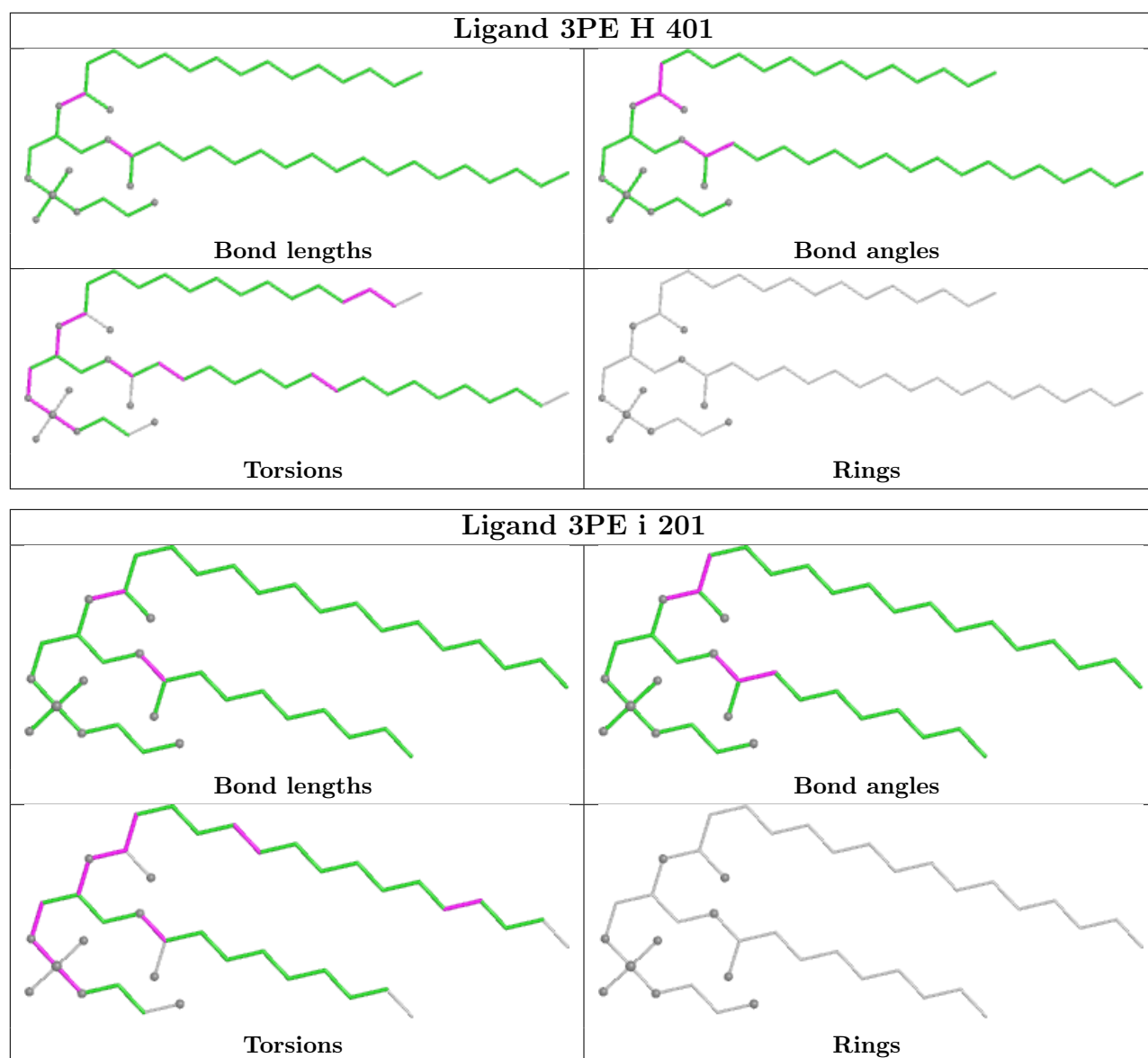
Ligand HEM Ac 402

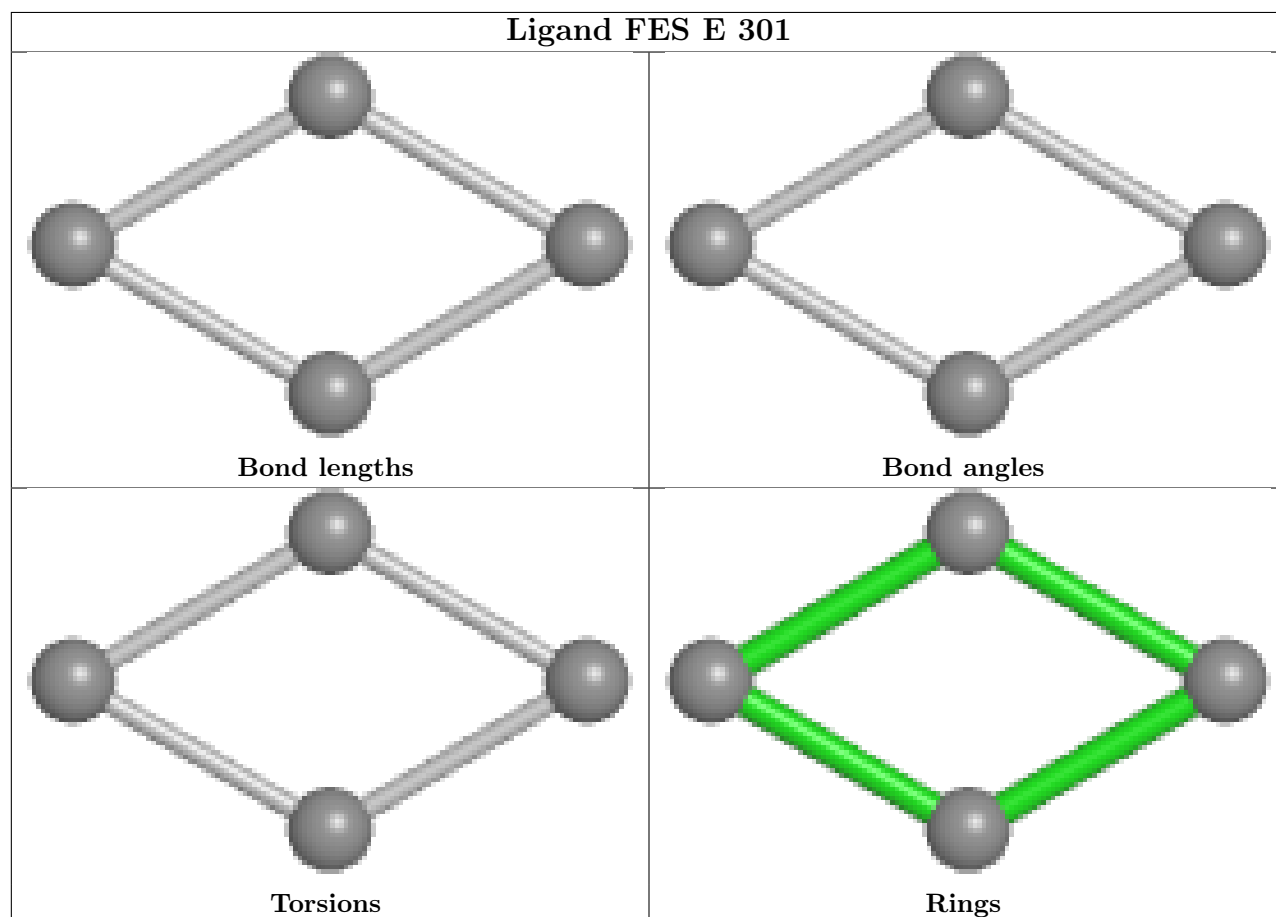
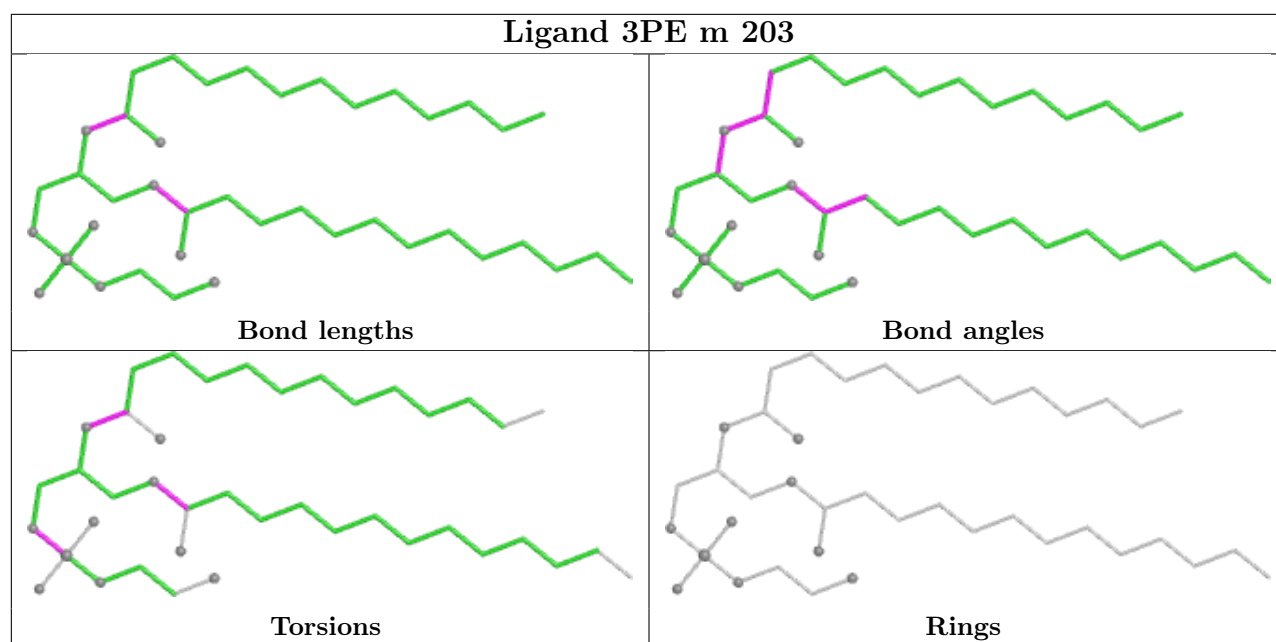


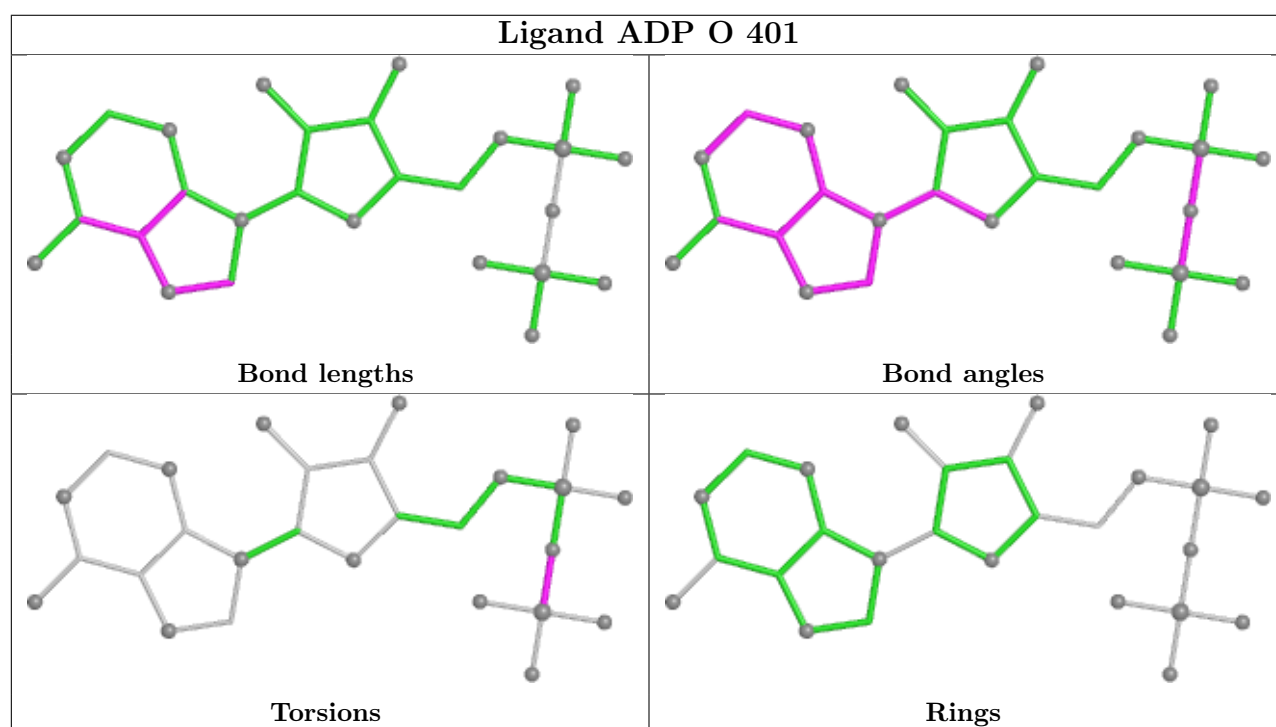
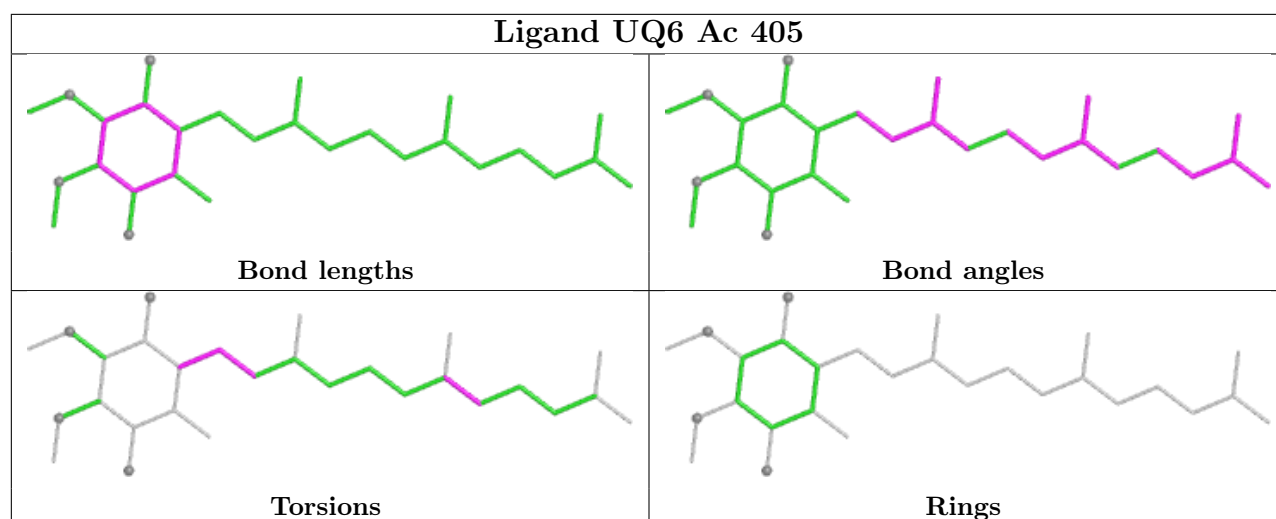
Ligand UQ9 H 400

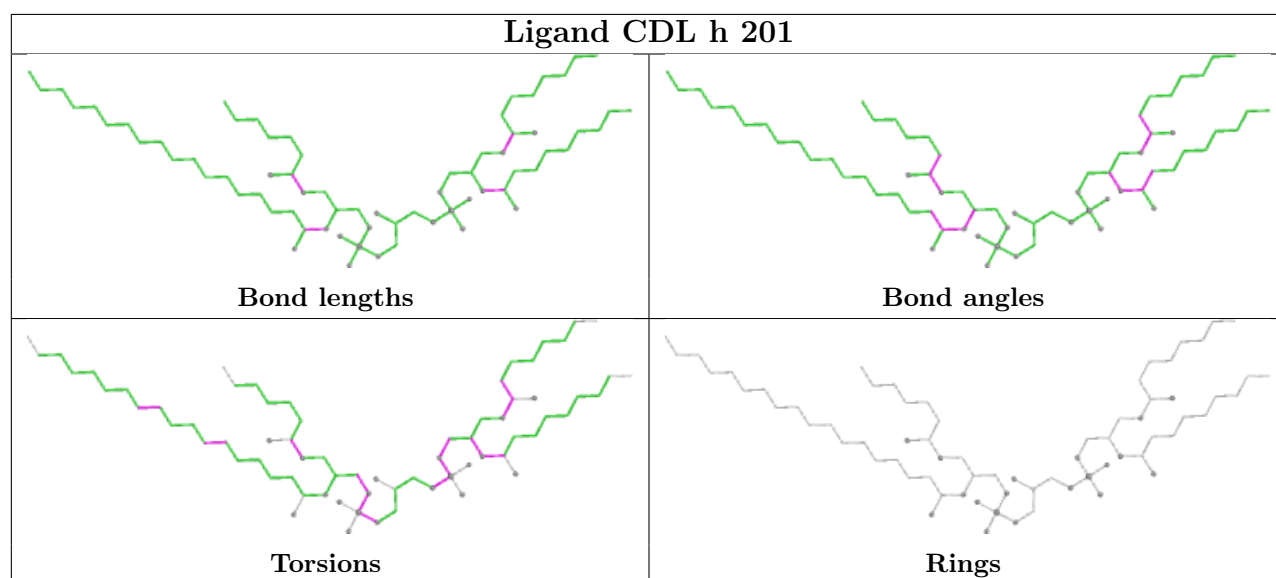
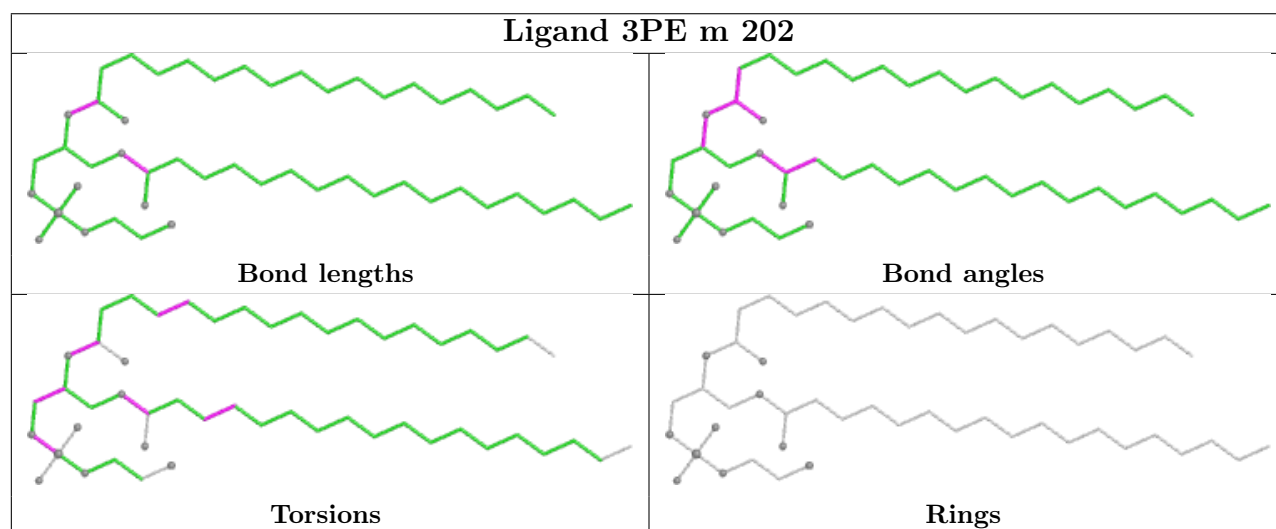
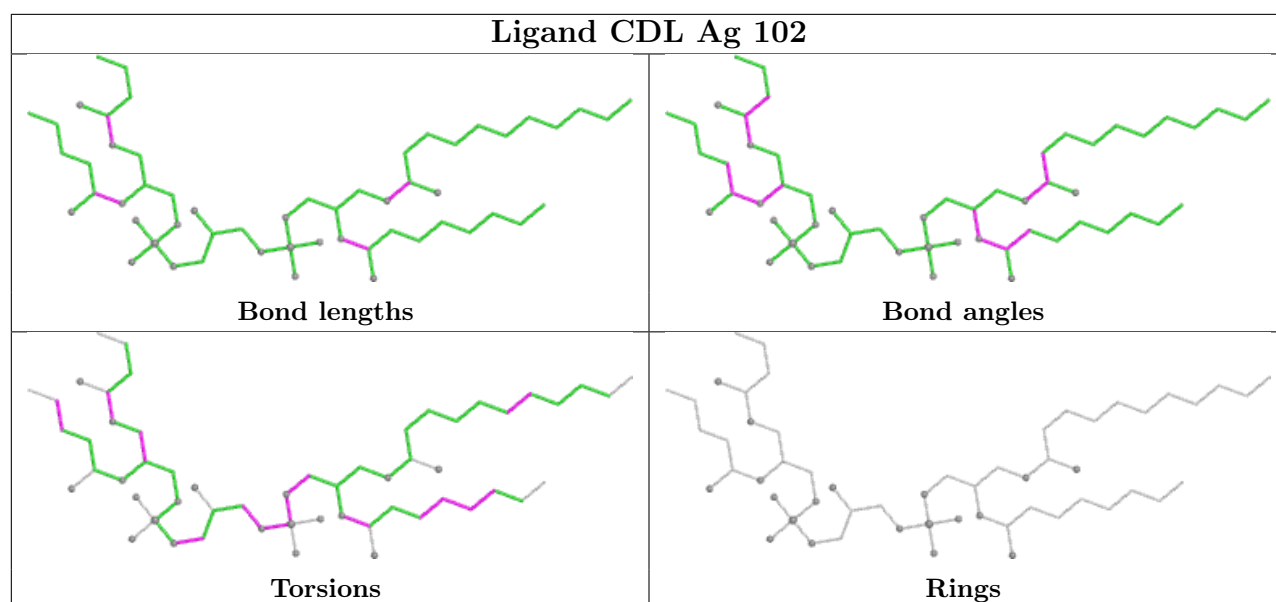




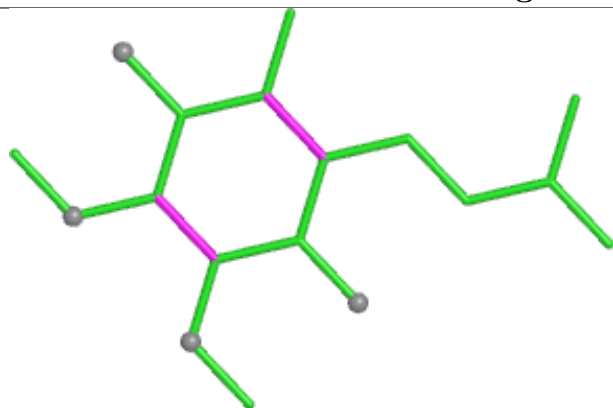




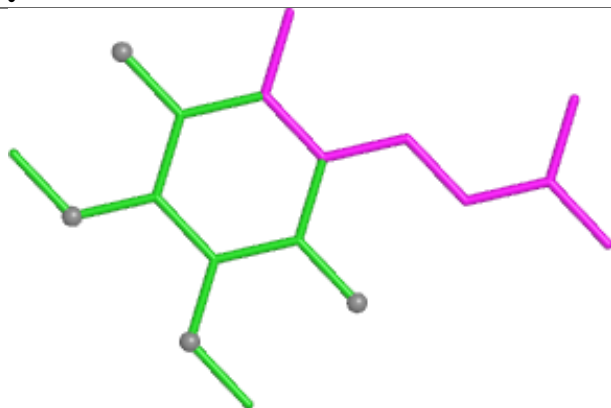




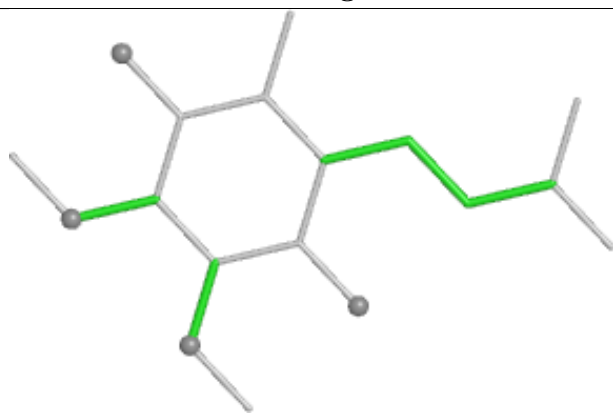
Ligand UQ1 B 302



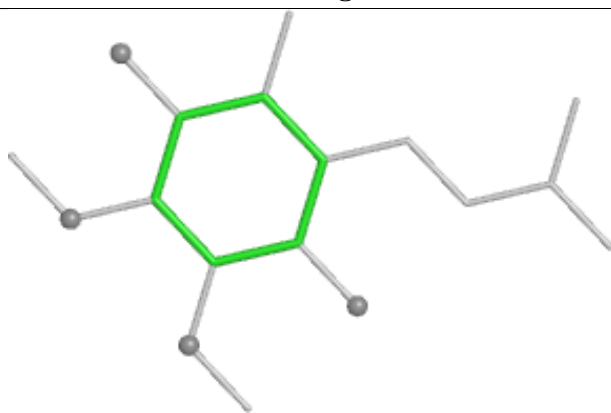
Bond lengths



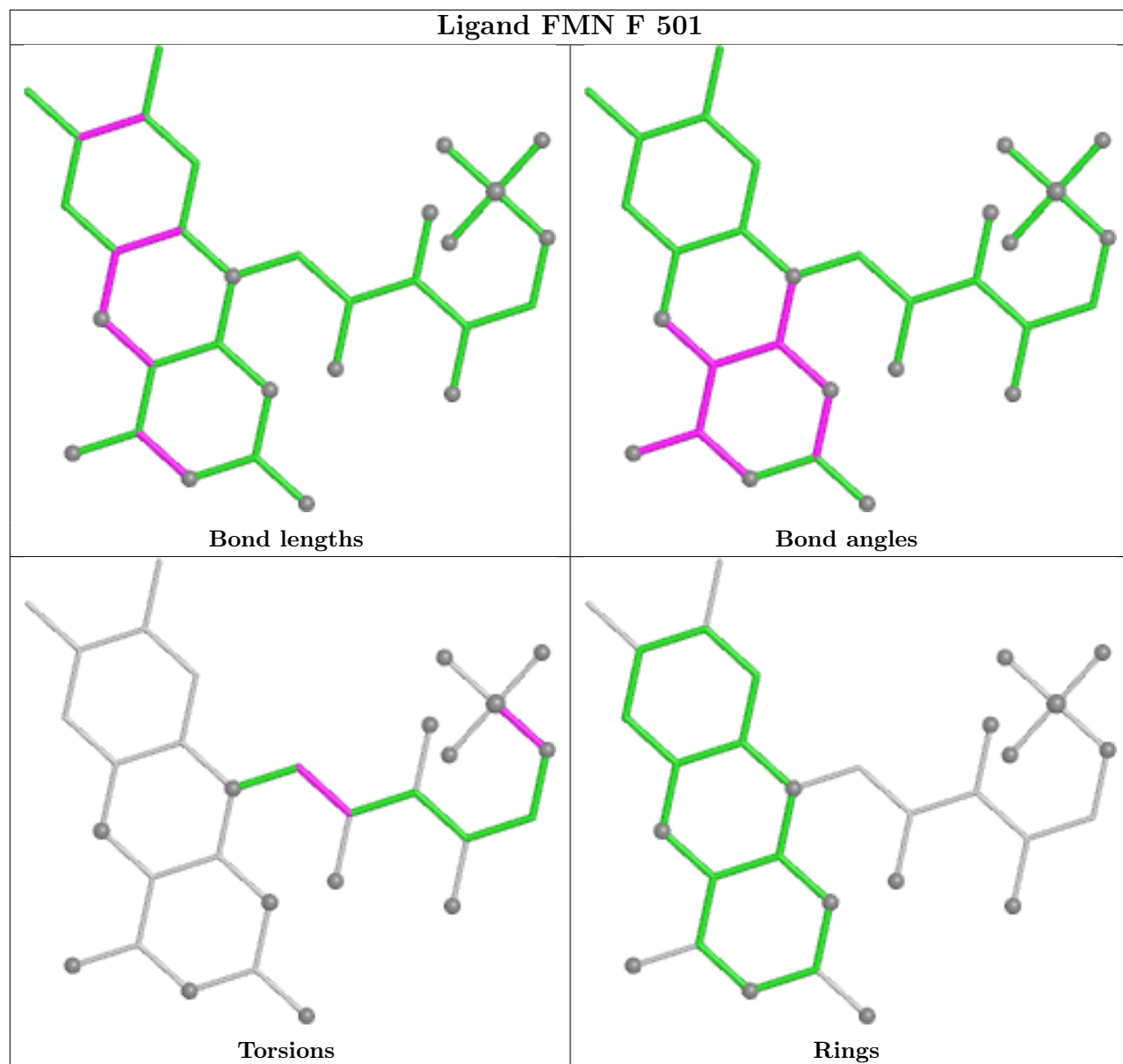
Bond angles

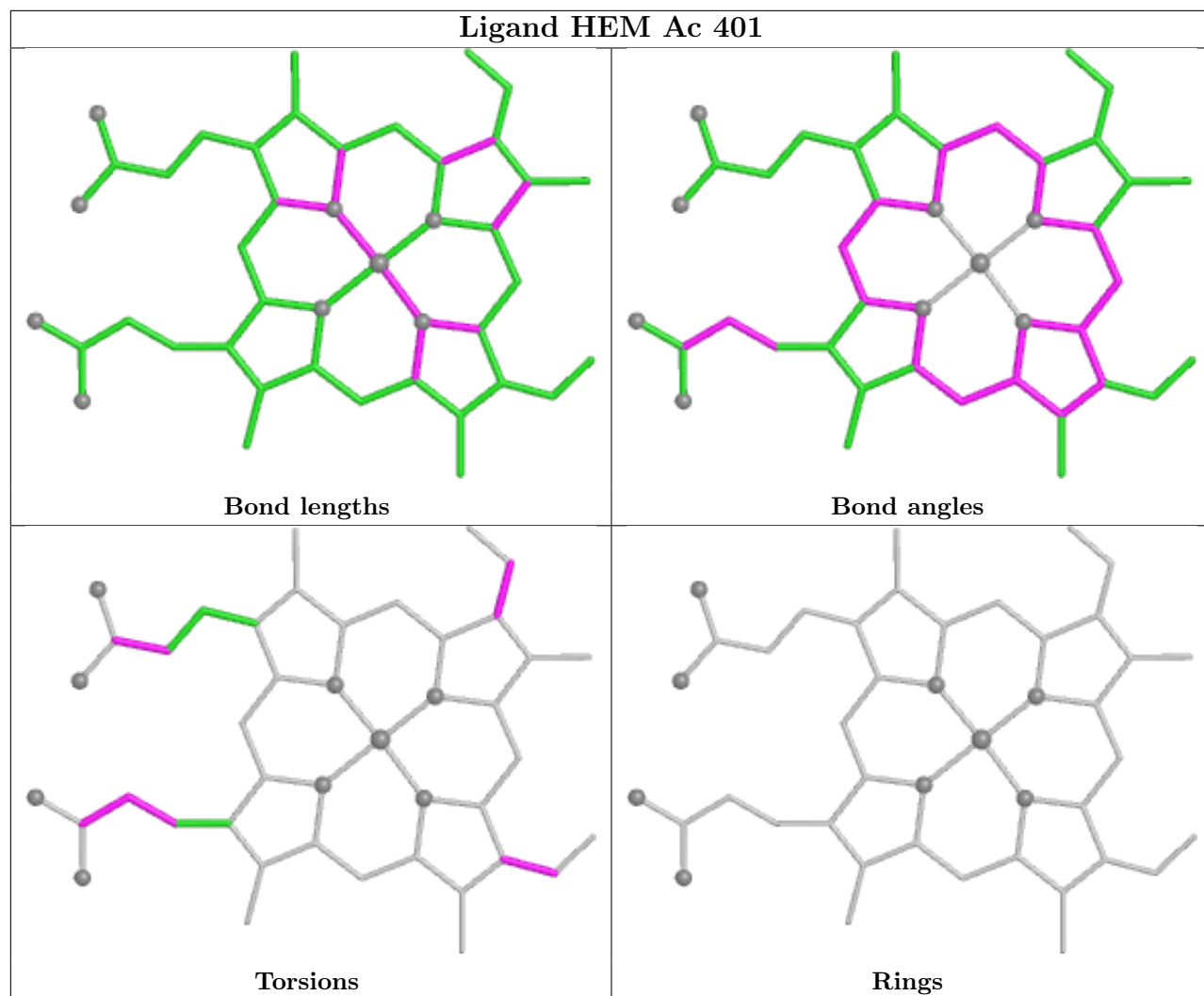


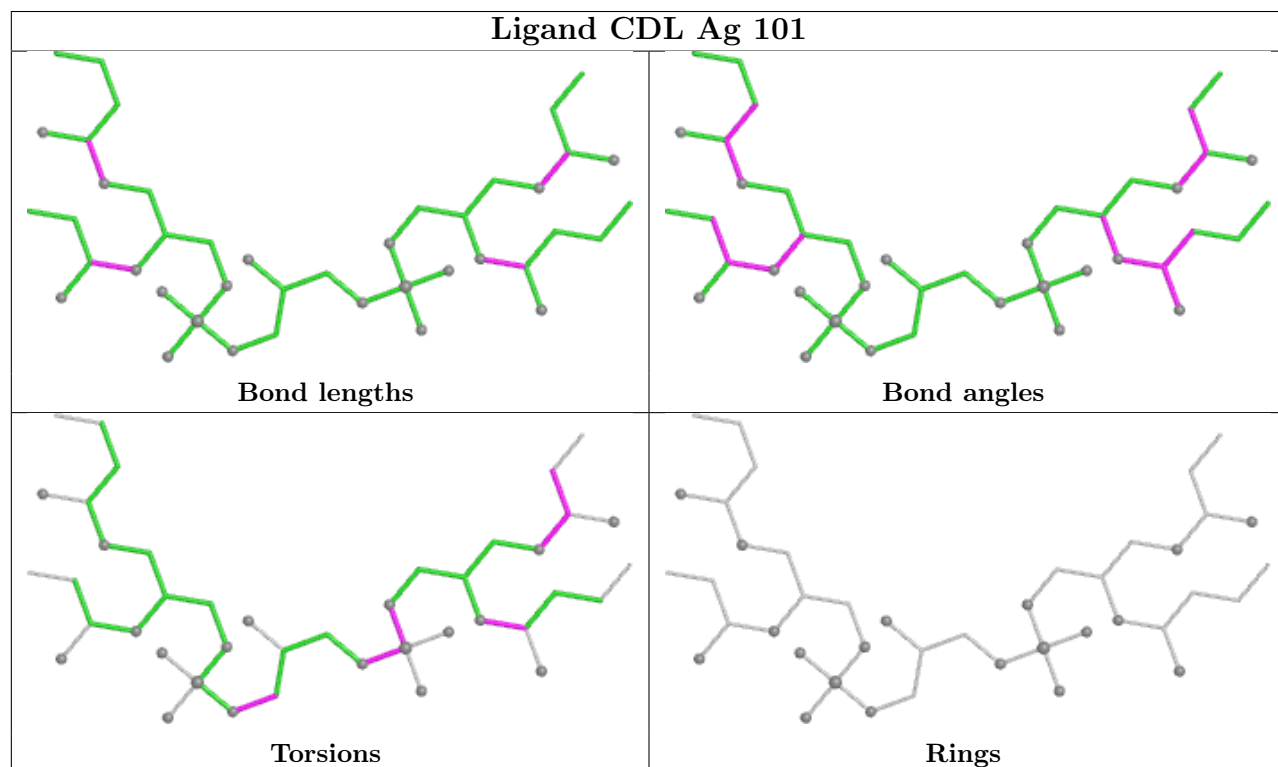
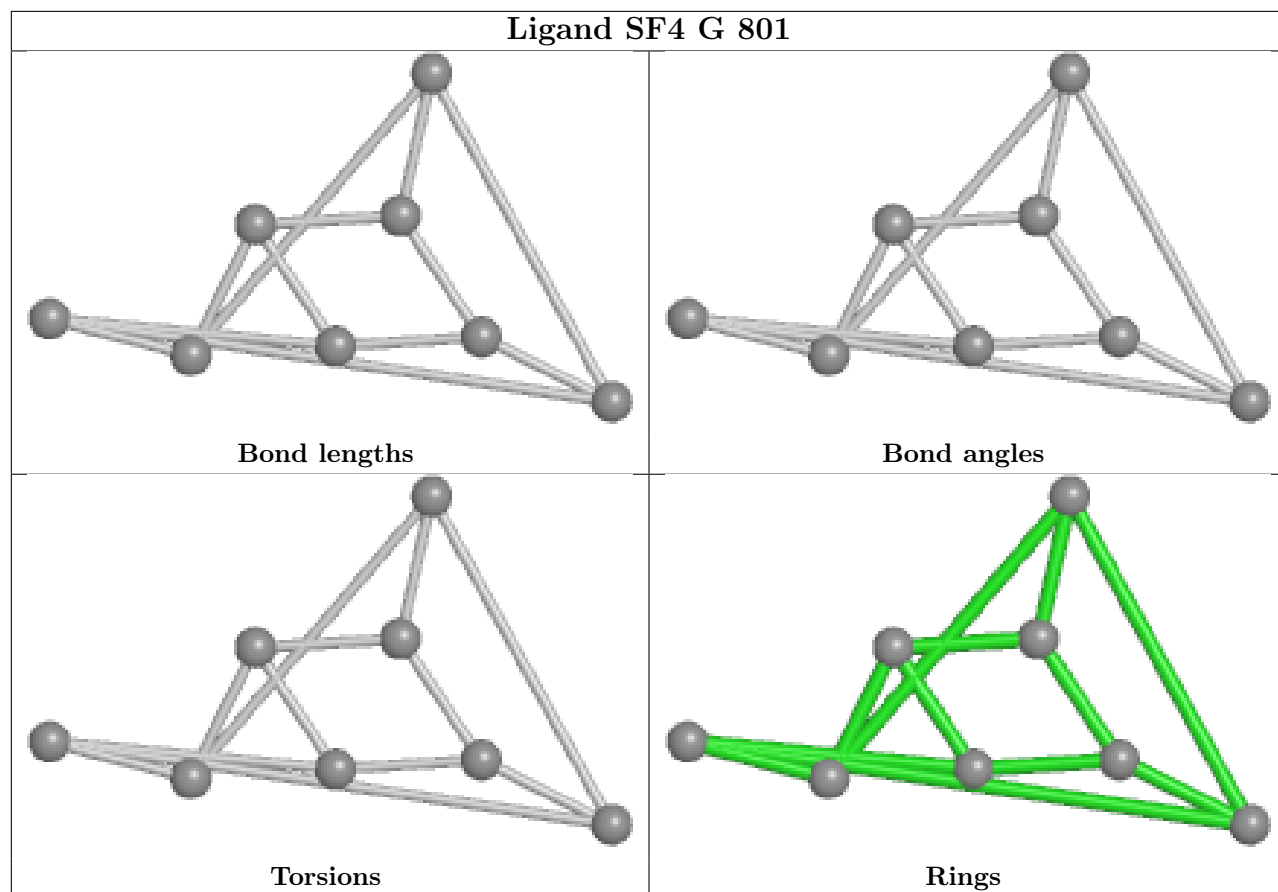
Torsions



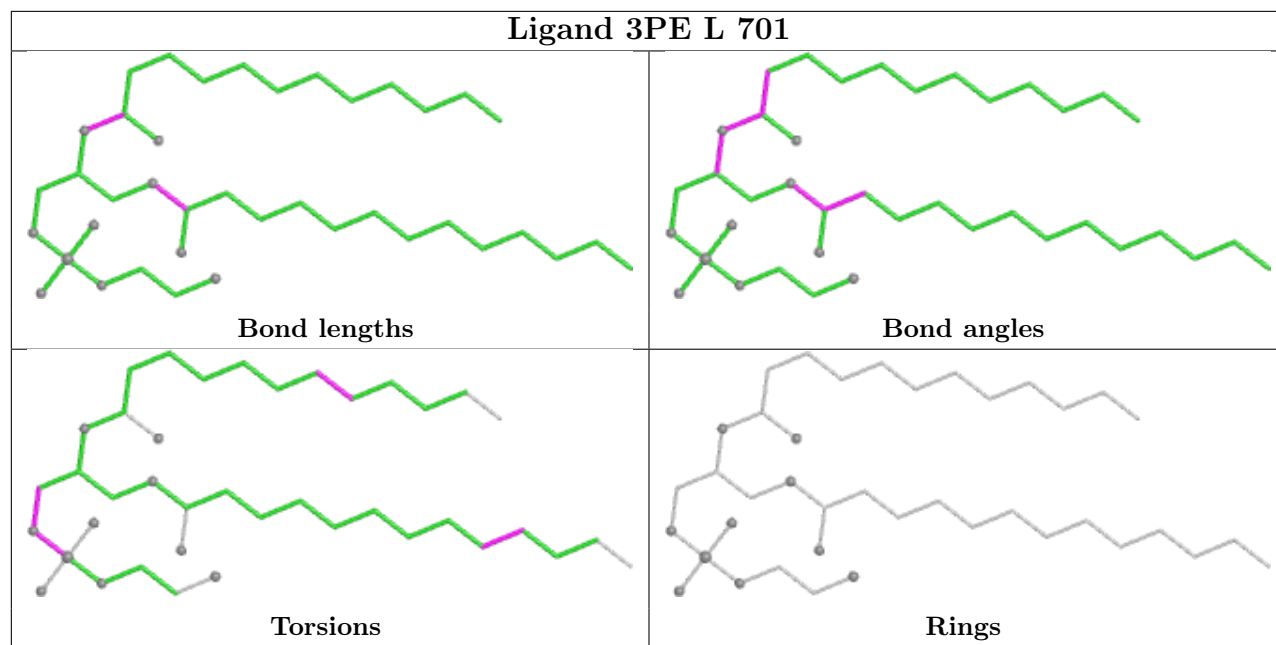
Rings



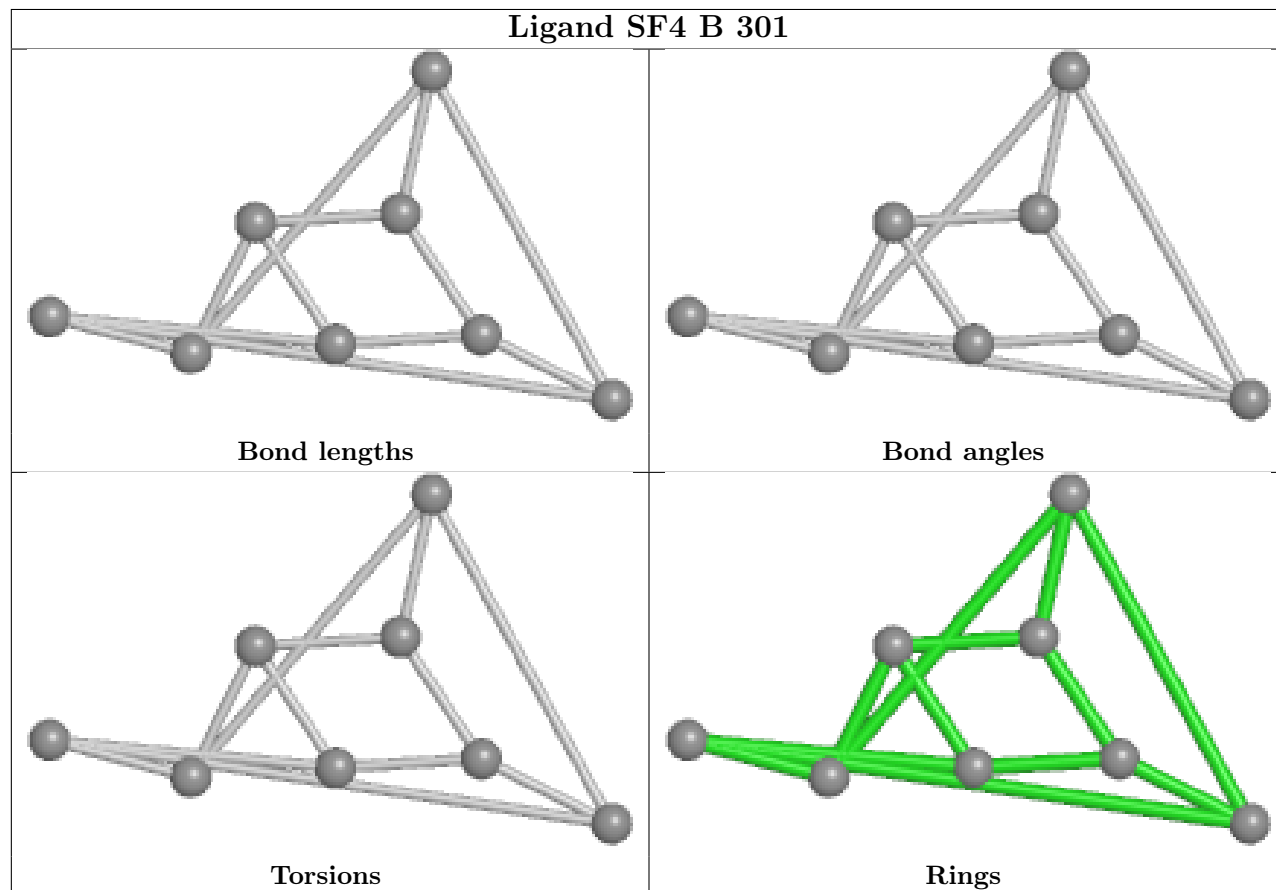


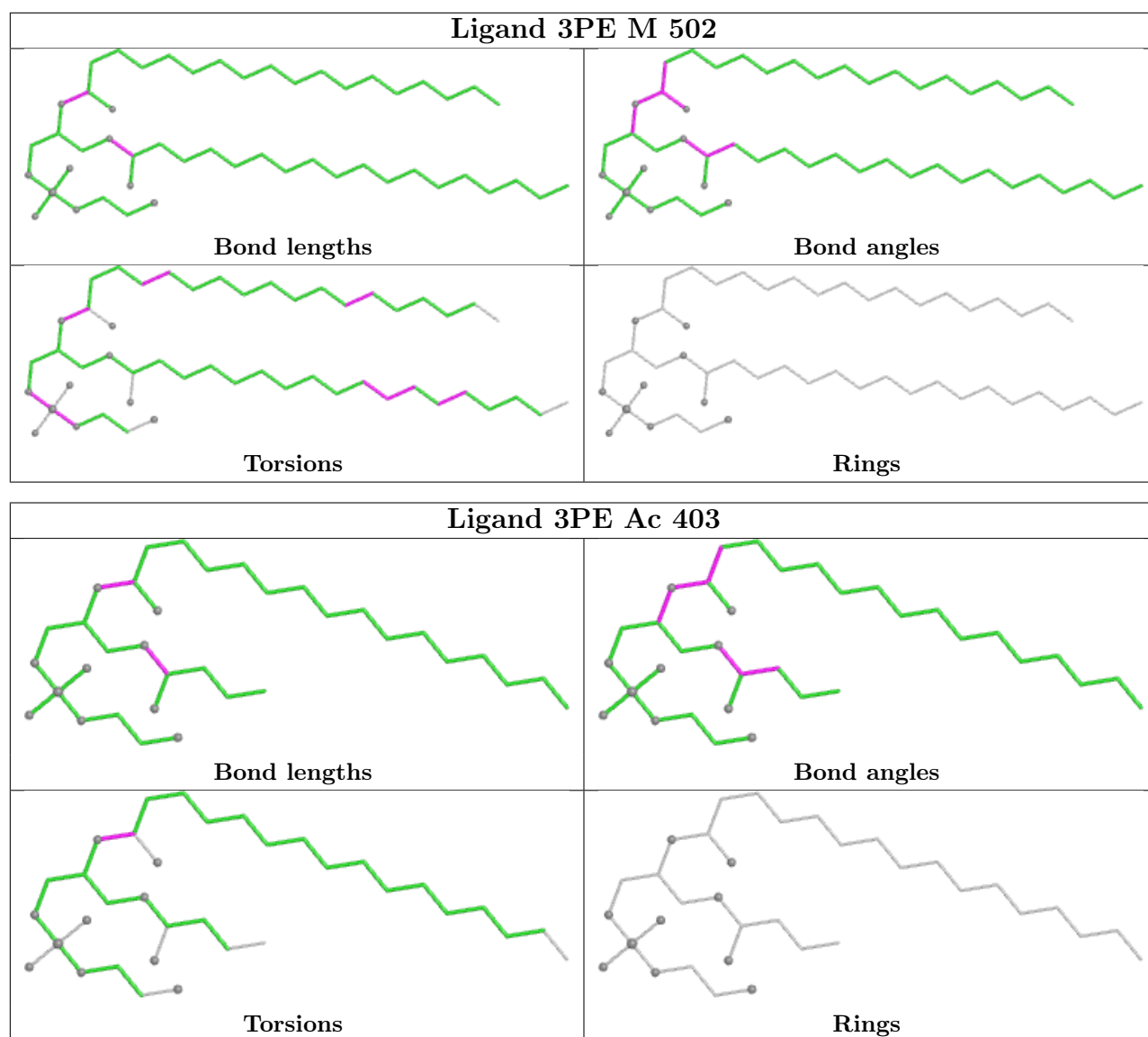


Ligand 3PE L 701

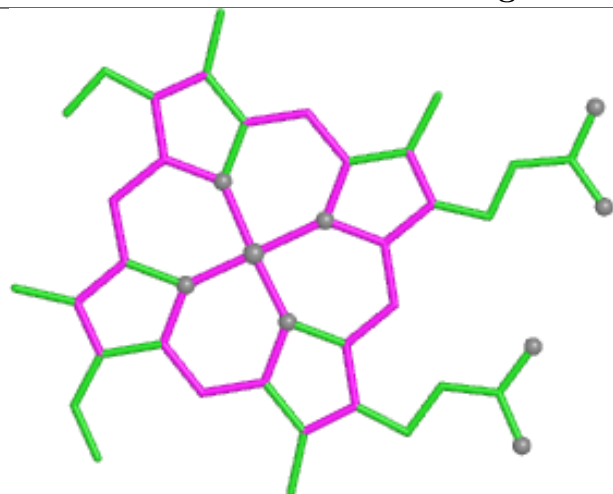


Ligand SF4 B 301

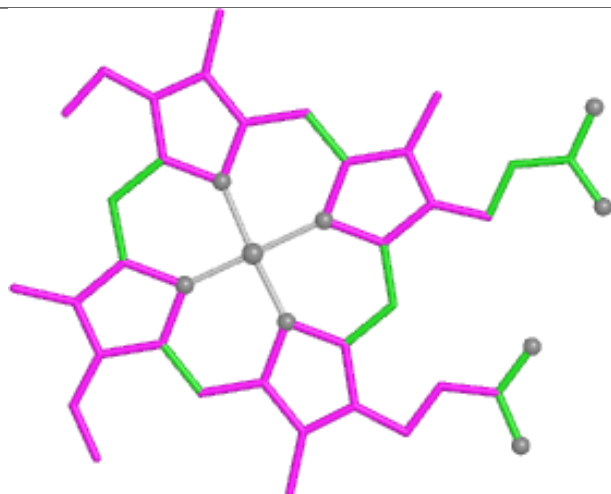




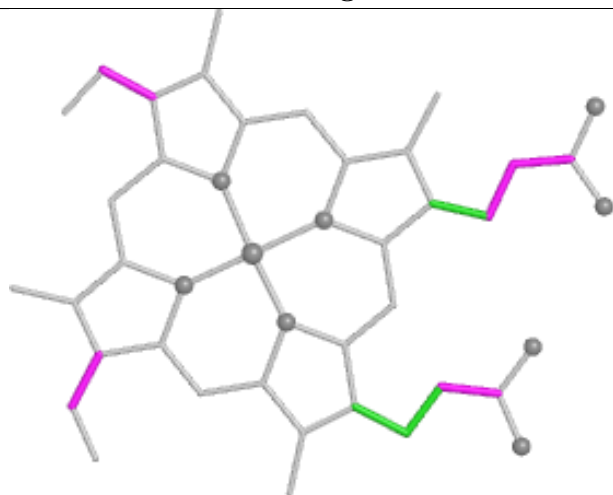
Ligand HEC AD 401



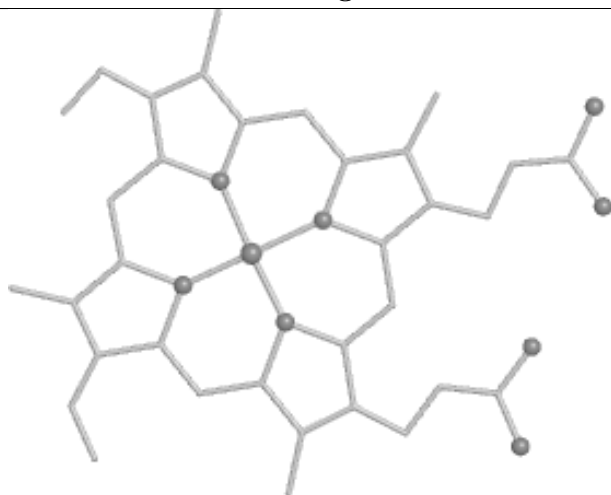
Bond lengths



Bond angles

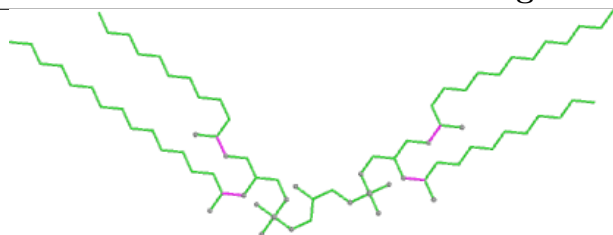


Torsions

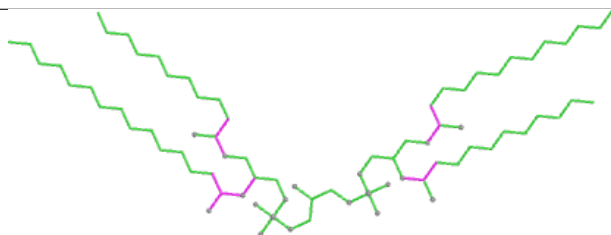


Rings

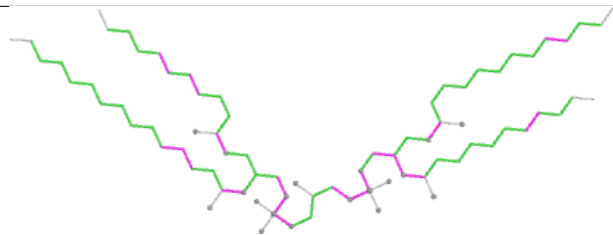
Ligand CDL L 704



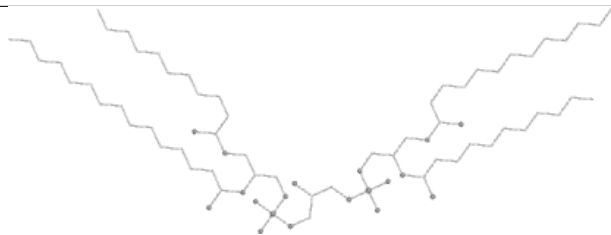
Bond lengths



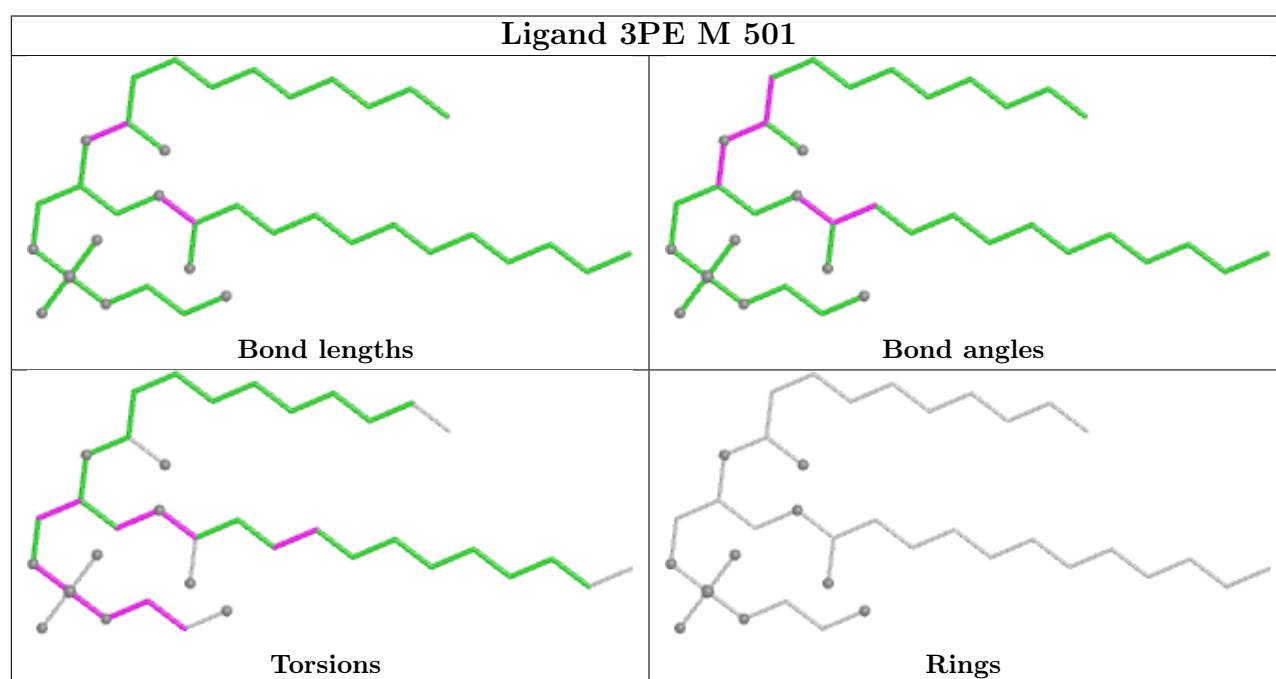
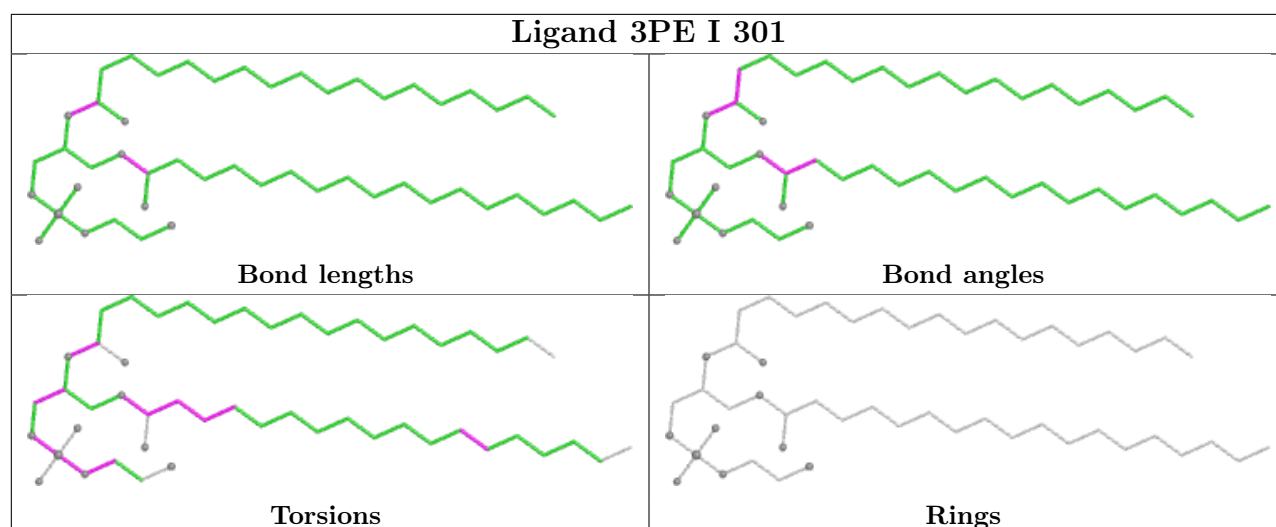
Bond angles

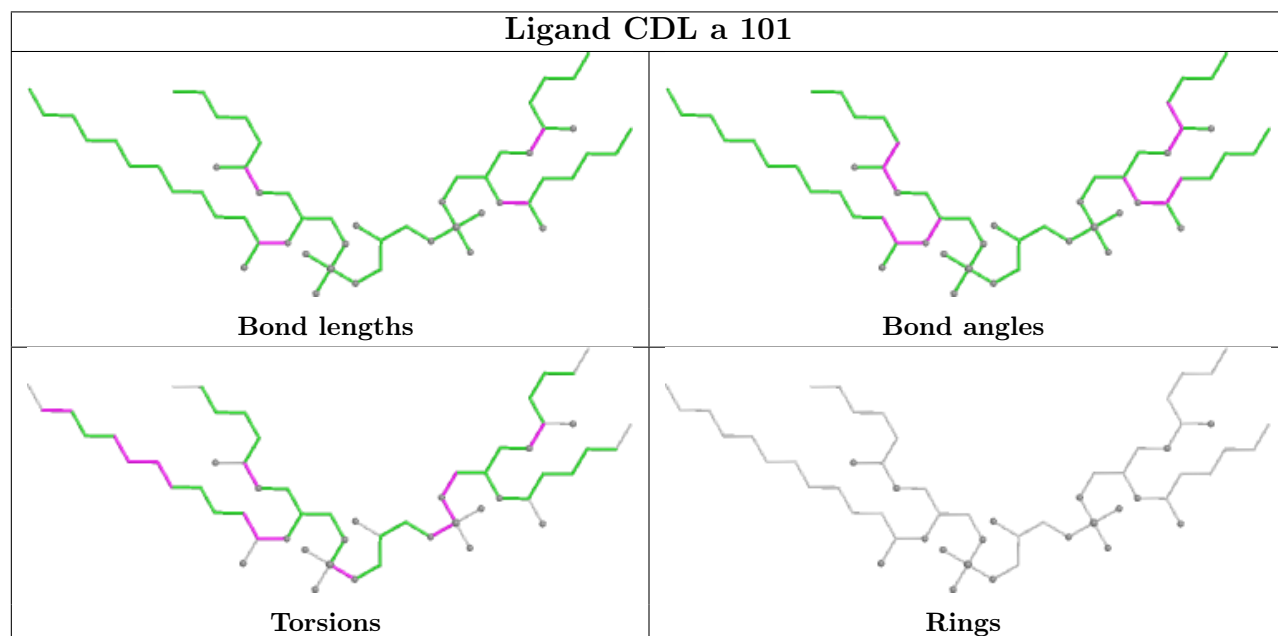
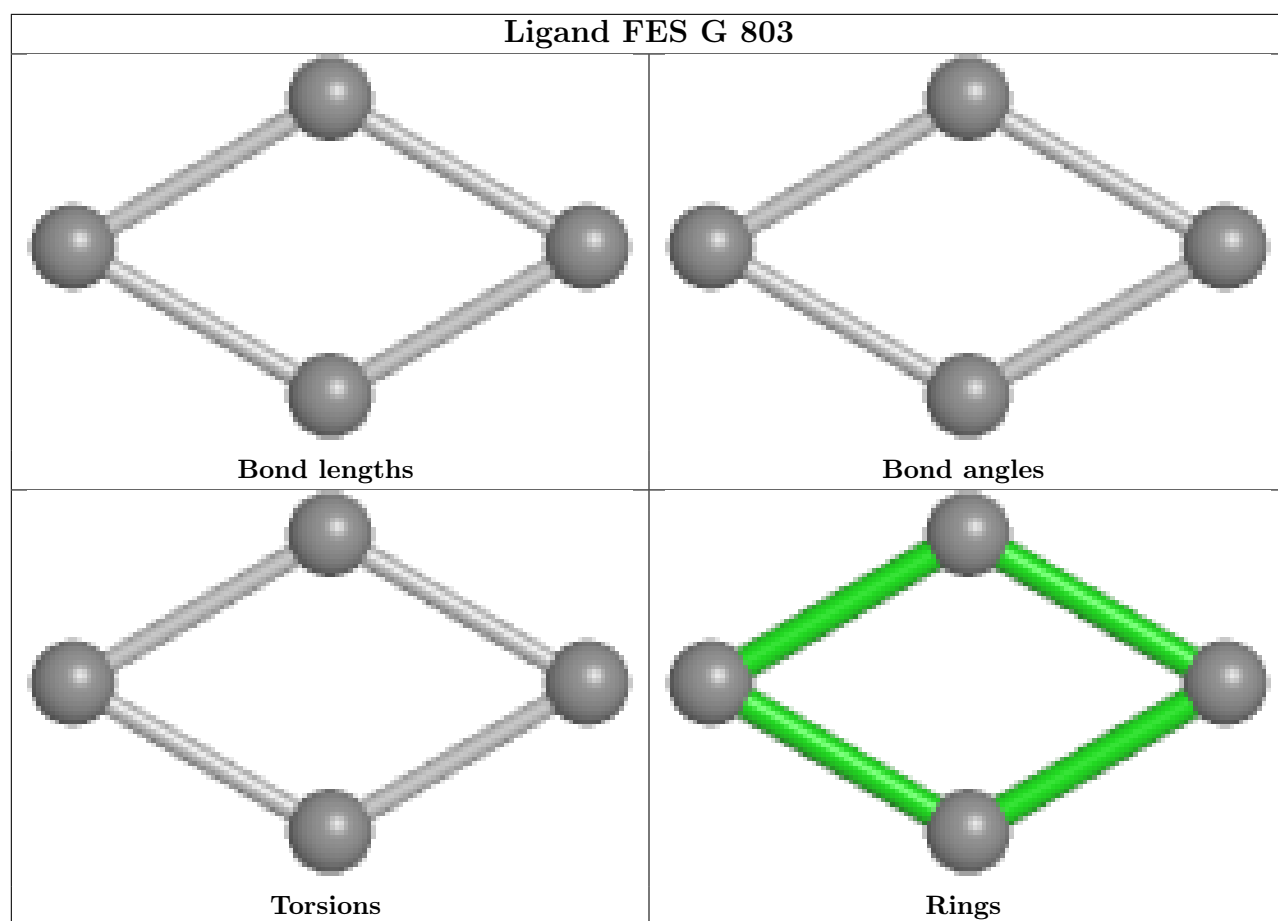


Torsions

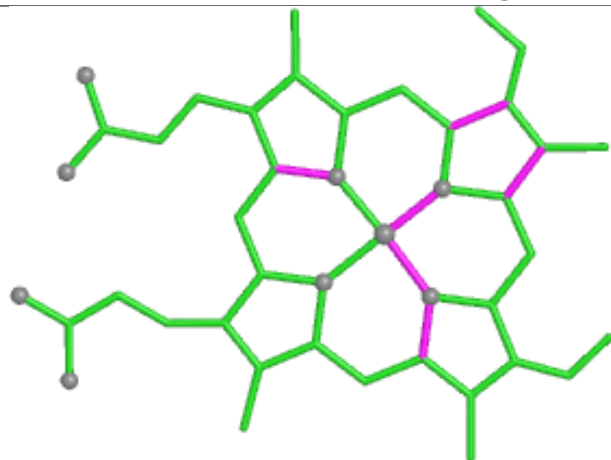


Rings

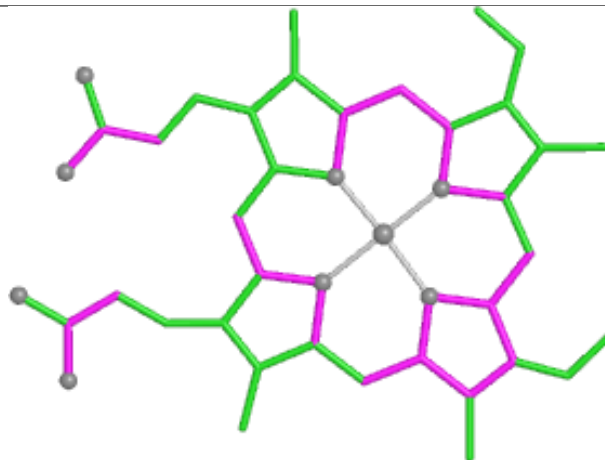




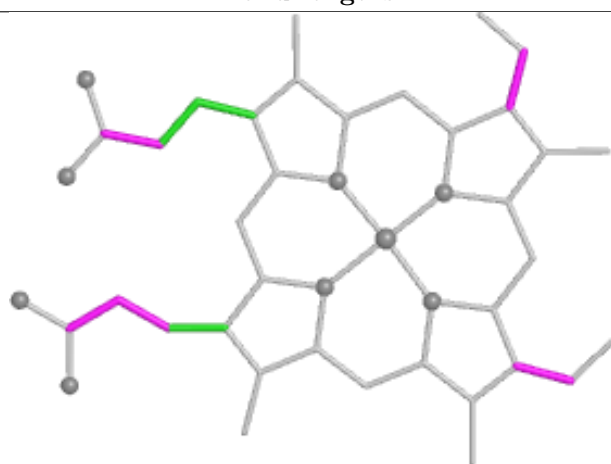
Ligand HEM AC 401



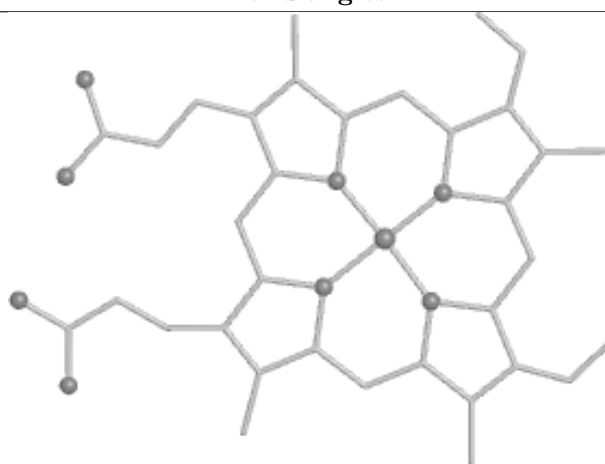
Bond lengths



Bond angles

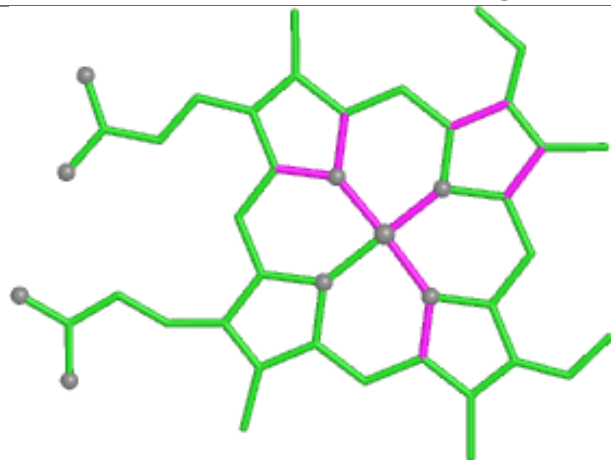


Torsions

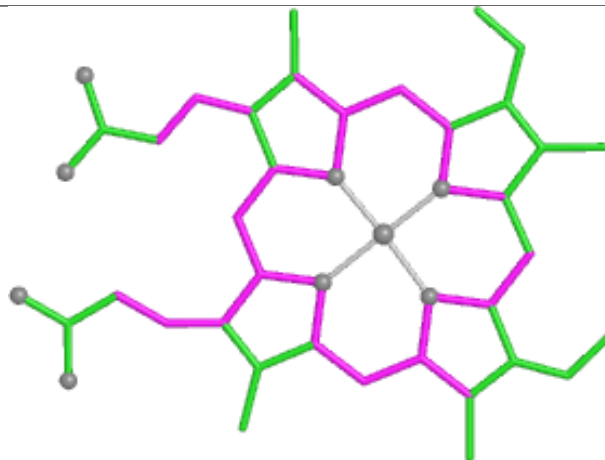


Rings

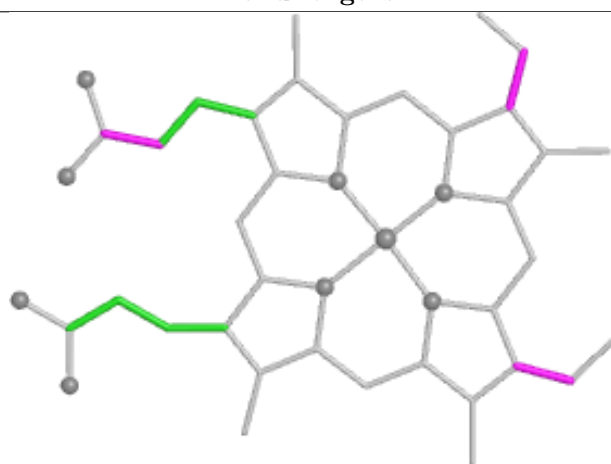
Ligand HEM AC 402



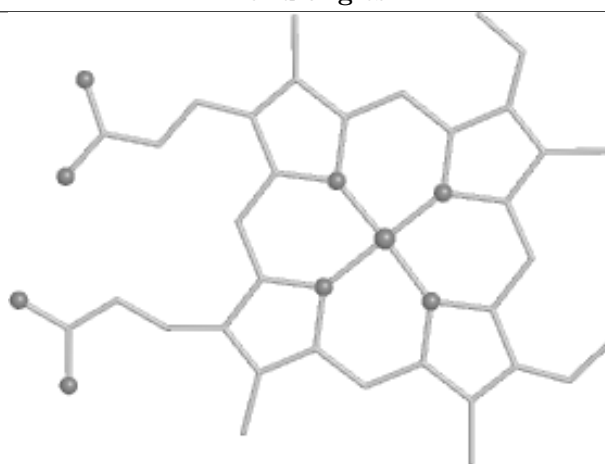
Bond lengths



Bond angles

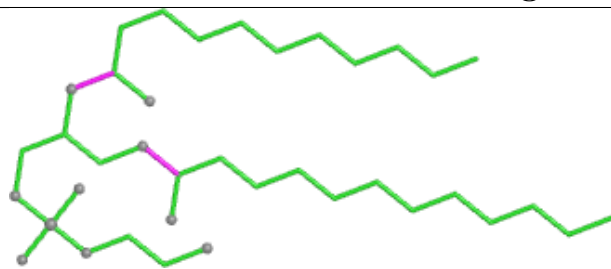


Torsions

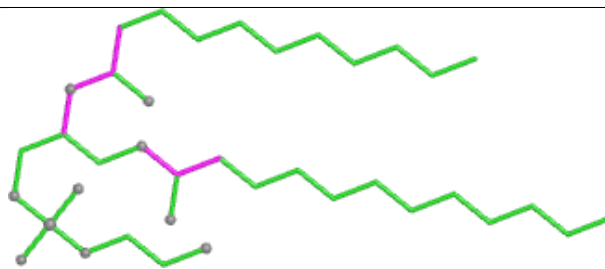


Rings

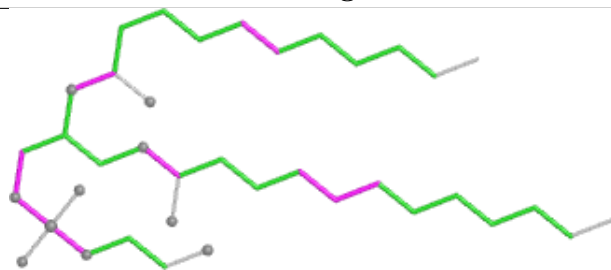
Ligand 3PE L 705



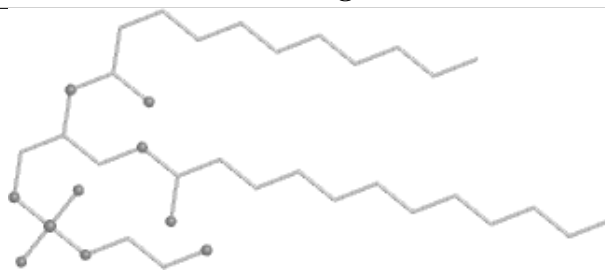
Bond lengths



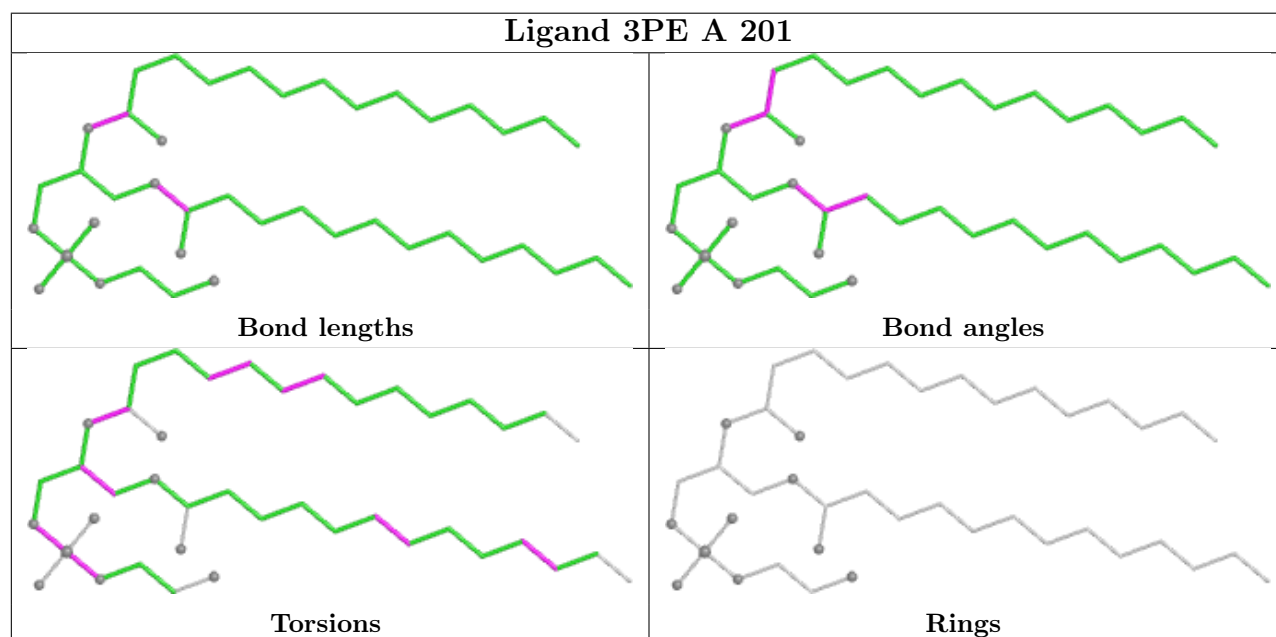
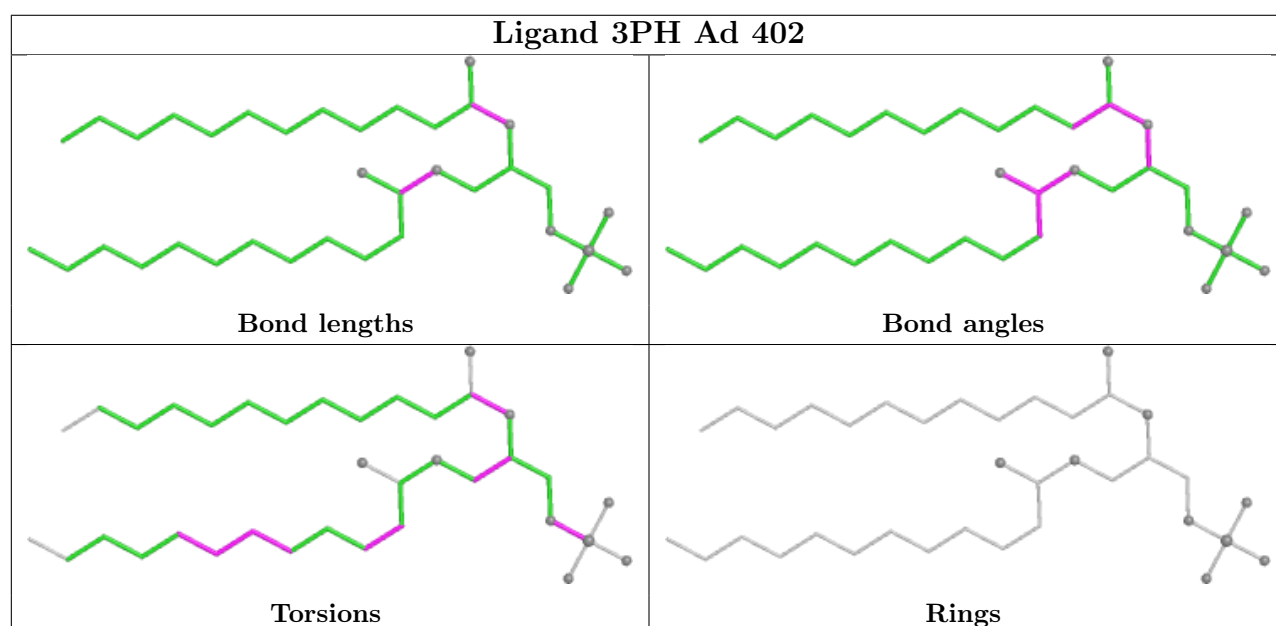
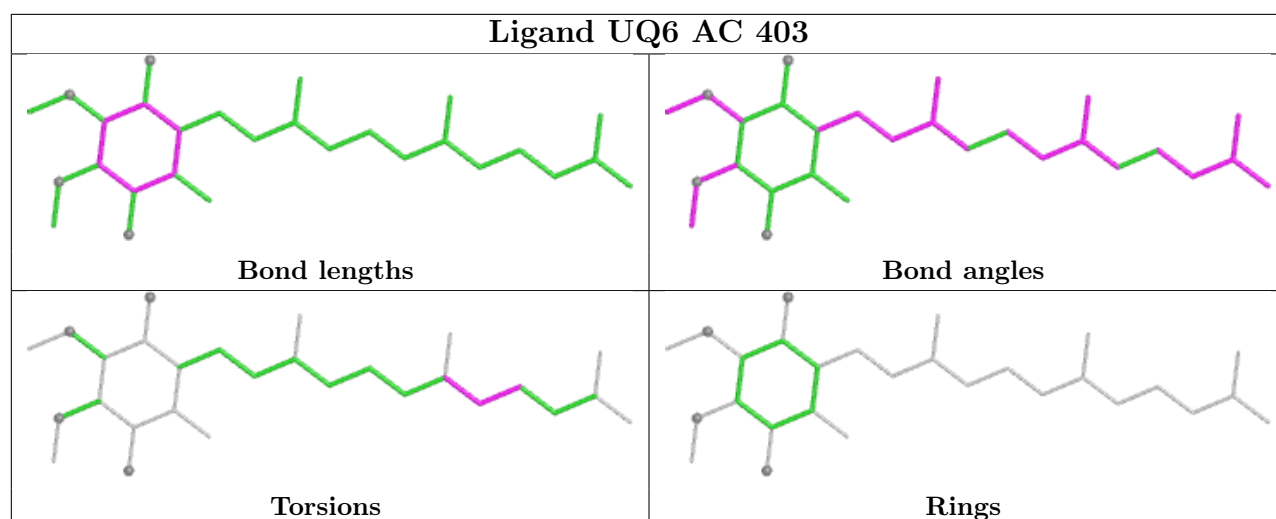
Bond angles

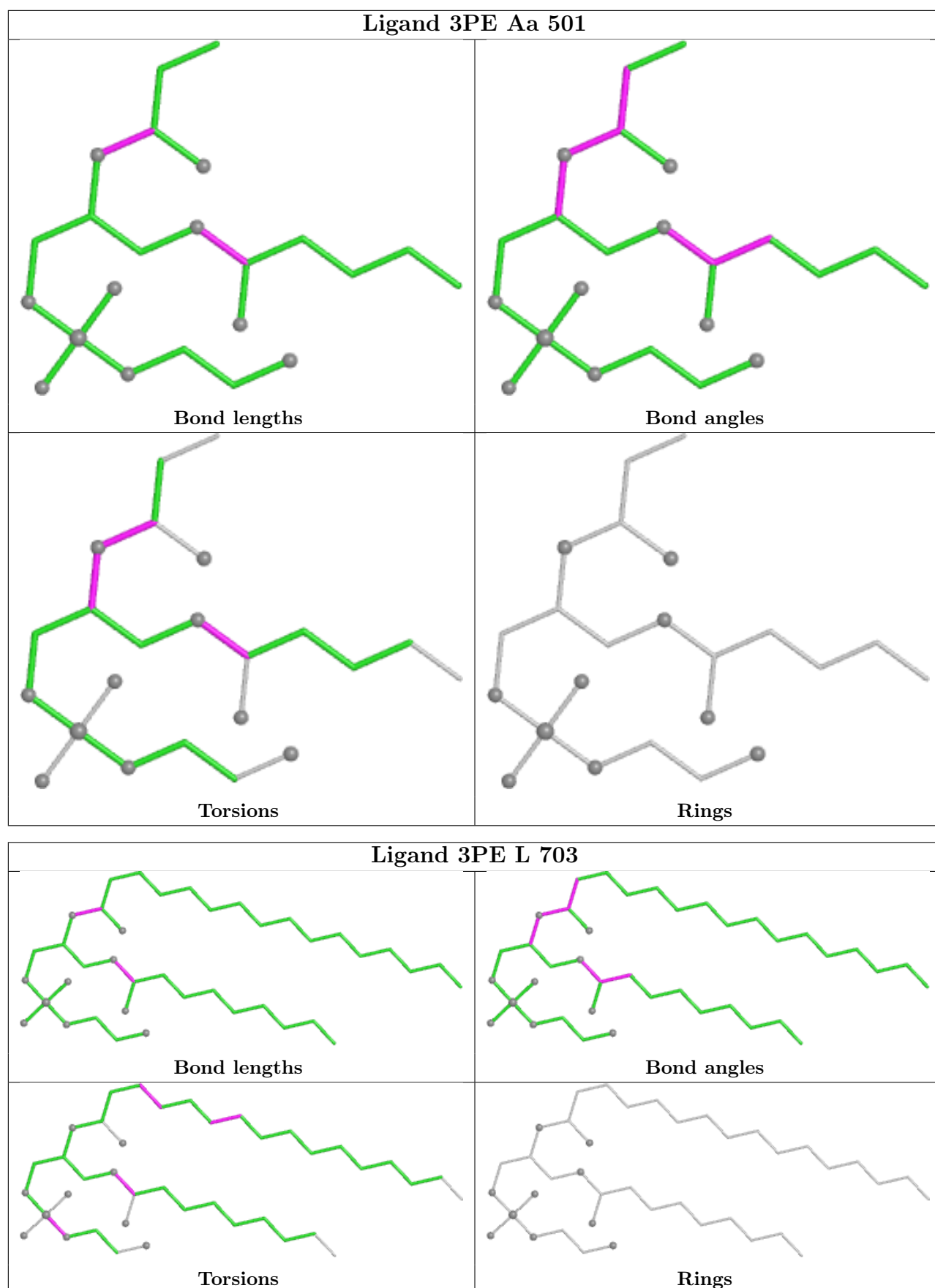


Torsions

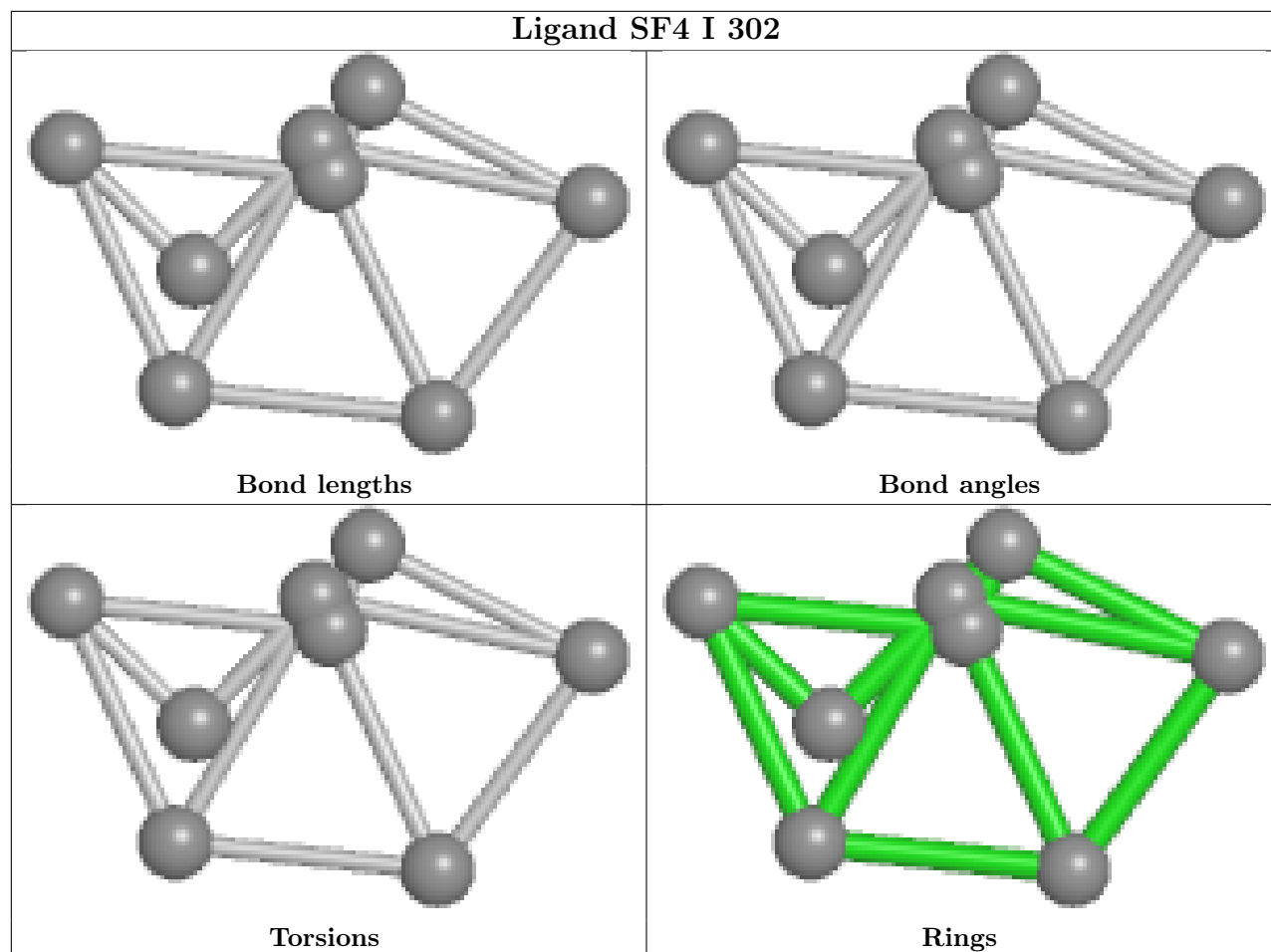


Rings

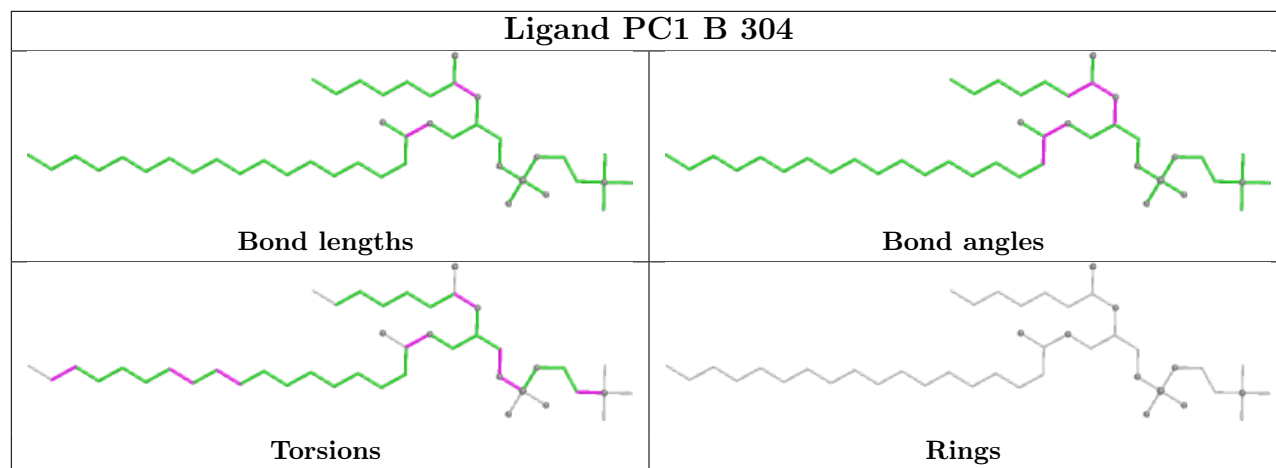


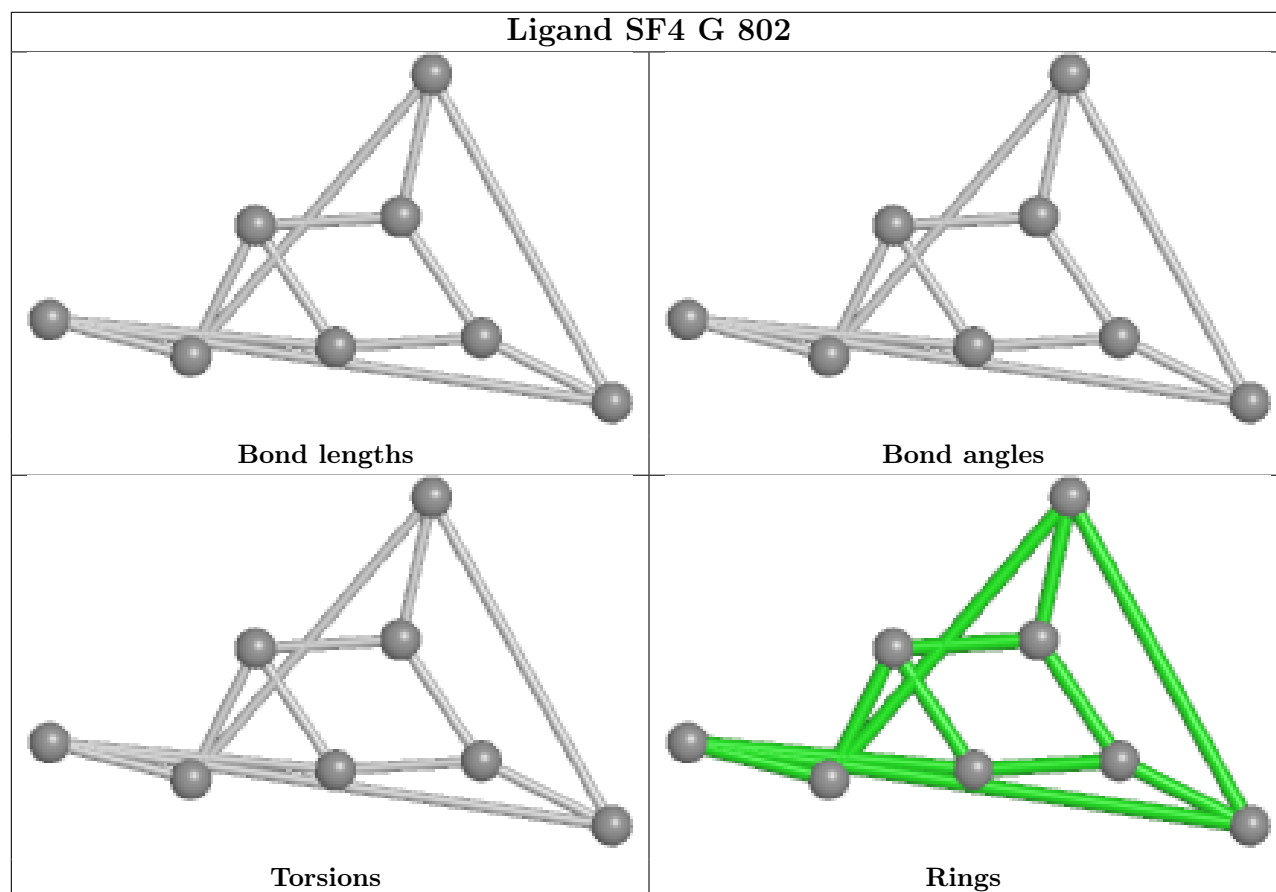
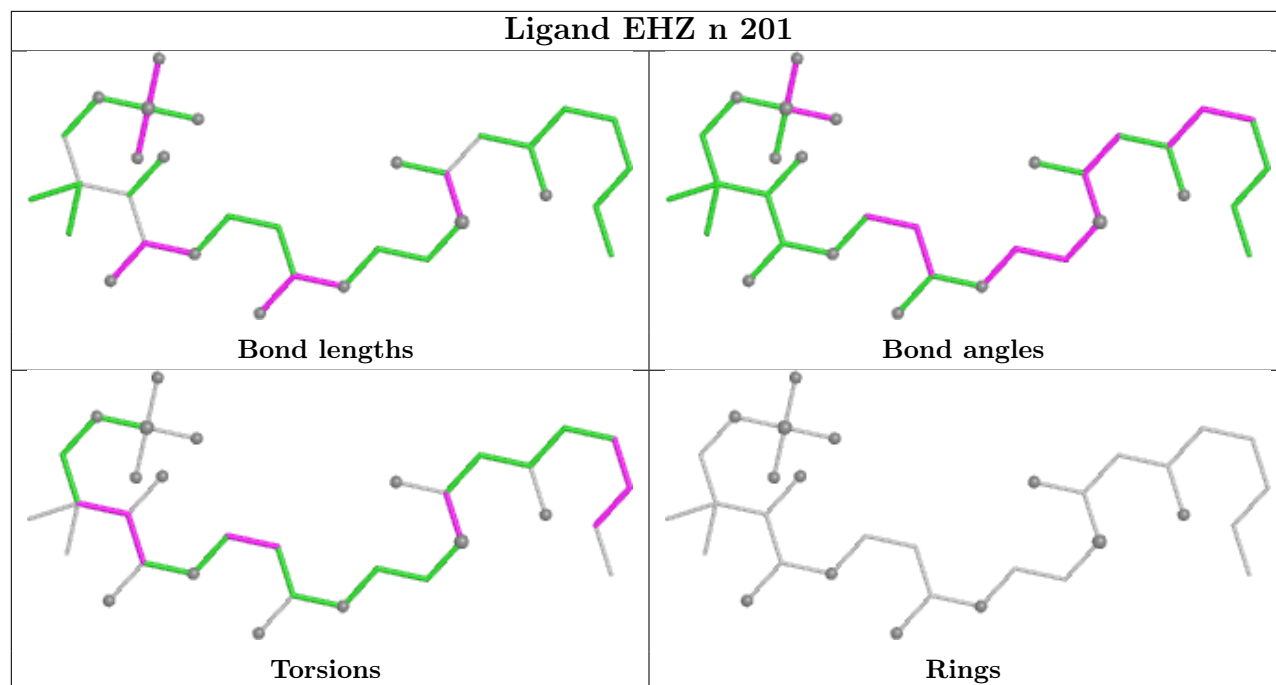


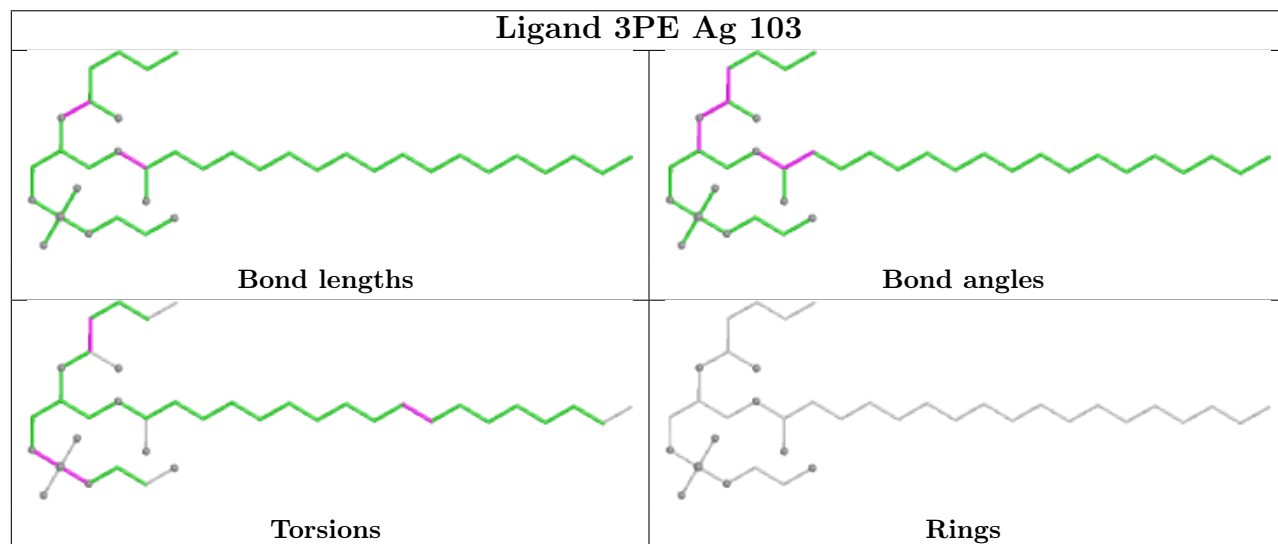
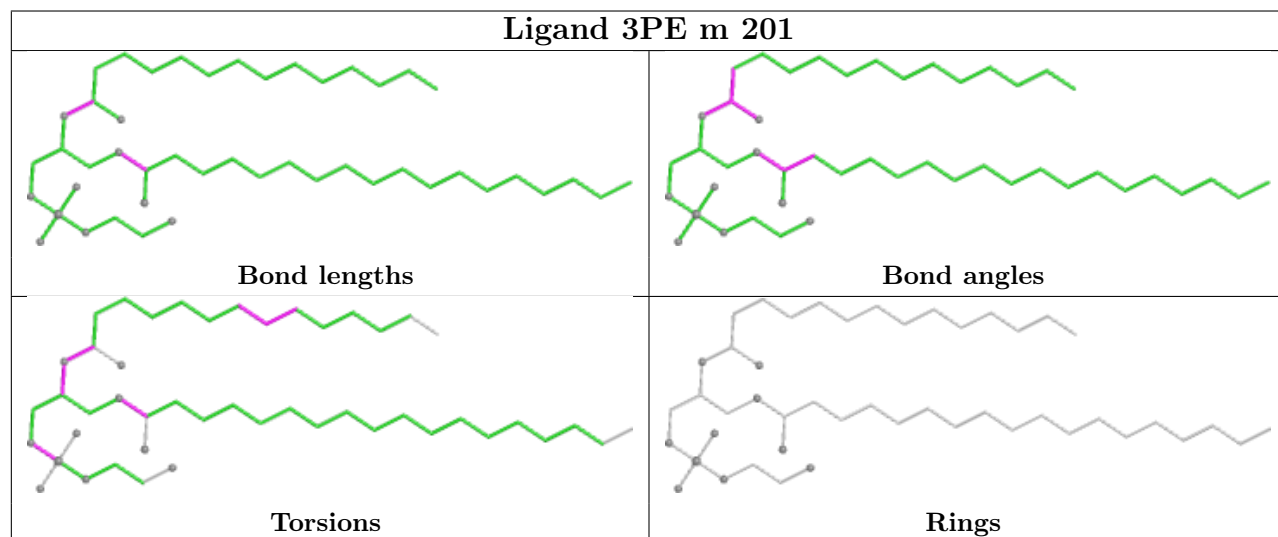
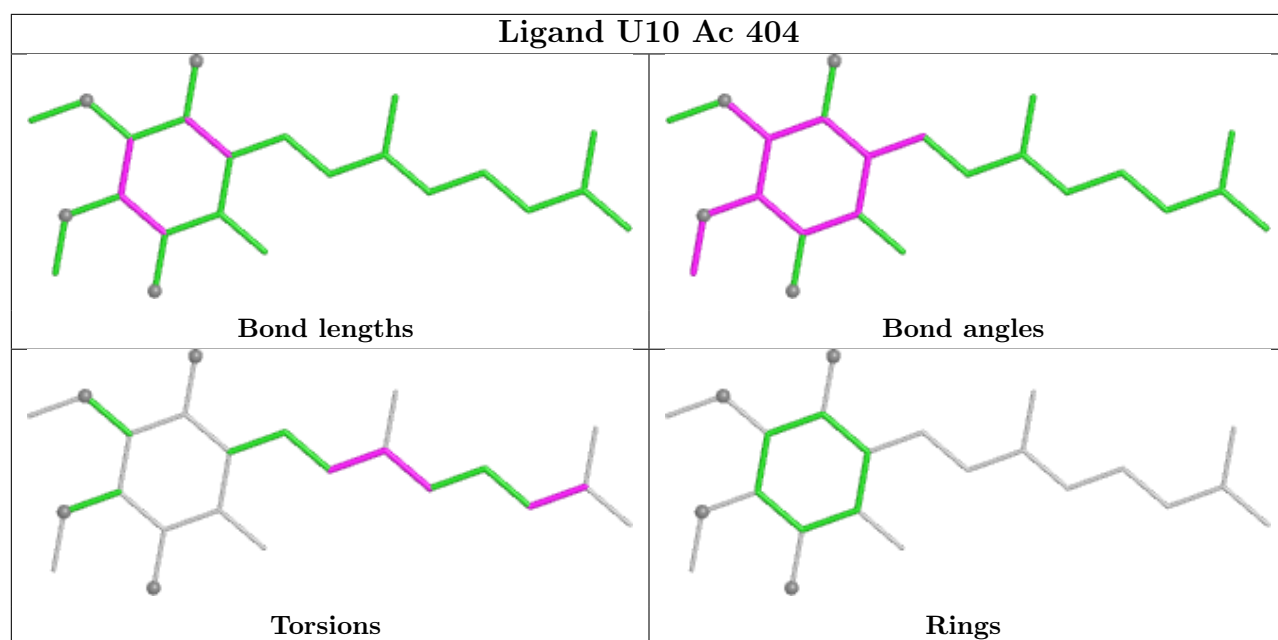
Ligand SF4 I 302

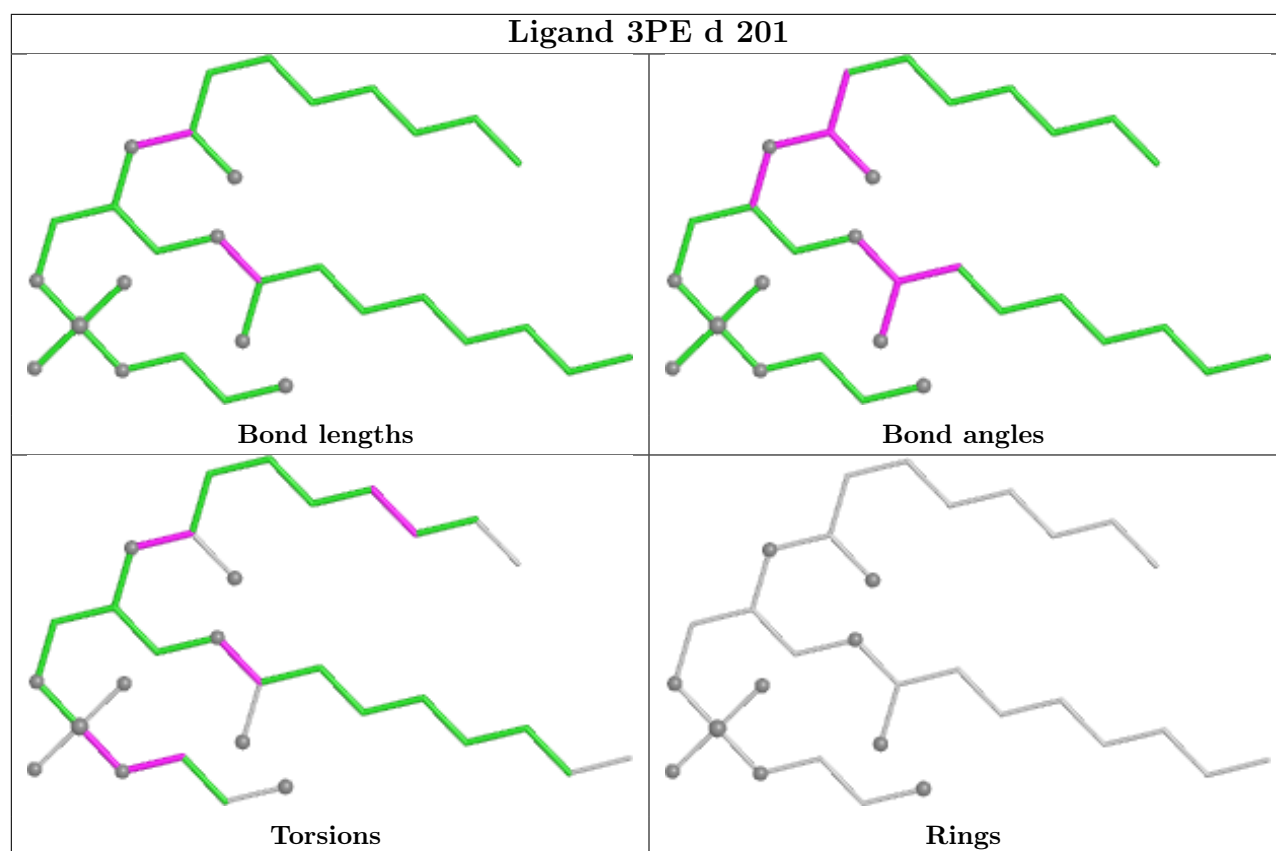


Ligand PC1 B 304









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

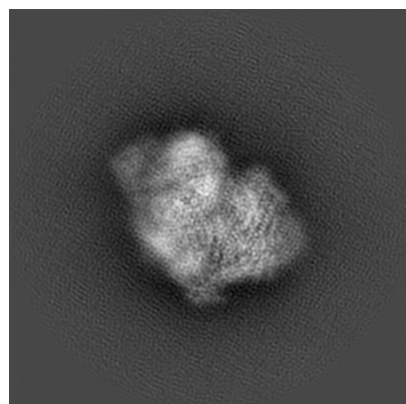
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35340. These allow visual inspection of the internal detail of the map and identification of artifacts.

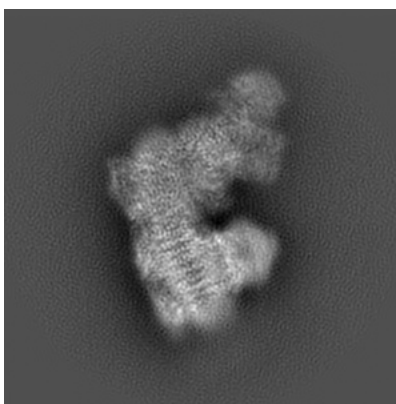
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

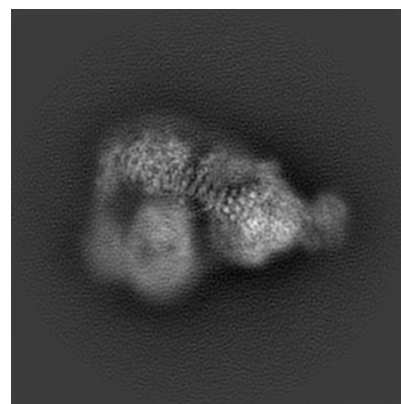
6.1.1 Primary map



X

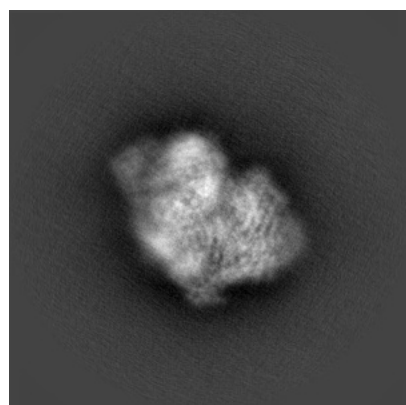


Y

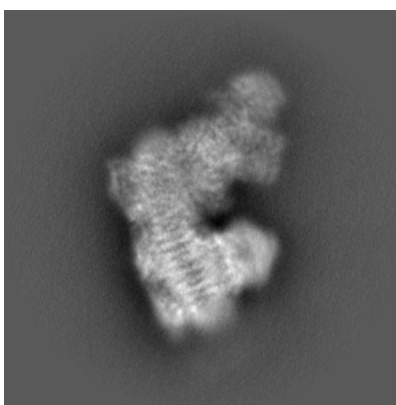


Z

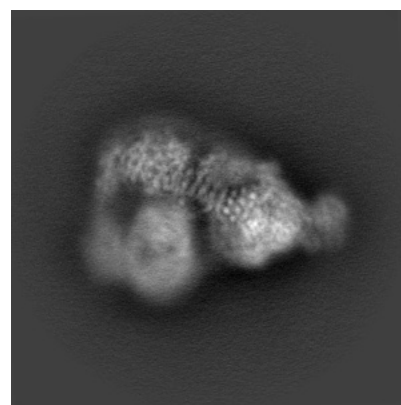
6.1.2 Raw map



X



Y

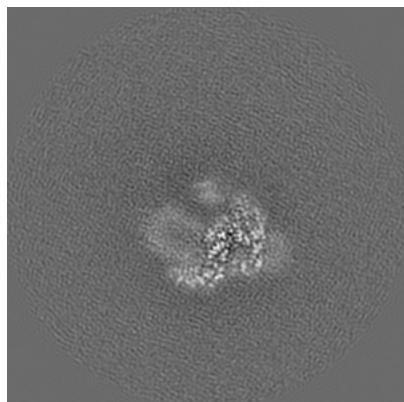


Z

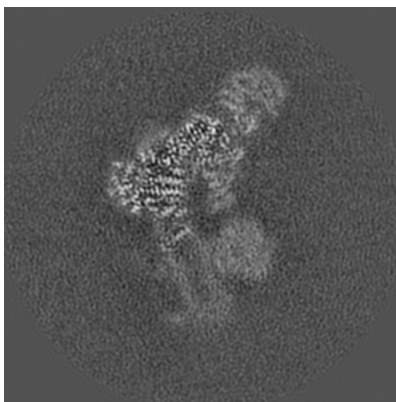
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

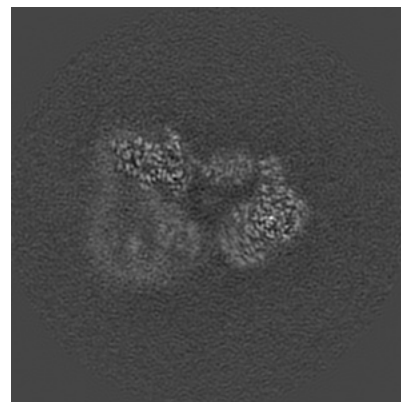
6.2.1 Primary map



X Index: 192

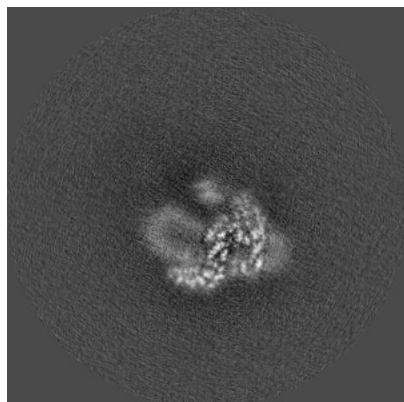


Y Index: 192

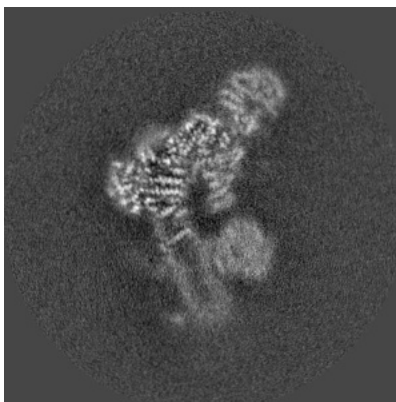


Z Index: 192

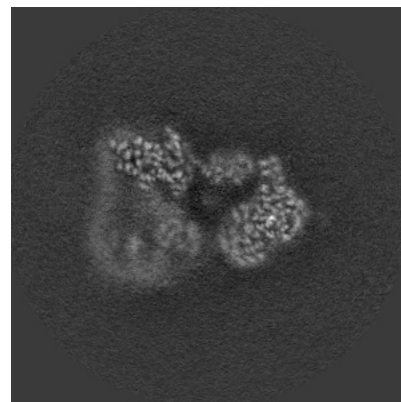
6.2.2 Raw map



X Index: 192



Y Index: 192

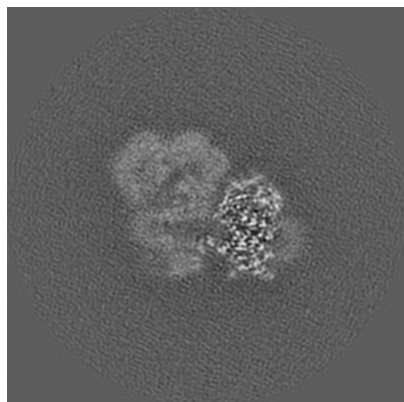


Z Index: 192

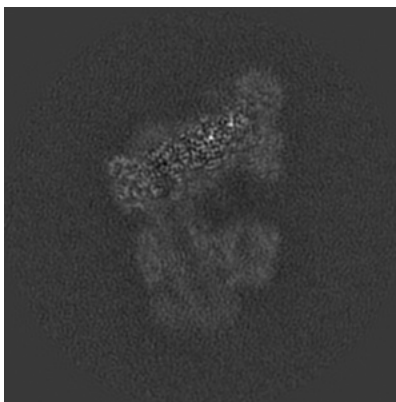
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

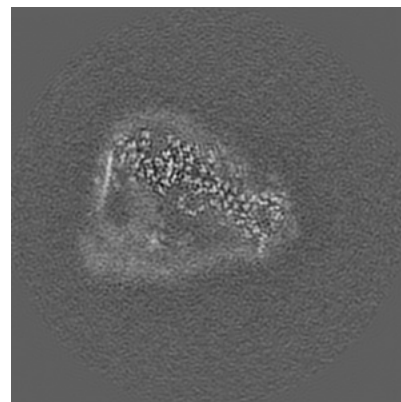
6.3.1 Primary map



X Index: 157

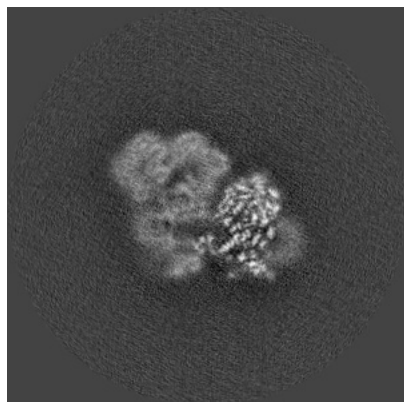


Y Index: 176

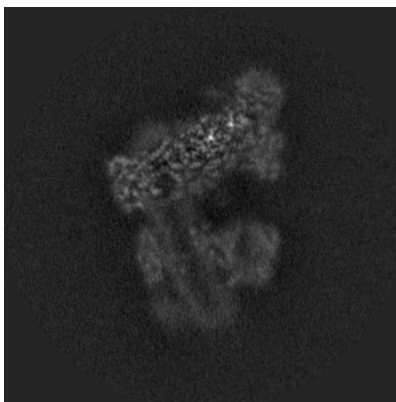


Z Index: 167

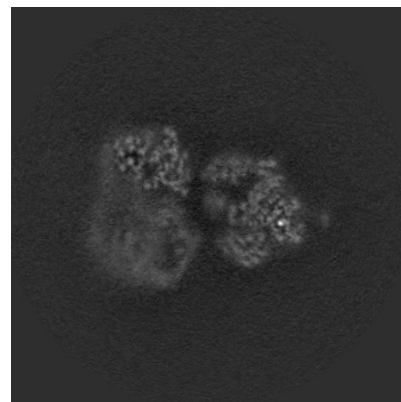
6.3.2 Raw map



X Index: 159



Y Index: 176

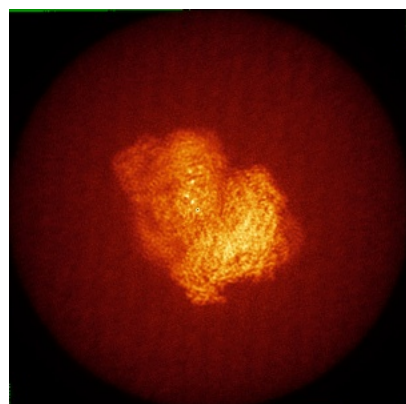


Z Index: 198

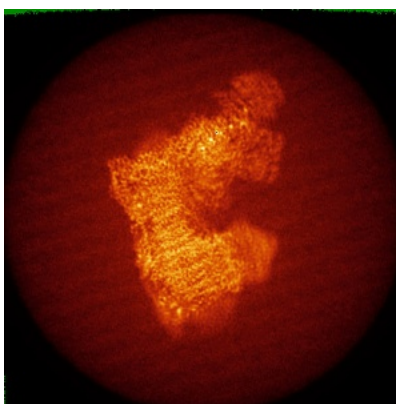
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

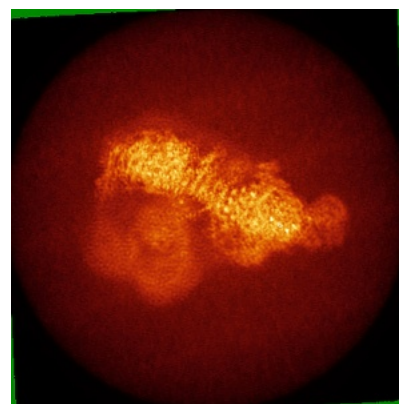
6.4.1 Primary map



X

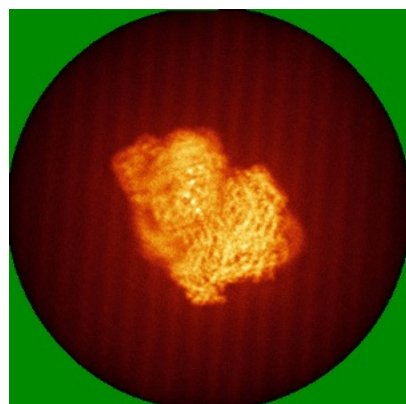


Y

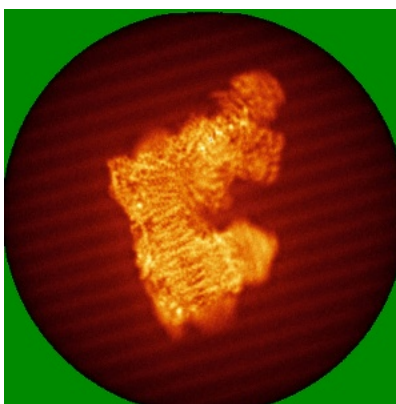


Z

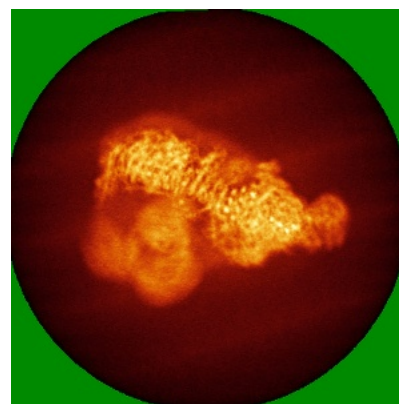
6.4.2 Raw map



X



Y

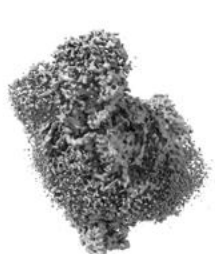


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



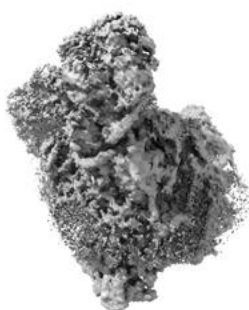
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

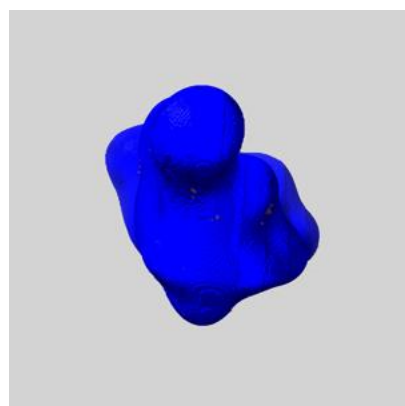
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

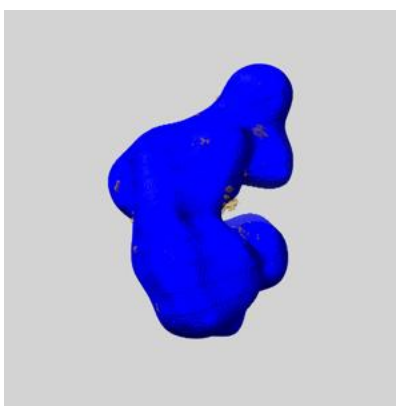
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

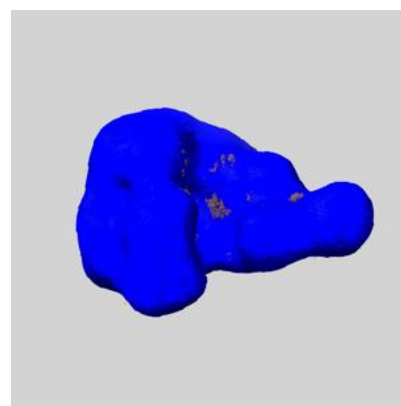
6.6.1 emd_35340_msk_1.map [i](#)



X



Y

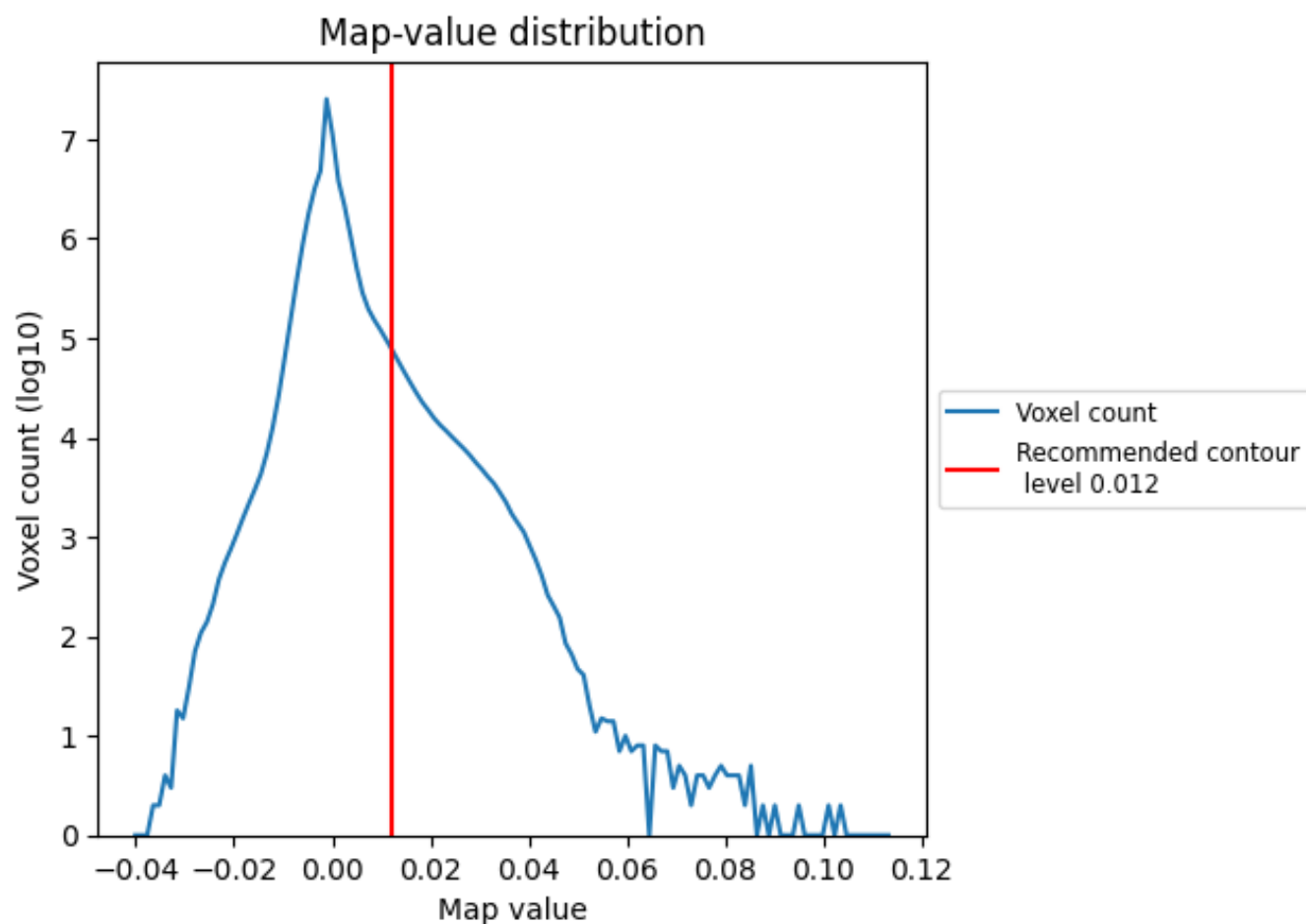


Z

7 Map analysis [i](#)

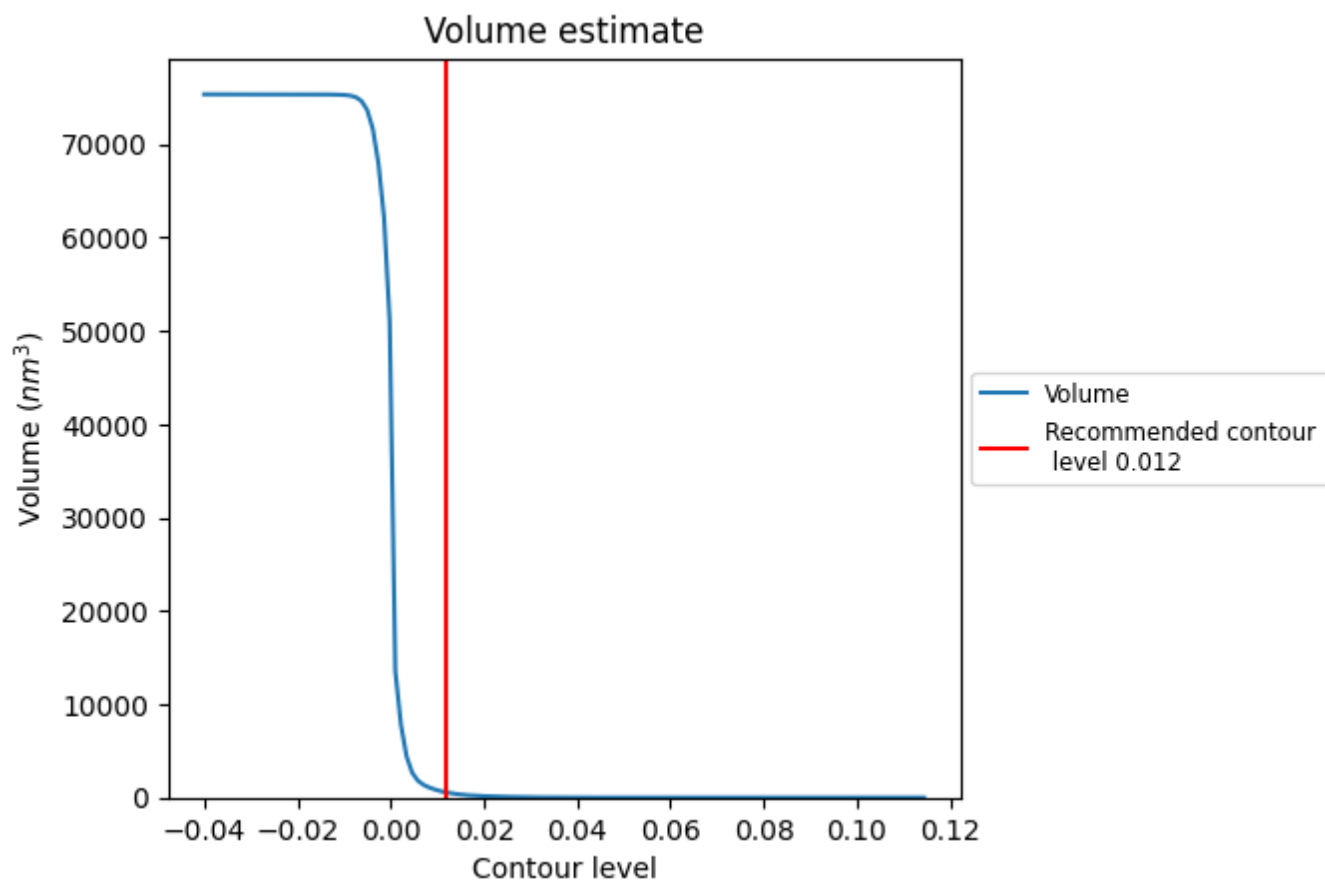
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

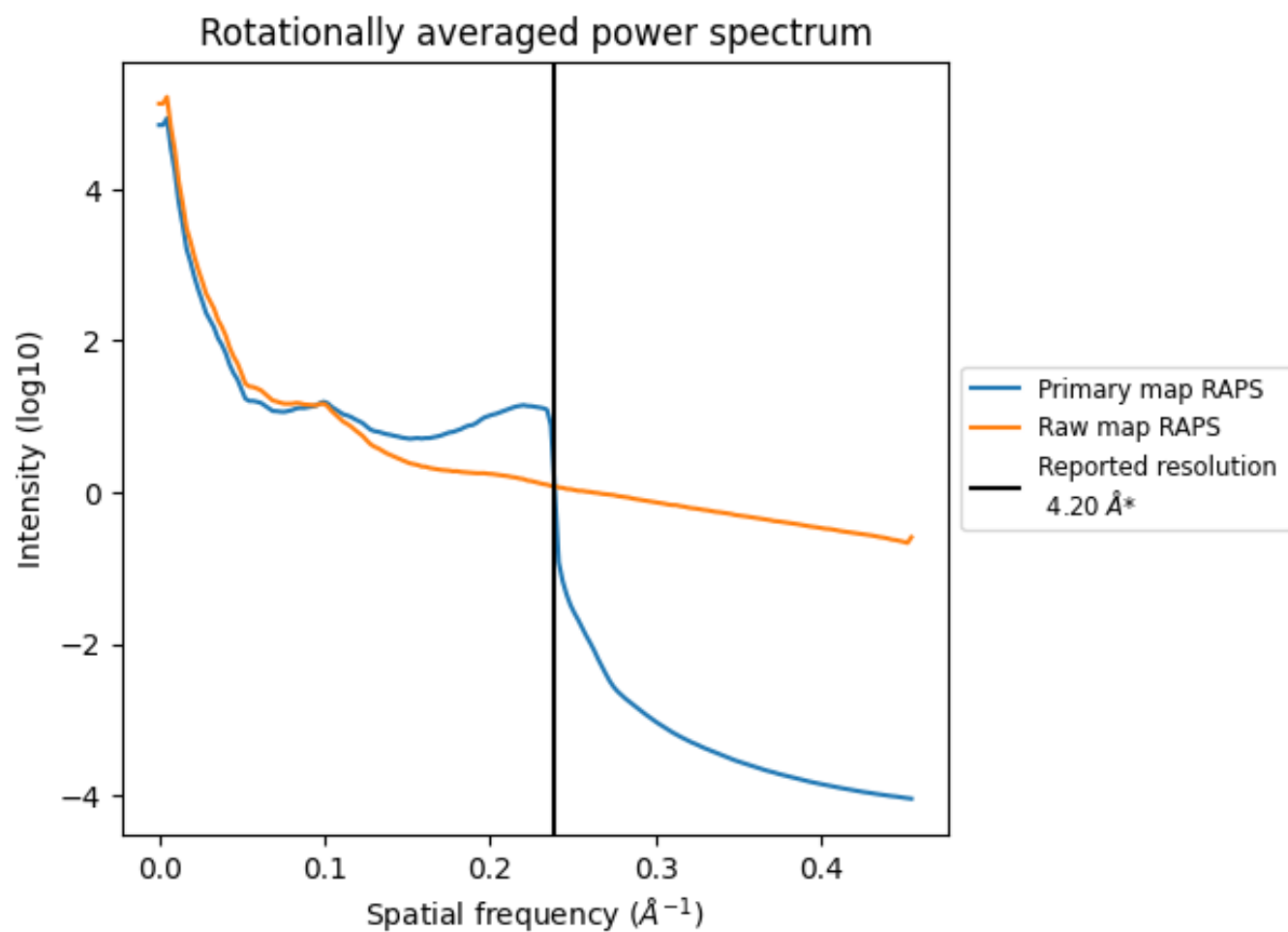
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 542 nm³; this corresponds to an approximate mass of 490 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

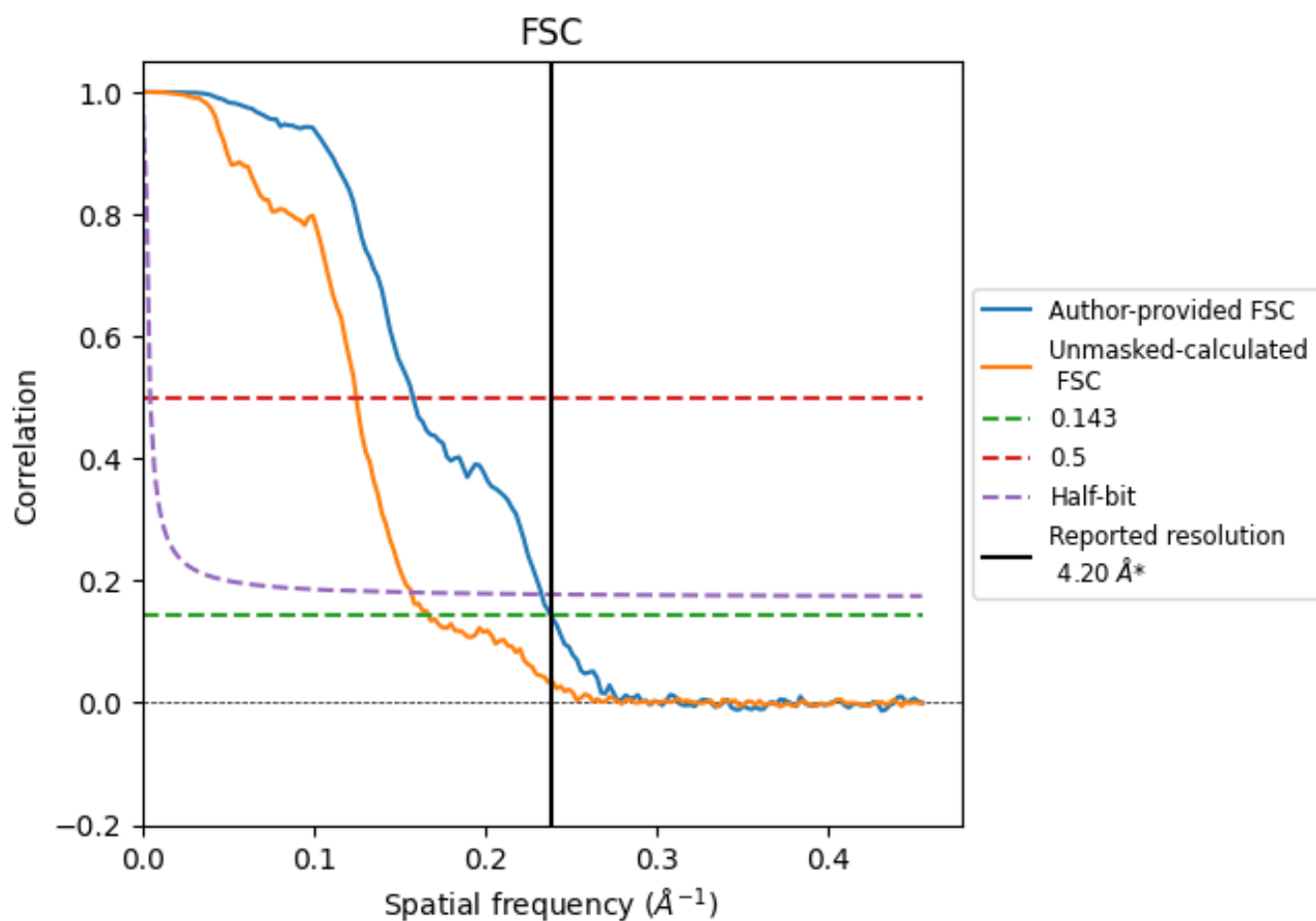


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

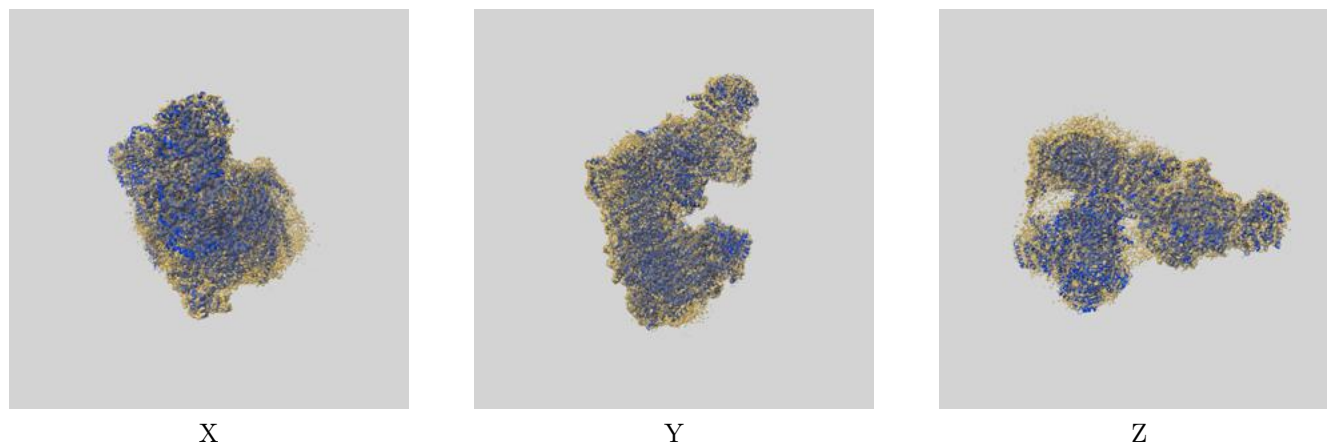
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.34	4.30
Unmasked-calculated*	6.00	8.02	6.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.00 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

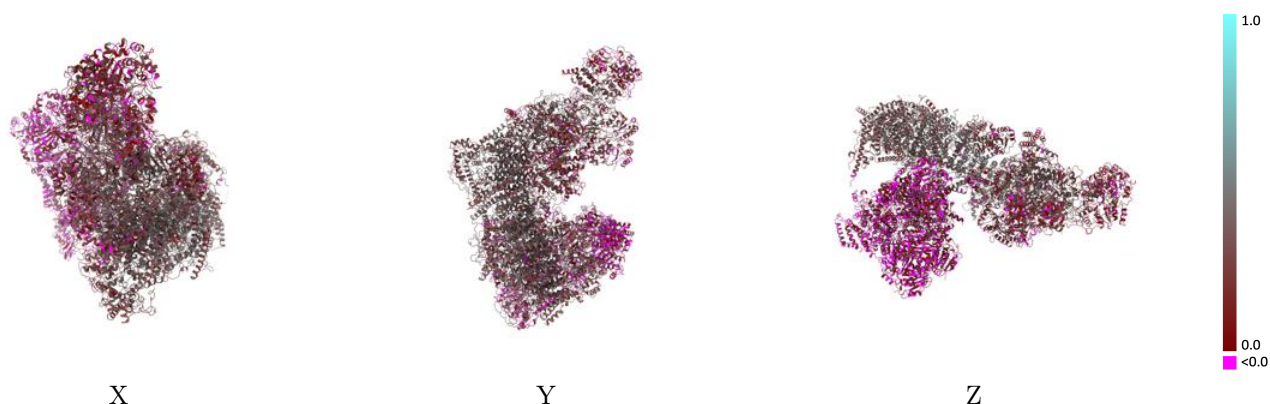
This section contains information regarding the fit between EMDB map EMD-35340 and PDB model 8IBD. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



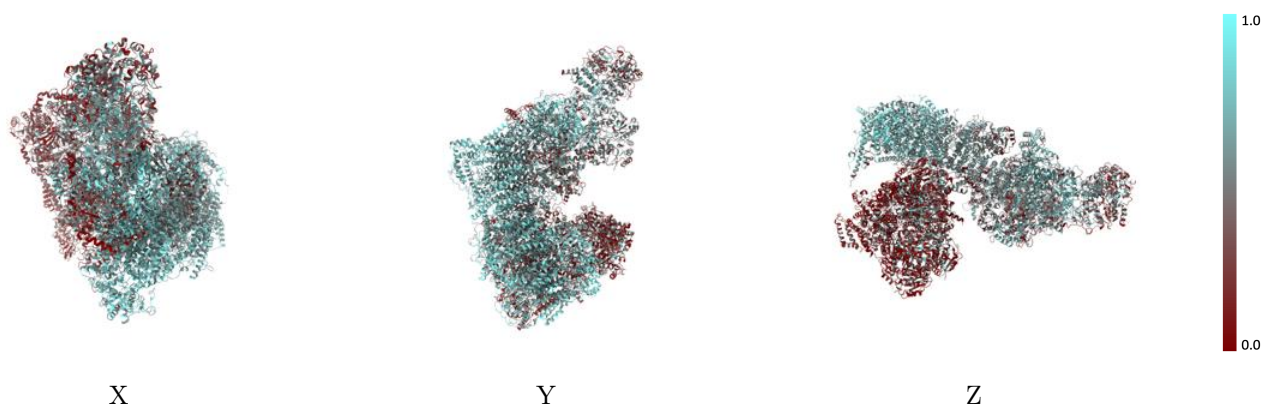
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



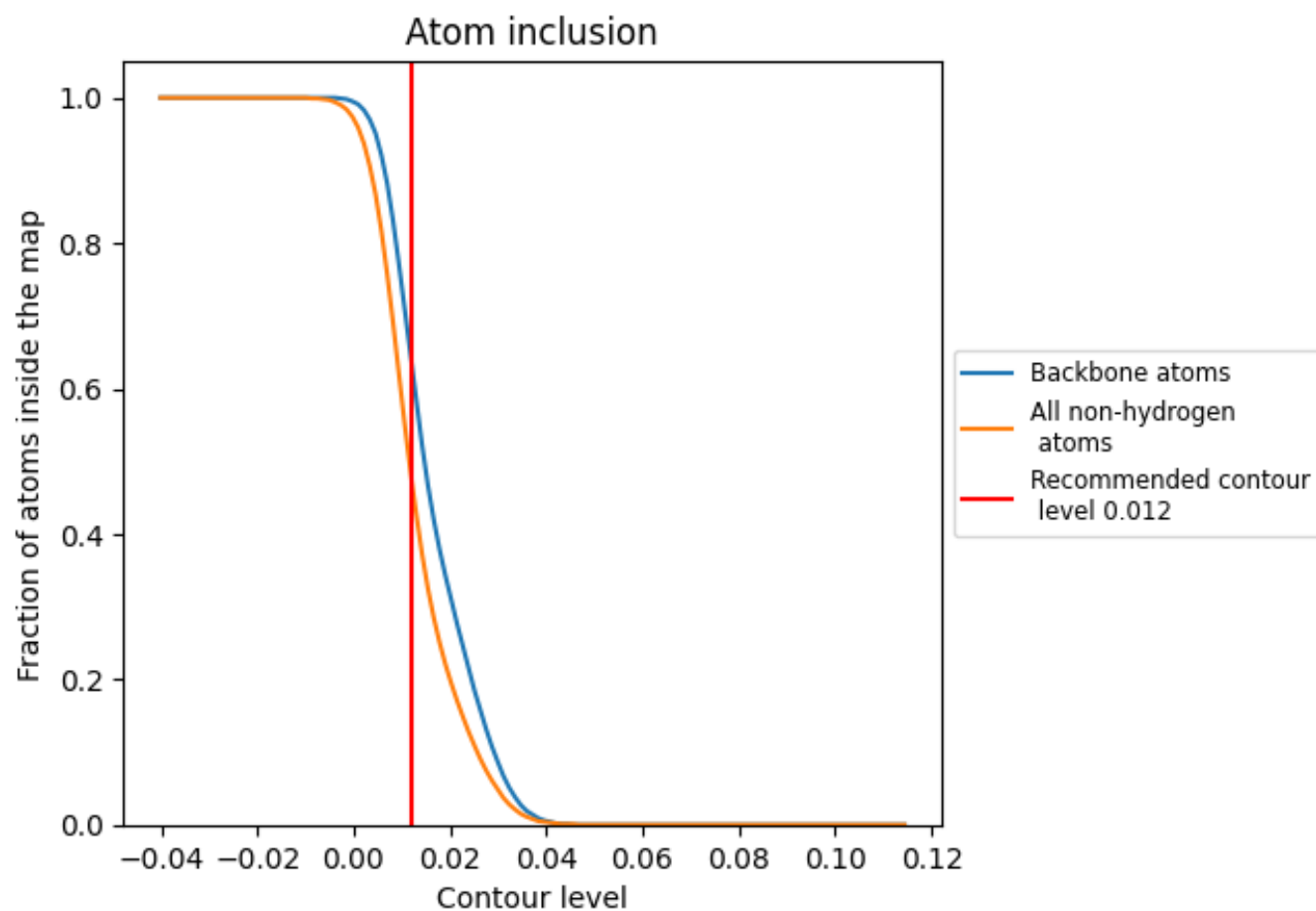
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4760	 0.2320
A	 0.5720	 0.3400
AA	 0.2260	 0.0500
AB	 0.2790	 0.0900
AC	 0.1360	 0.0600
AD	 0.1840	 0.0400
AE	 0.0400	 0.0110
AF	 0.2120	 0.0620
AG	 0.1030	 0.0200
AH	 0.1380	 0.0390
AI	 0.0610	 0.0570
AJ	 0.0870	 -0.0090
AK	 0.0170	 -0.0420
Aa	 0.2460	 0.0880
Ab	 0.2610	 0.0640
Ac	 0.2520	 0.1320
Ad	 0.3300	 0.1260
Ae	 0.0650	 0.0450
Af	 0.2580	 0.1320
Ag	 0.1940	 0.1060
Ah	 0.2590	 0.0910
Ai	 0.0400	 0.0720
Aj	 0.1070	 0.1090
Ak	 0.0240	 0.0290
B	 0.6760	 0.3570
C	 0.6330	 0.2840
D	 0.6690	 0.3480
E	 0.3820	 0.1930
F	 0.4370	 0.1890
G	 0.5440	 0.2330
H	 0.6730	 0.3720
I	 0.7440	 0.3600
J	 0.5640	 0.3220
K	 0.6160	 0.3800
L	 0.6650	 0.3660



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
M	 0.7000	 0.3940
N	 0.6830	 0.3940
O	 0.4740	 0.2590
P	 0.4870	 0.2060
Q	 0.4780	 0.2770
R	 0.2910	 0.1840
S	 0.4200	 0.1130
T	 0.2970	 0.1400
U	 0.7030	 0.3250
V	 0.5450	 0.2120
W	 0.4600	 0.1940
X	 0.7290	 0.3370
Y	 0.5570	 0.3280
Z	 0.7300	 0.3220
a	 0.6740	 0.3380
b	 0.7270	 0.3520
c	 0.6160	 0.2950
d	 0.6980	 0.3570
e	 0.7060	 0.3520
f	 0.6930	 0.3500
g	 0.6790	 0.3590
h	 0.7020	 0.3620
i	 0.6860	 0.3330
j	 0.7040	 0.3200
k	 0.7240	 0.3210
l	 0.7000	 0.3590
m	 0.6240	 0.3380
n	 0.7220	 0.3400
o	 0.6530	 0.2710
p	 0.7140	 0.3460
q	 0.1400	 0.1820
r	 0.1940	 0.1580
s	 0.1220	 0.1140