



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:01 AM UTC

PDB ID : 8IC2 / pdb_00008ic2
EMDB ID : EMD-35352
Title : Respiratory complex CI:CIII2, type I, PERK -/- mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 6.30 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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 EMD 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) : 2.49

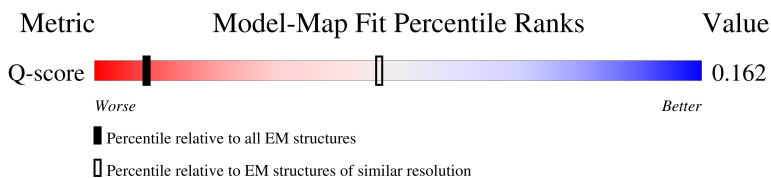
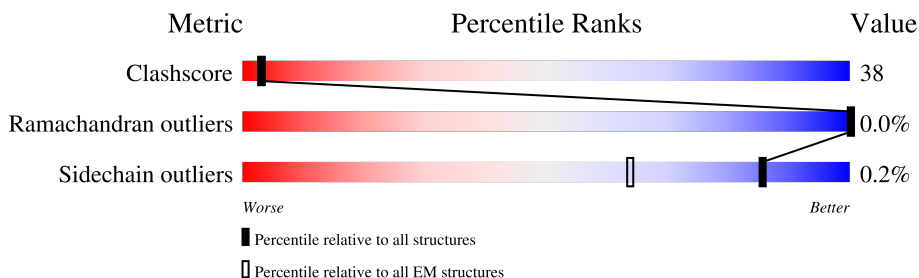
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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.



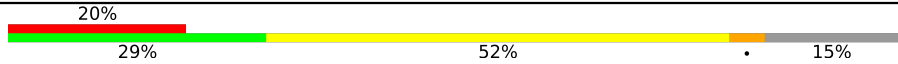
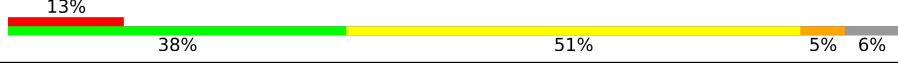
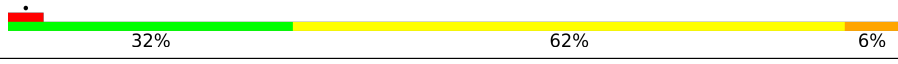
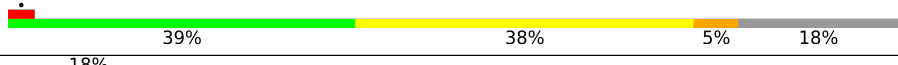
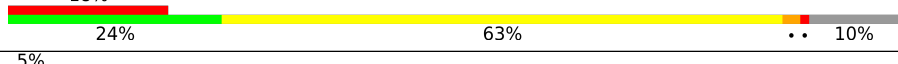
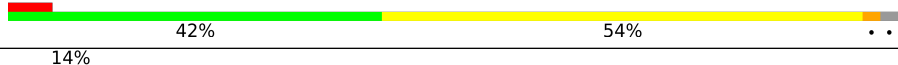
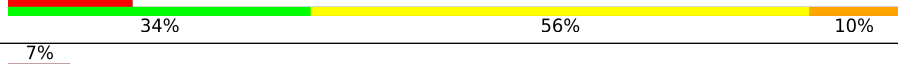
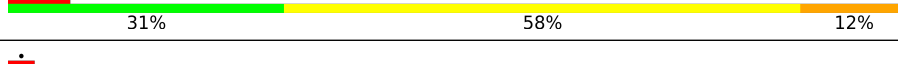
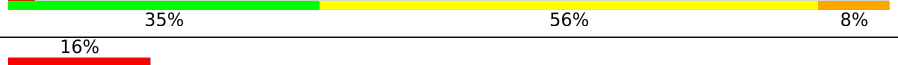
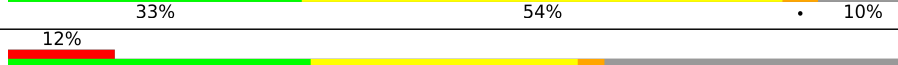
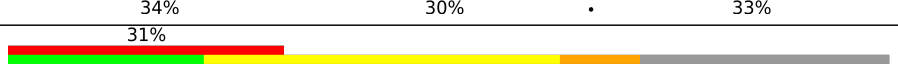
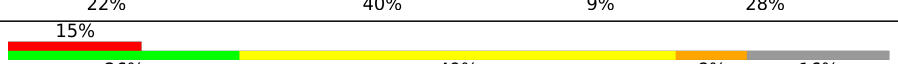
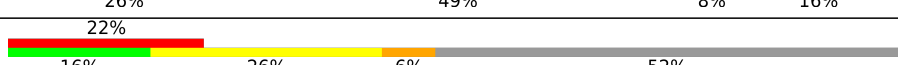
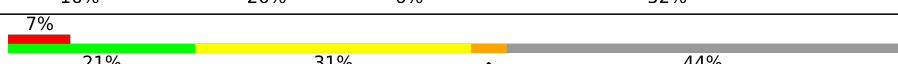
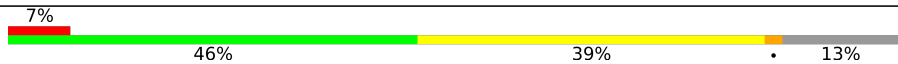
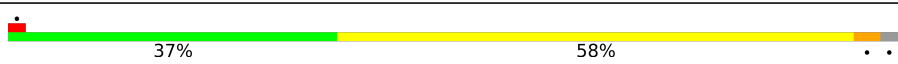
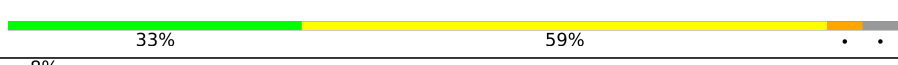
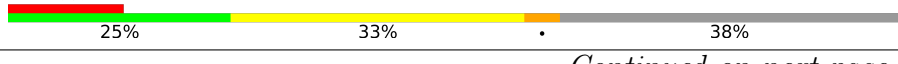
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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	

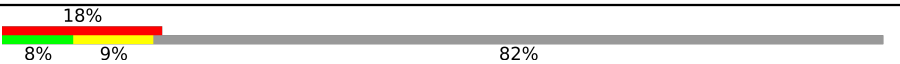
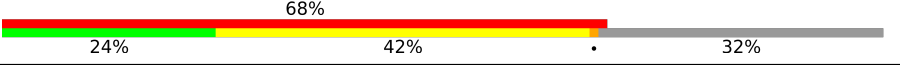
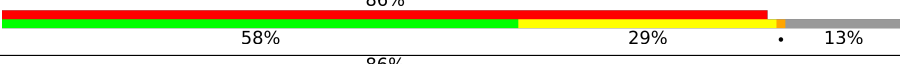
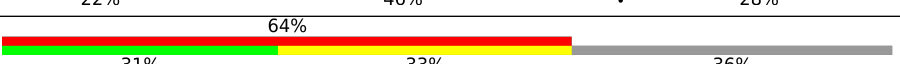
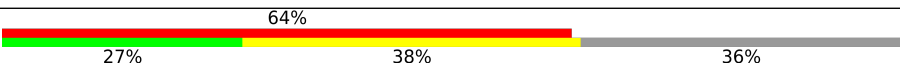
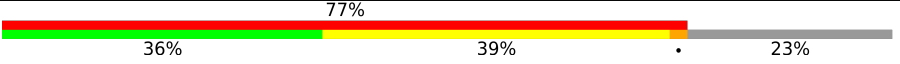
Continued on next page...

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	
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
55	SF4	B	301	-	-	X	-
55	SF4	F	502	-	-	X	-
55	SF4	G	802	-	-	X	-
55	SF4	I	303	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
61	UQ9	H	401	-	-	X	-
62	CDL	q	201	-	-	X	-
67	HEM	AC	402	-	-	X	-
68	UQ6	AC	403	-	-	X	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 97017 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	91	Total	C	N	O	S	0	0
			737	511	102	118	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	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
			1641	1060	279	299	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
			3443	2201	592	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	424	Total	C	N	O	S	0	0
			3273	2062	586	603	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
			2531	1701	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	173	Total	C	N	O	S	0	0
			1389	875	239	263	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- 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	318	Total	C	N	O	S	0	0
			2588	1662	426	490	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	118	Total	C	N	O	S	0	0
			957	608	165	180	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	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 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 sub-unit 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 sub-unit 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 sub-unit 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 sub-unit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 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	79	Total	C	N	O	S	0	0
			620	408	98	110	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	103	Total	C	N	O	S	0	0
			859	544	157	150	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	99	Total	C	N	O	S	0	0
			835	541	134	156	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	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	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	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	122	Total	C	N	O	S	0	0
			1020	655	180	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	29	Total	C	N	O	0	0
			238	151	39	48		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	403	Total	C	N	O	S	0	0
			3157	1971	562	608	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	400	Total	C	N	O	S	0	0
			3131	1957	554	604	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	413	Total	C	N	O	S	0	0
			3097	1949	542	597	9		
46	Ab	417	Total	C	N	O	S	0	0
			3128	1965	550	604	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	369	Total	C	N	O	S	0	0
			2956	1995	457	484	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
48	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	181	Total	C	N	O	S	0	0
			1397	885	243	263	6		
49	AI	48	Total	C	N	O		0	0
			328	210	61	57			
49	Ae	186	Total	C	N	O	S	0	0
			1436	907	251	271	7		

- 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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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	75	Total	C	N	O	S	0	0
			634	413	115	105	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	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	64	Total	C	N	O	S	0	0
			527	321	98	103	5		

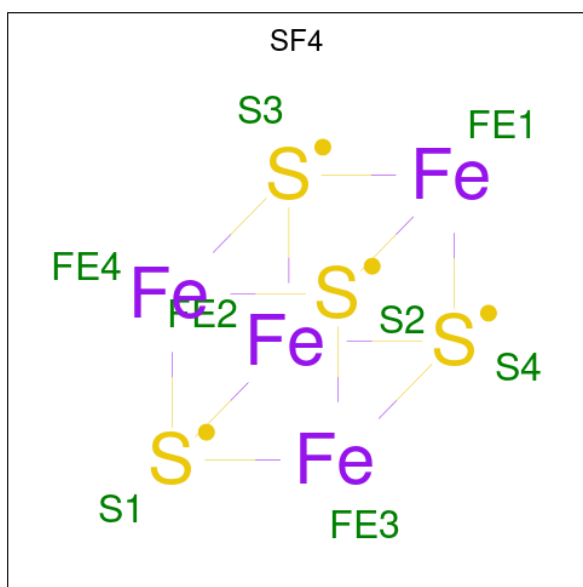
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AJ	41	Total	C	N	O		0	0
			332	216	57	59			
53	Aj	41	Total	C	N	O		0	0
			332	216	57	59			

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

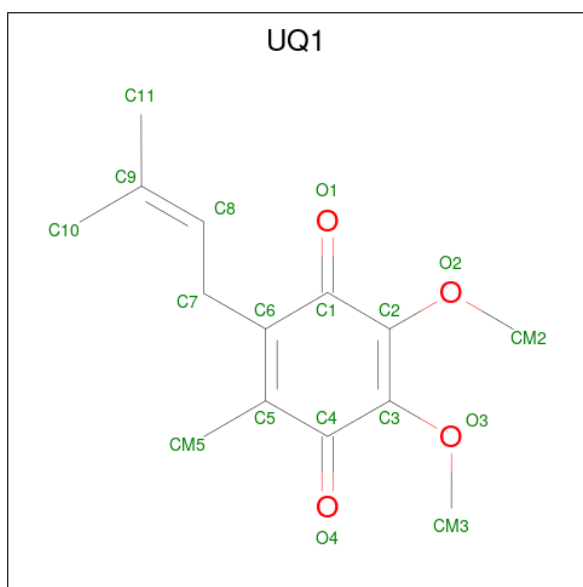
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	43	Total	C	N	O	S	0	0
			355	235	64	55	1		
54	Ak	45	Total	C	N	O	S	0	0
			365	242	64	58	1		

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



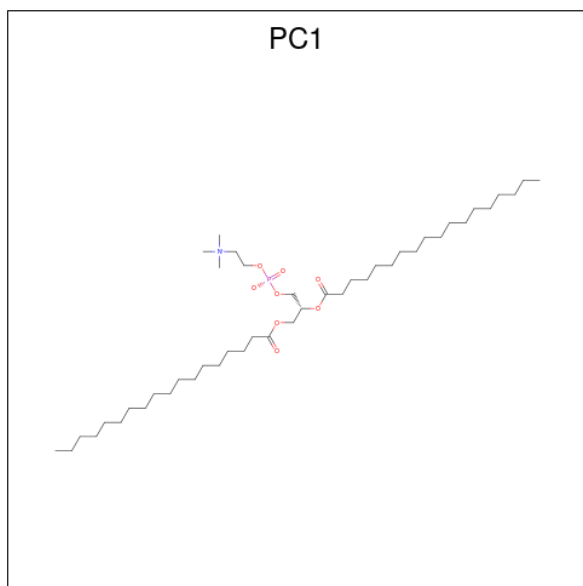
Mol	Chain	Residues	Atoms			AltConf
55	B	1	Total	Fe	S	0
			8	4	4	
55	F	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 56 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



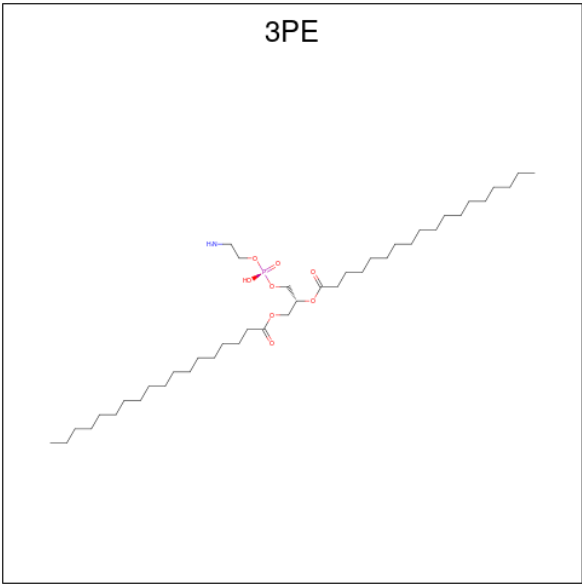
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	C	O	0
			18	14	4	

- Molecule 57 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
57	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
57	I	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



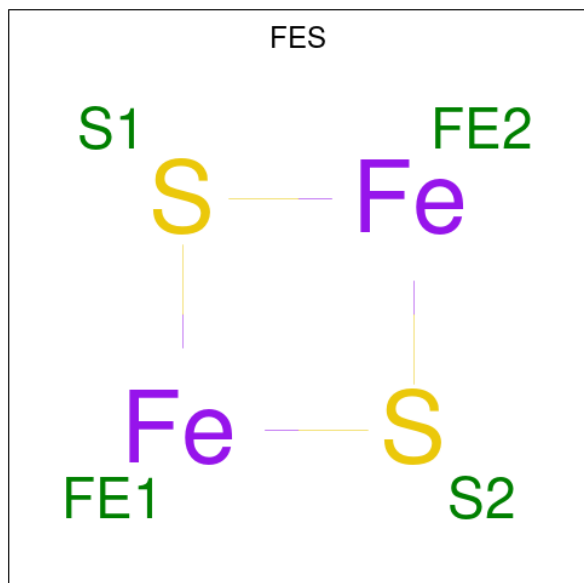
Mol	Chain	Residues	Atoms					AltConf
58	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
58	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
58	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
58	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
58	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
58	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	

Continued on next page...

Continued from previous page...

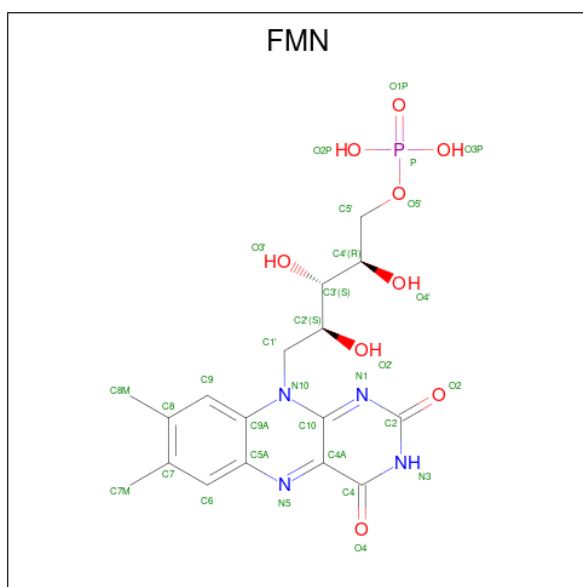
Mol	Chain	Residues	Atoms					AltConf
58	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



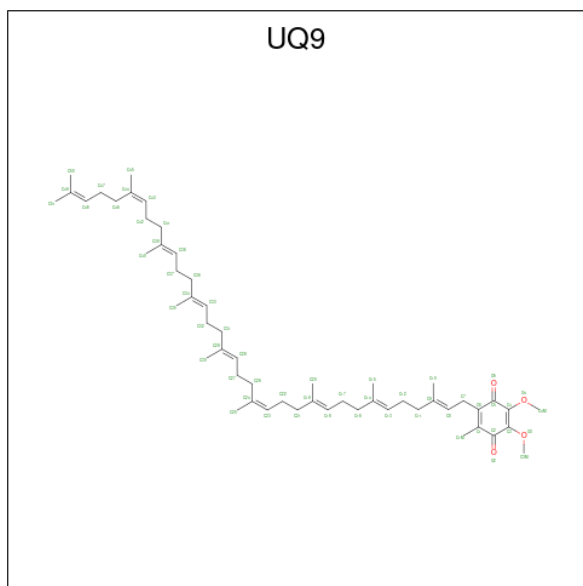
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



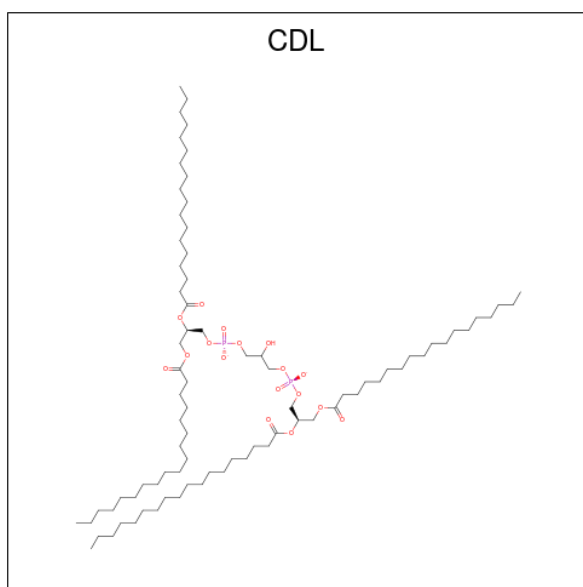
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).

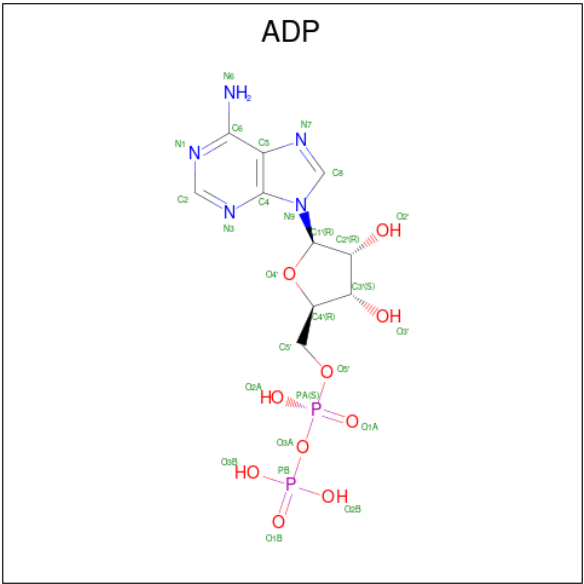


Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			73	54	17	2	
62	M	1	Total	C	O	P	0
			82	63	17	2	
62	Y	1	Total	C	O	P	0
			71	52	17	2	
62	d	1	Total	C	O	P	0
			65	46	17	2	
62	h	1	Total	C	O	P	0
			68	49	17	2	
62	q	1	Total	C	O	P	0
			57	38	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ag	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

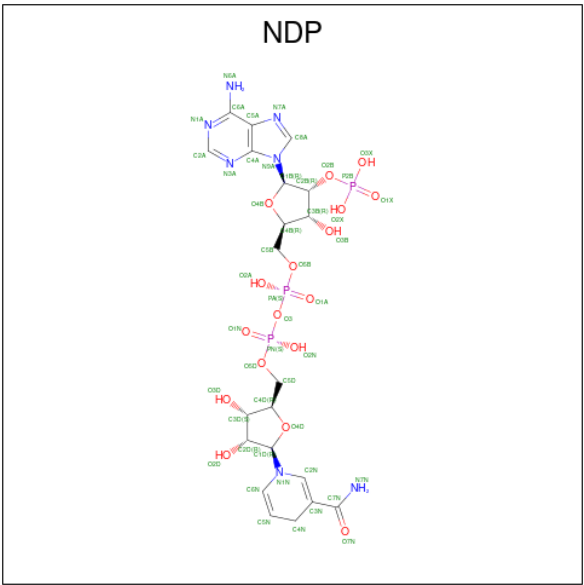
Mol	Chain	Residues	Atoms		AltConf
63	L	1	Total	Zn	0
			1	1	
63	R	1	Total	Zn	0
			1	1	

- Molecule 64 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



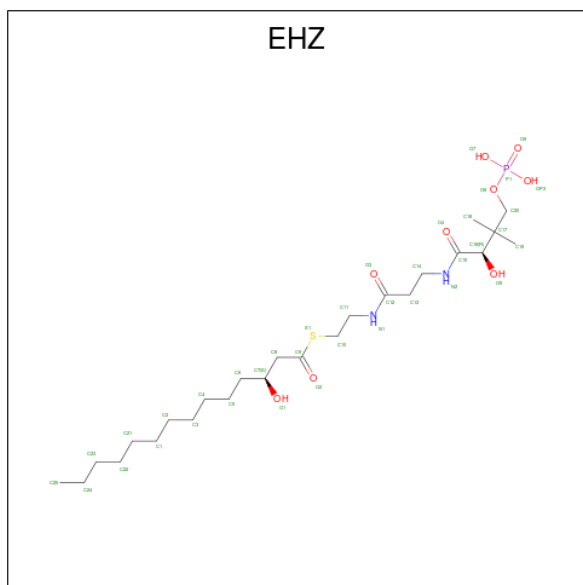
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	O	1	27	10	5	10	2	0

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



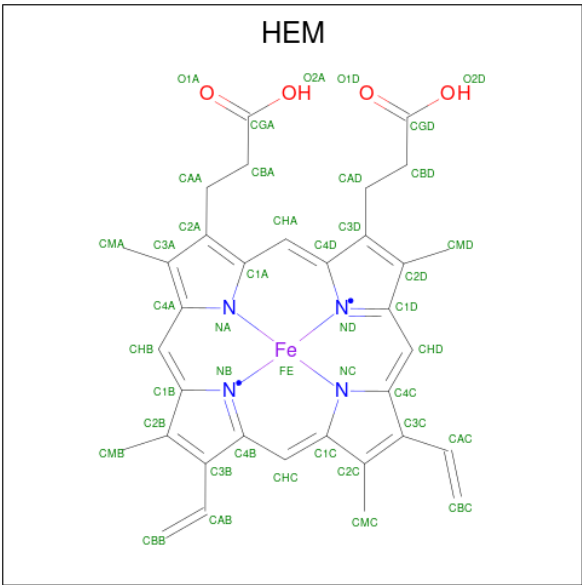
Mol	Chain	Residues	Atoms					AltConf
65	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- 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).



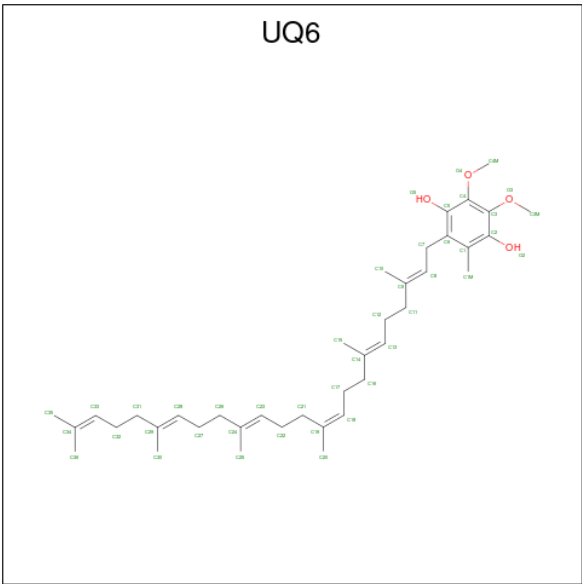
Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



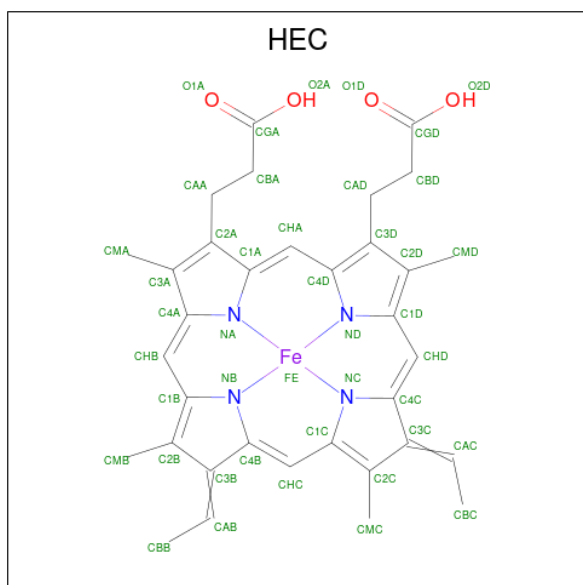
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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: C₃₉H₆₀O₄) (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
			23	19	4	

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



Mol	Chain	Residues	Atoms					AltConf
69	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

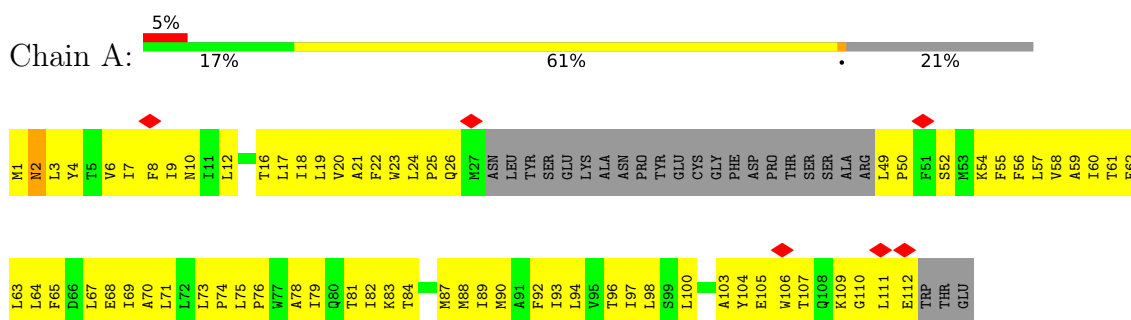
- Molecule 70 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



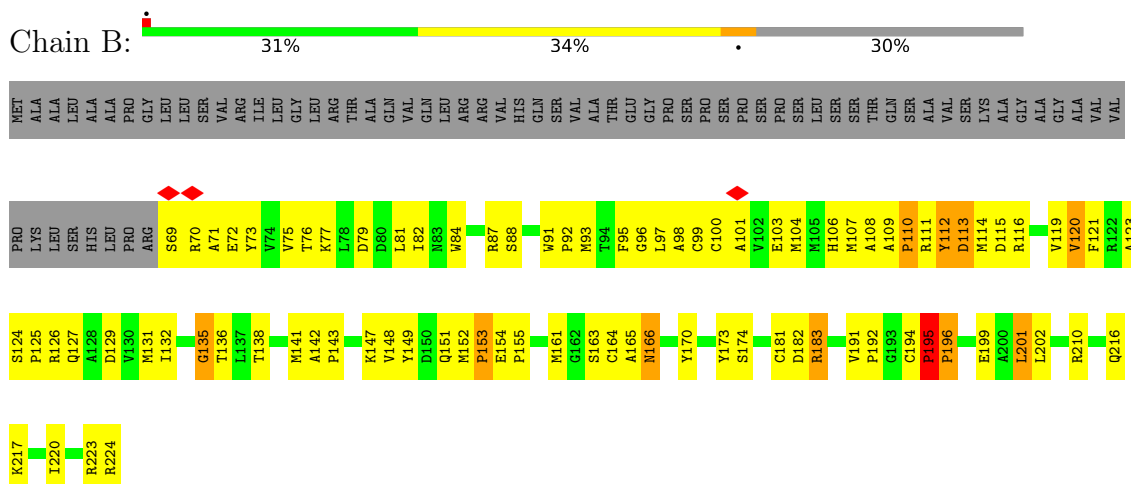
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

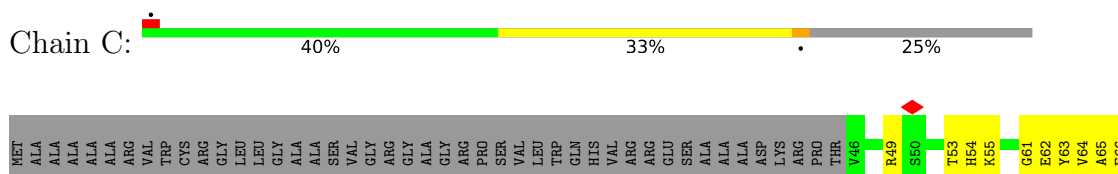
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

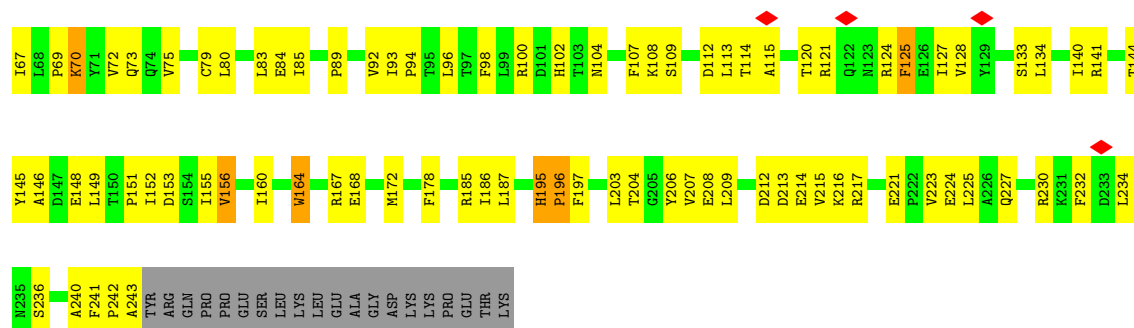


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

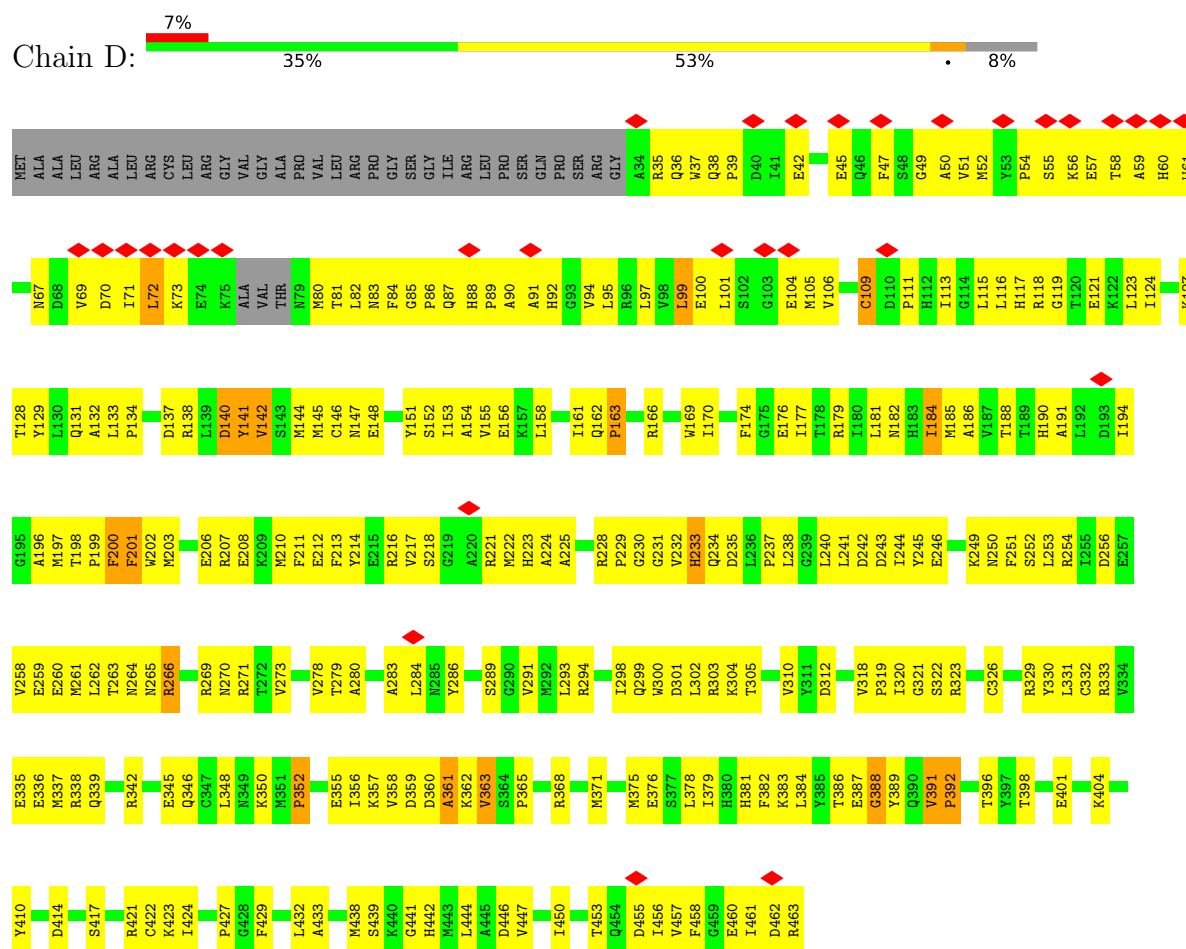


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

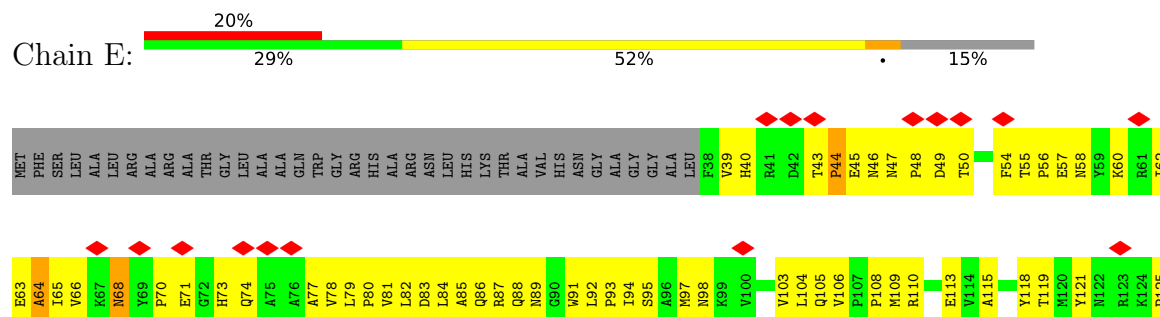


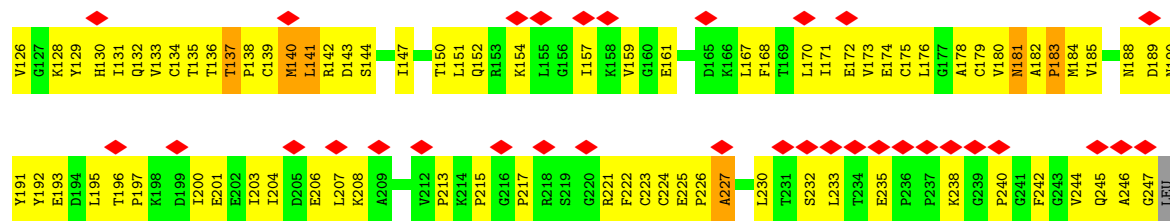


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

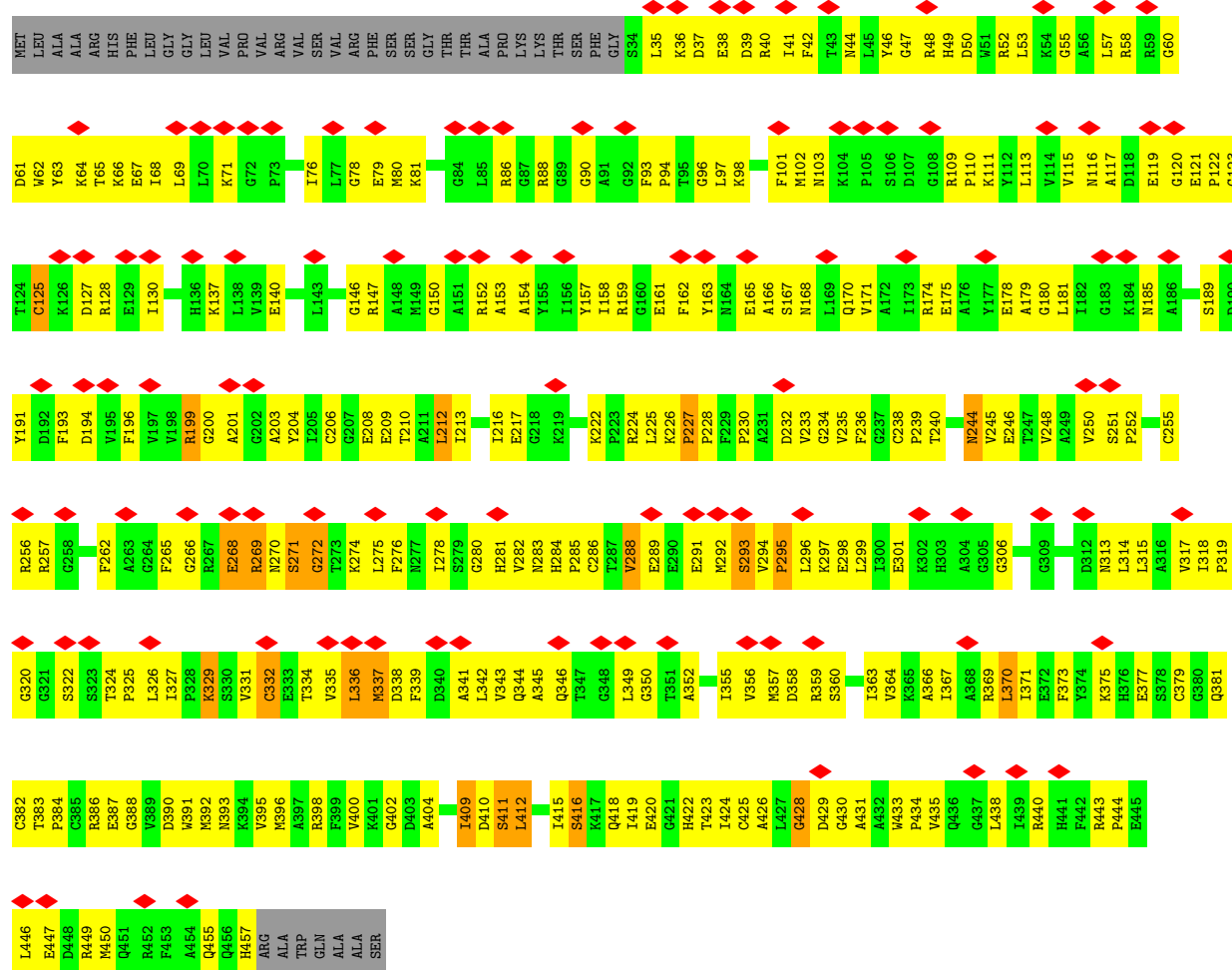


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

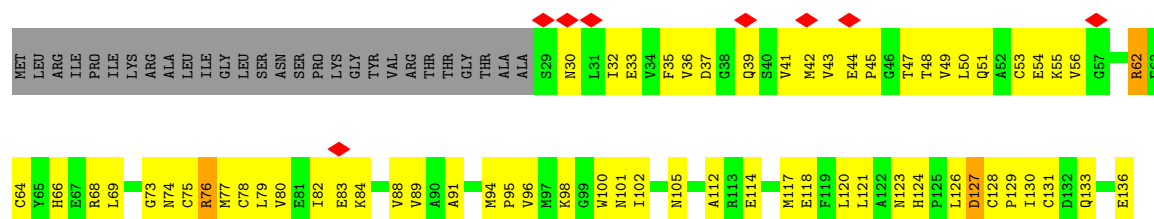


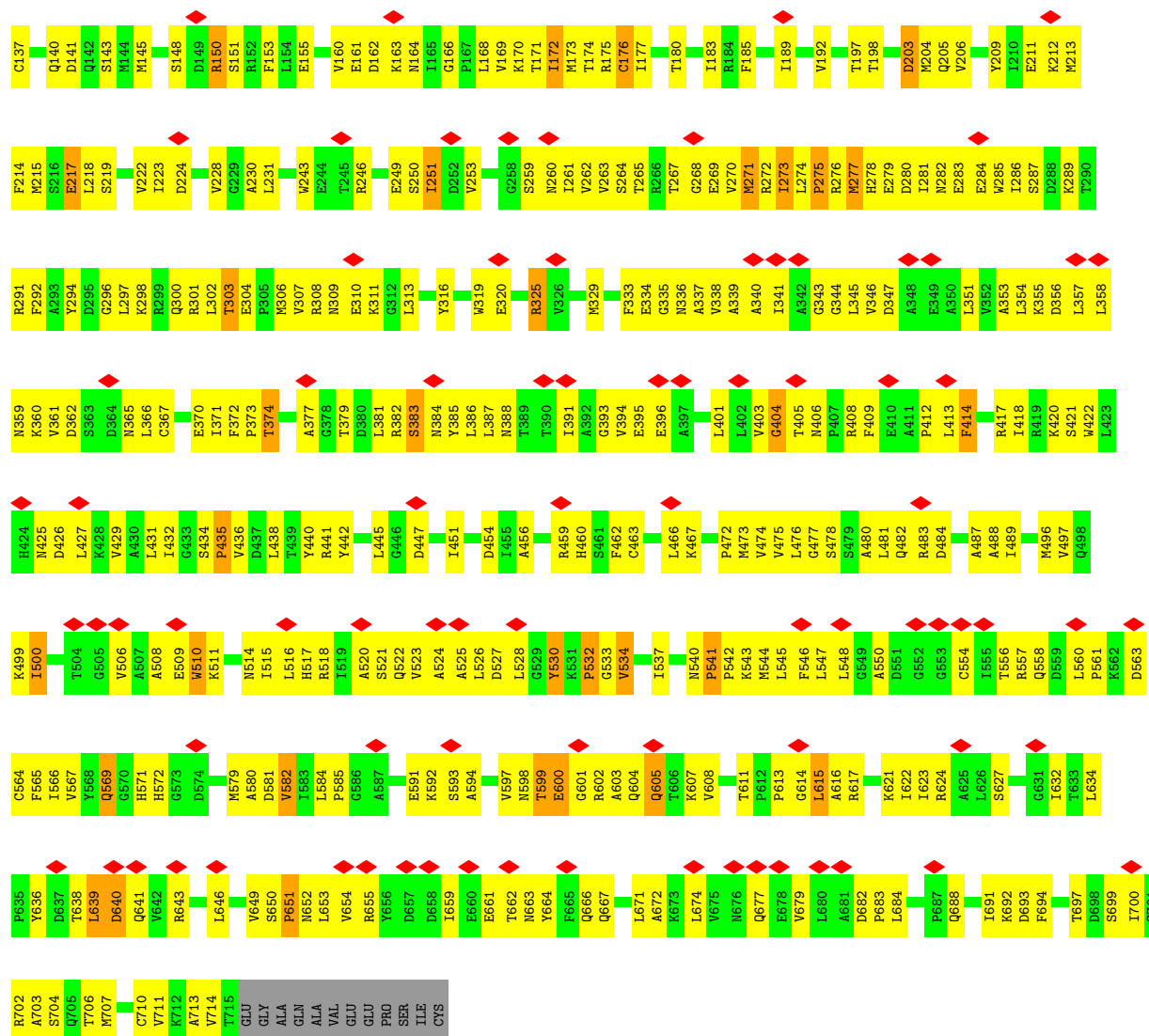


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



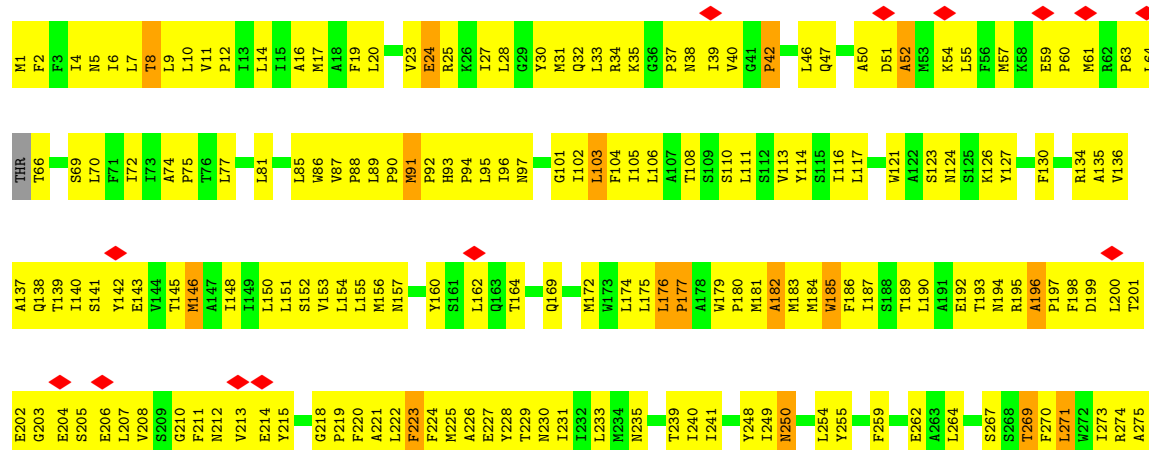
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

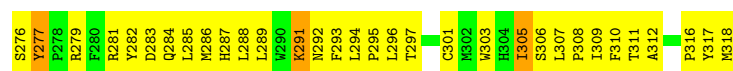




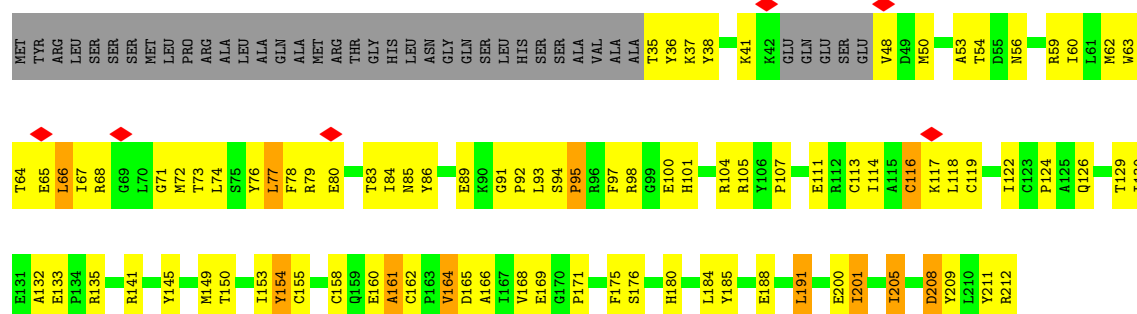
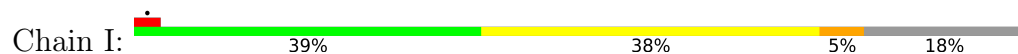
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 32% 62% 6%

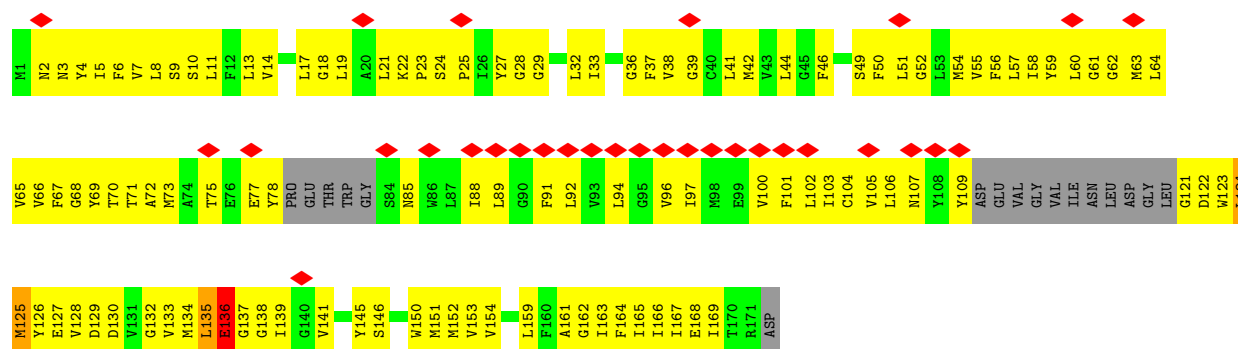




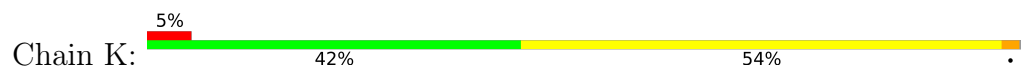
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



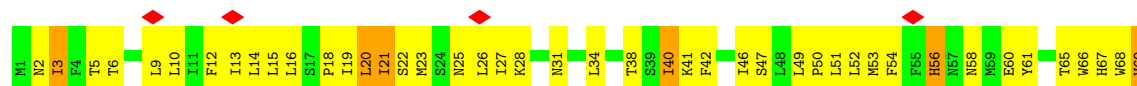
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

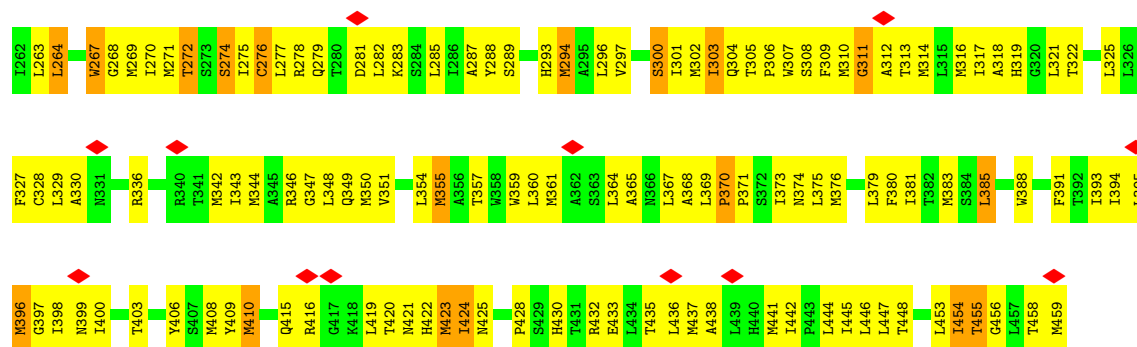


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

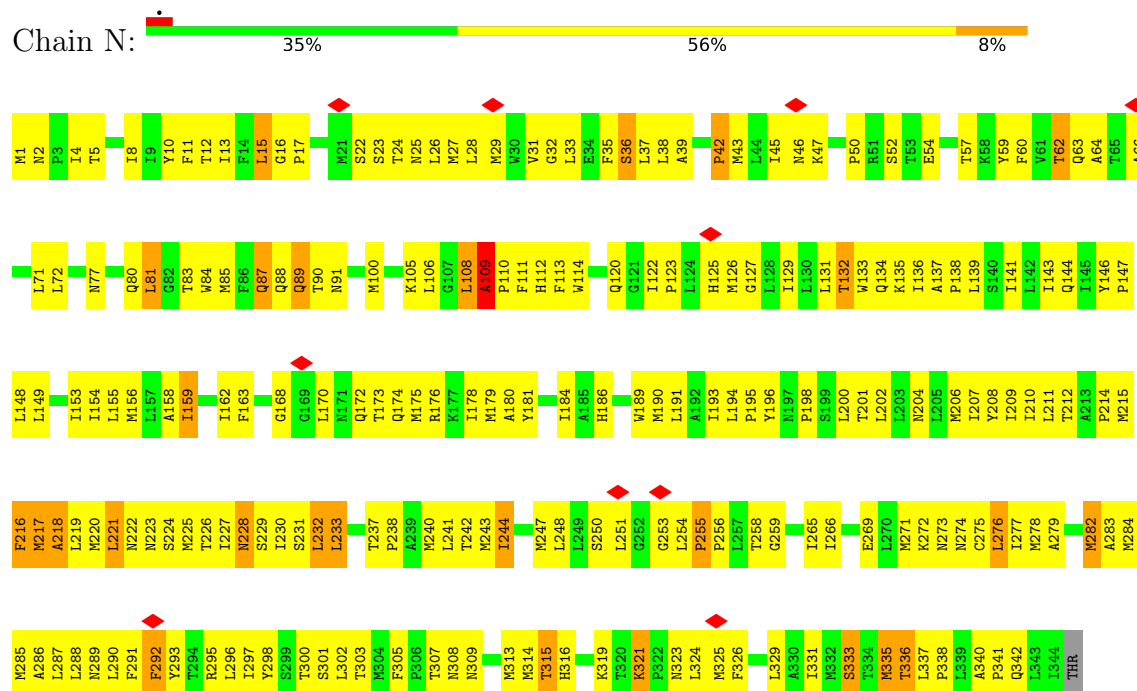


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

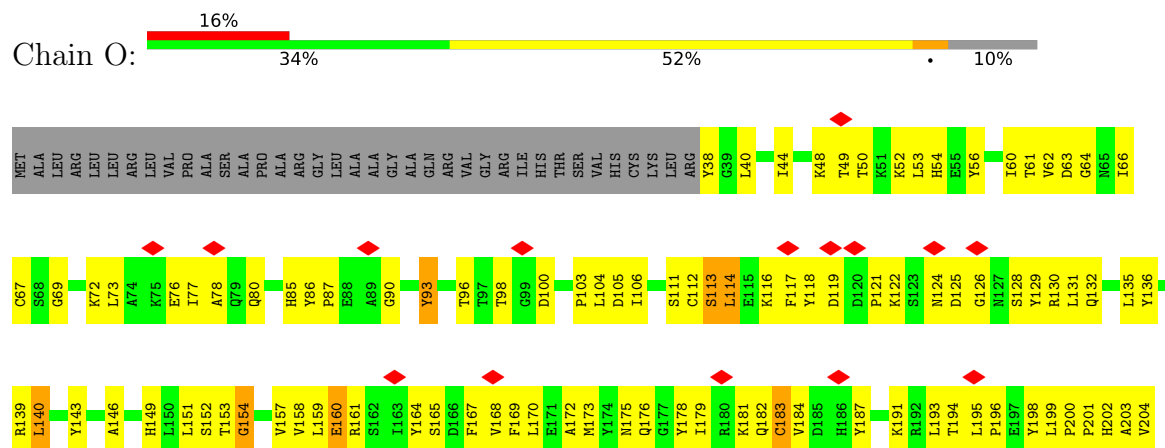


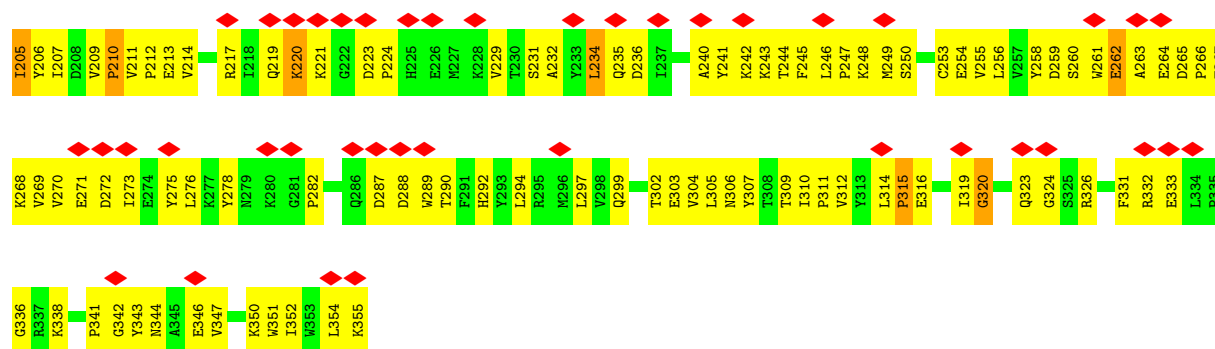


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

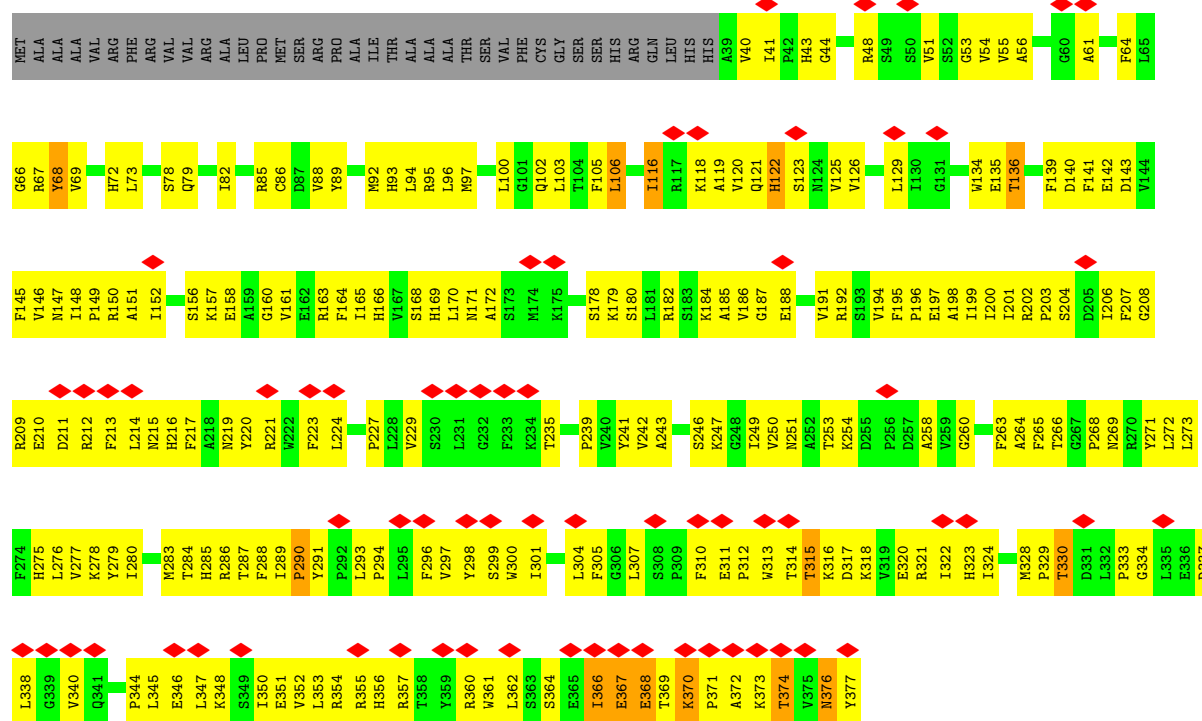


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

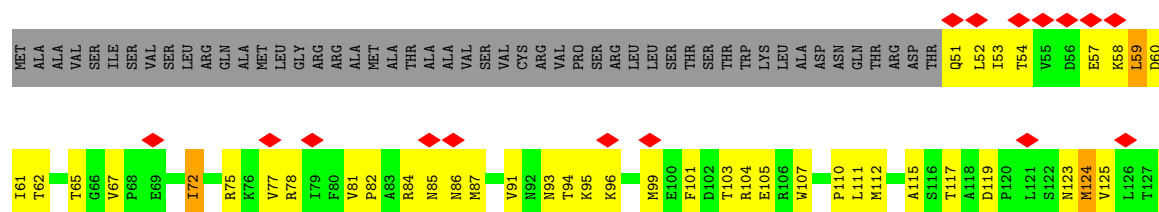


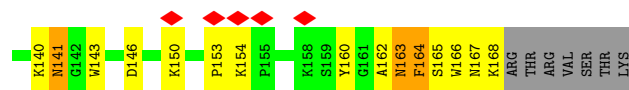


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

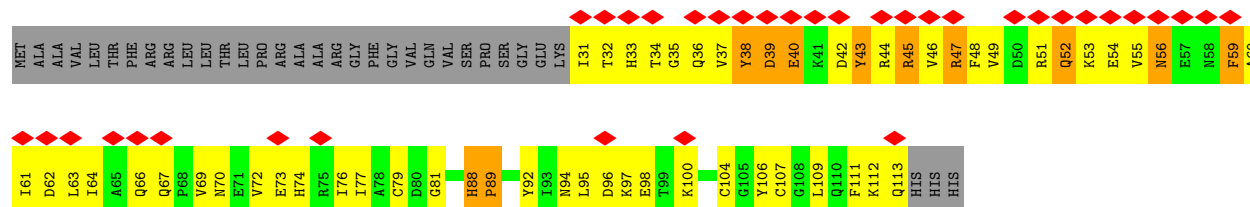
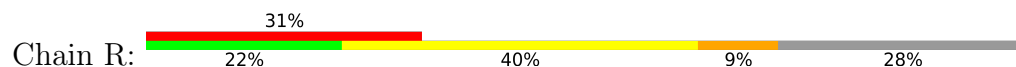


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

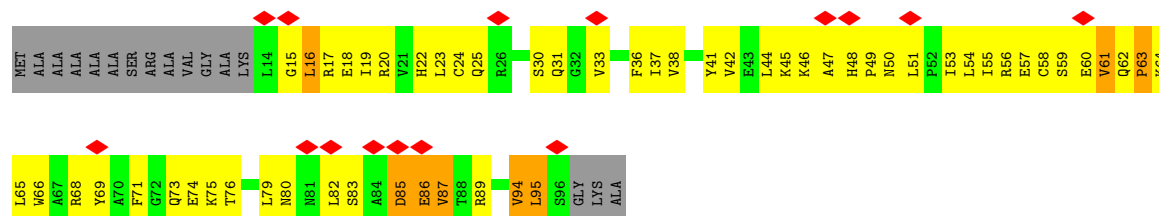




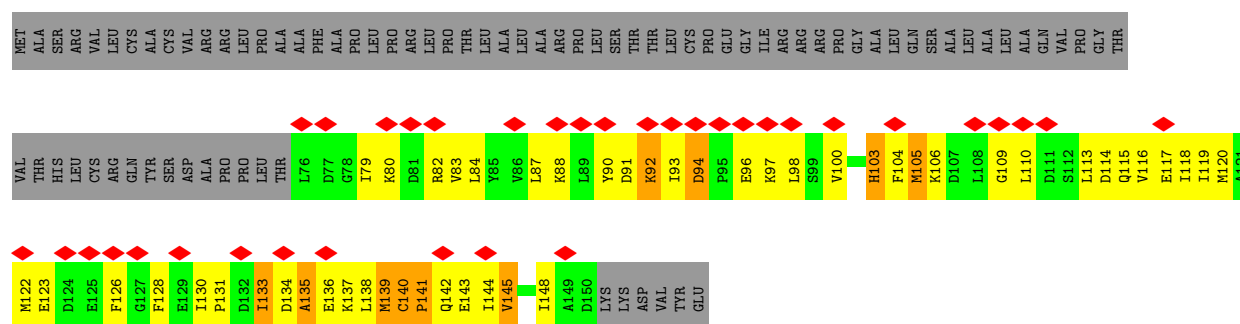
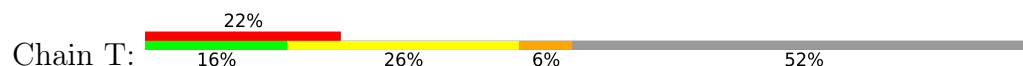
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

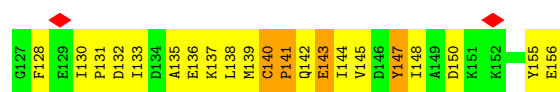


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

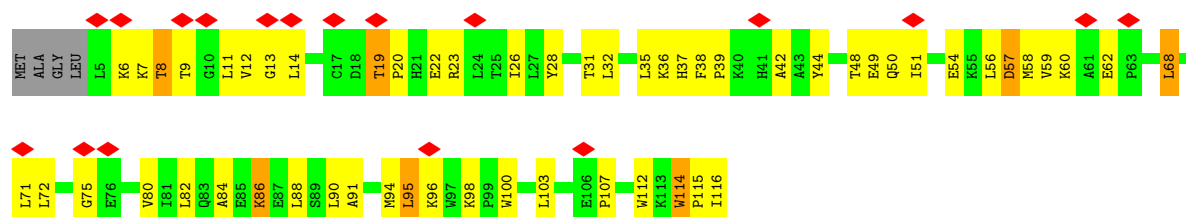


- Molecule 20: Acyl carrier protein, mitochondrial

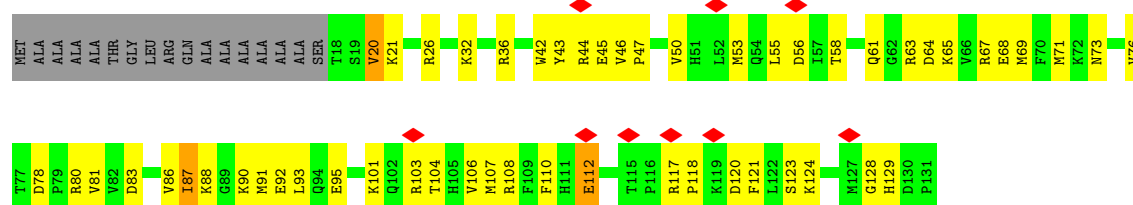




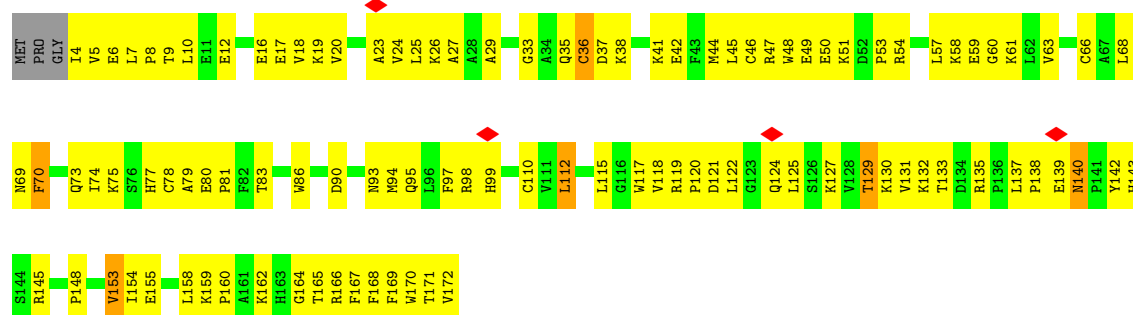
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



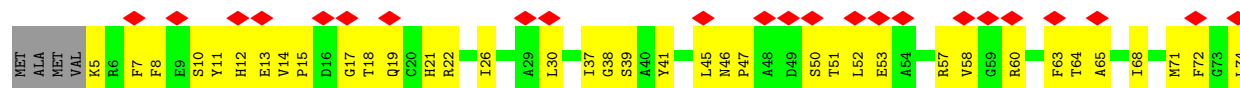
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

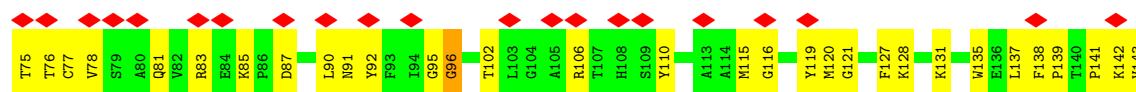


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

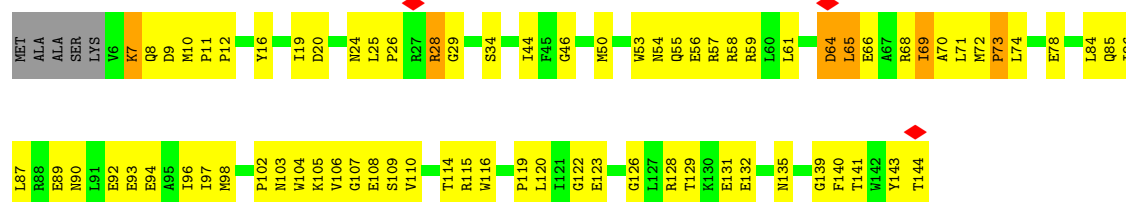


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

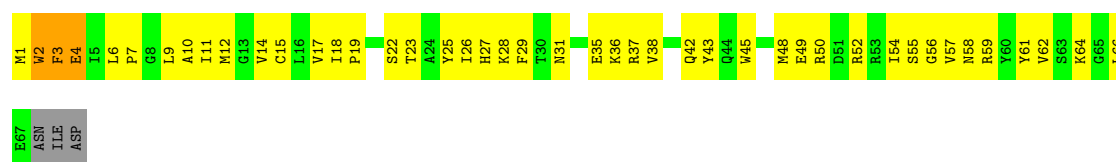




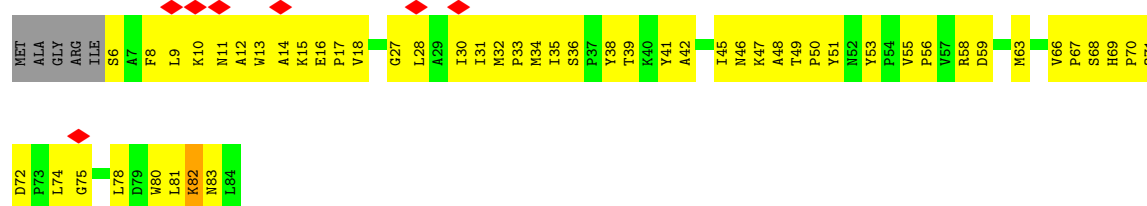
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



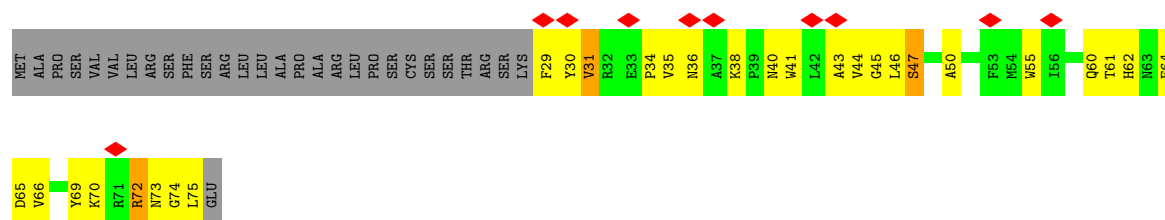
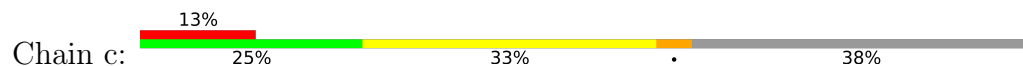
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

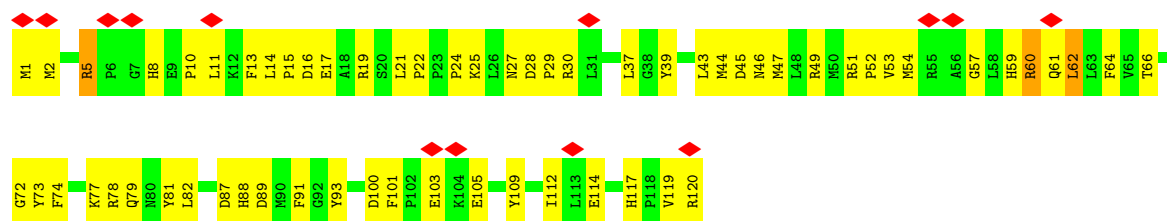


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

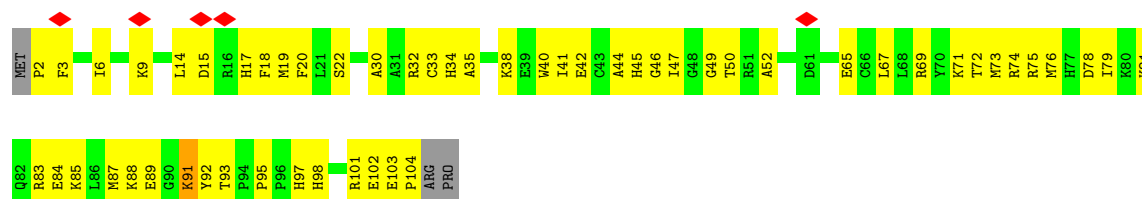
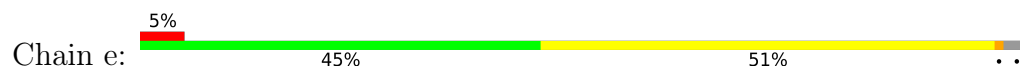


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2





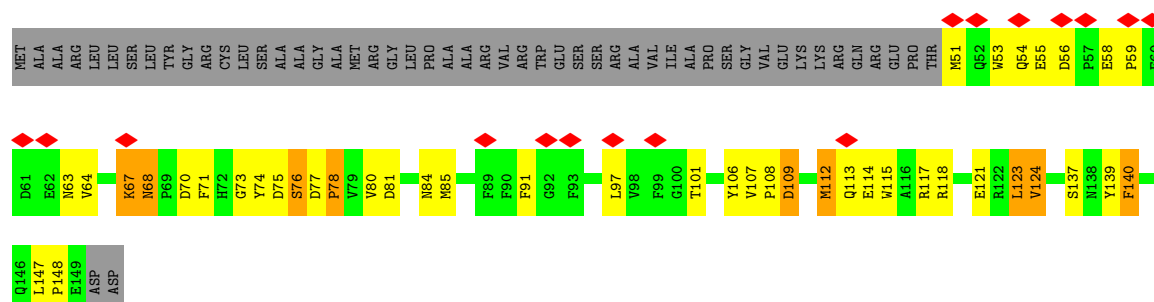
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



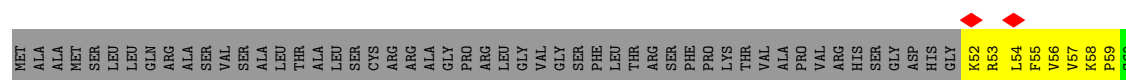
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

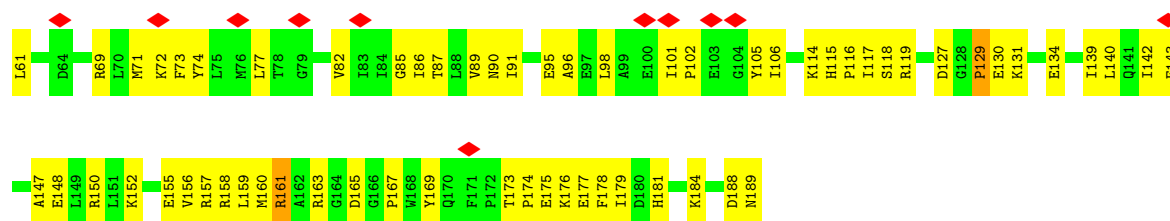


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

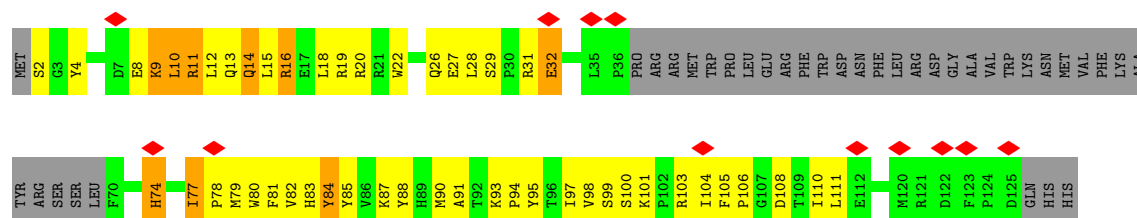


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

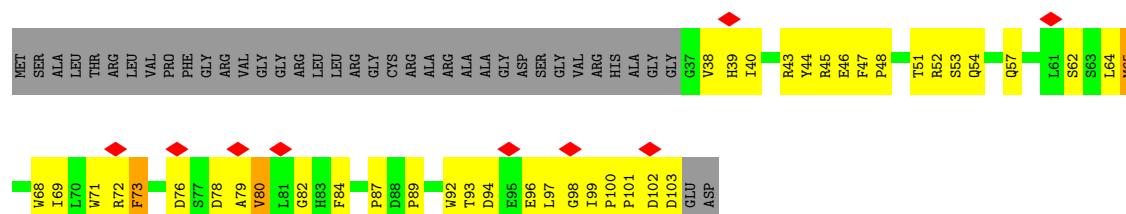
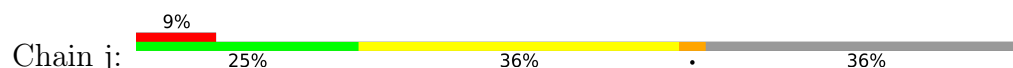




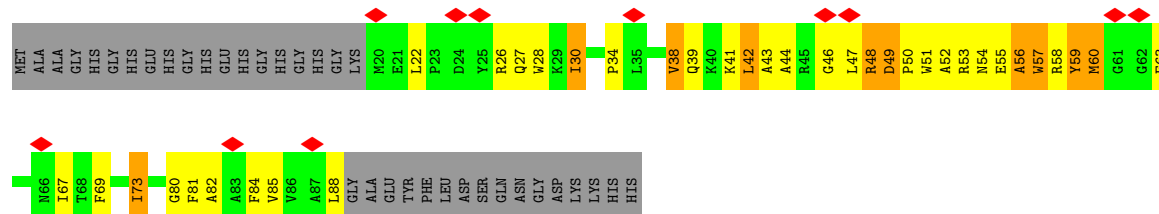
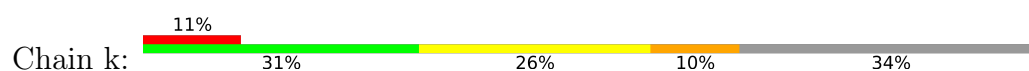
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



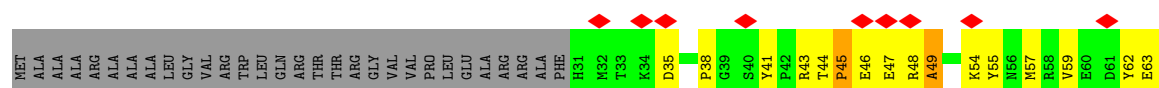
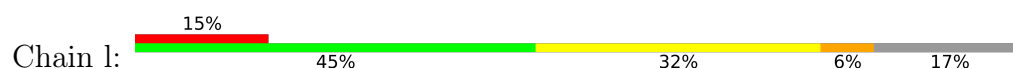
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

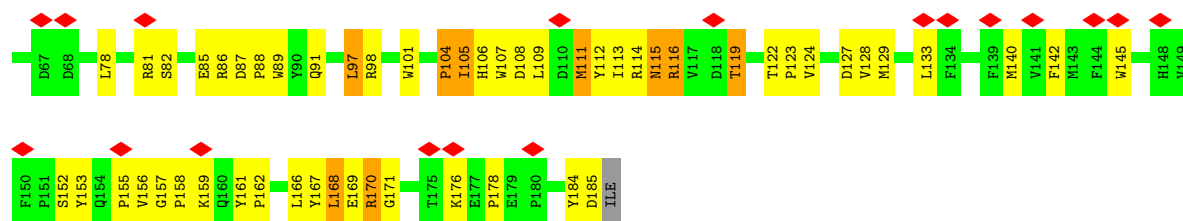


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

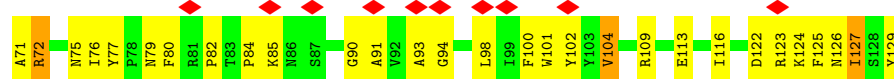


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

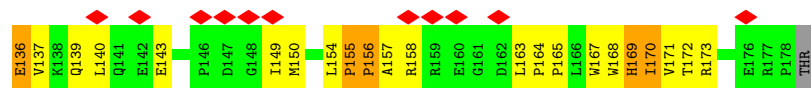
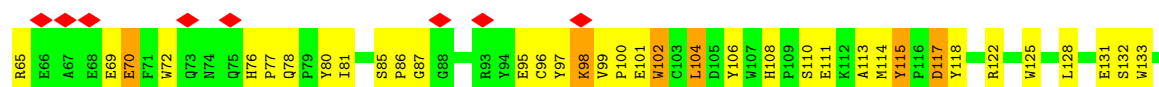
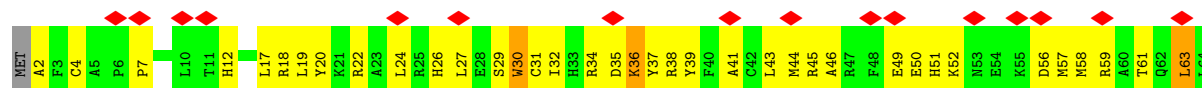




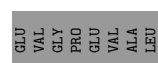
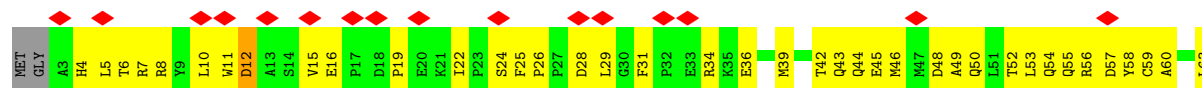
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

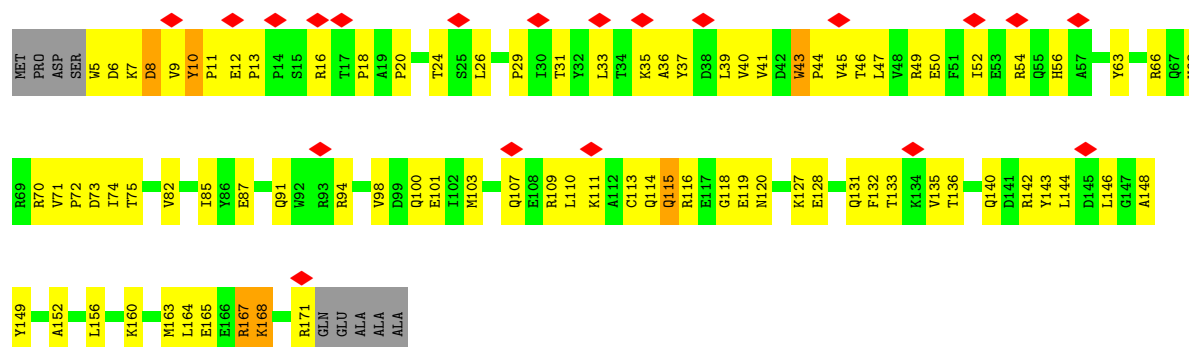


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

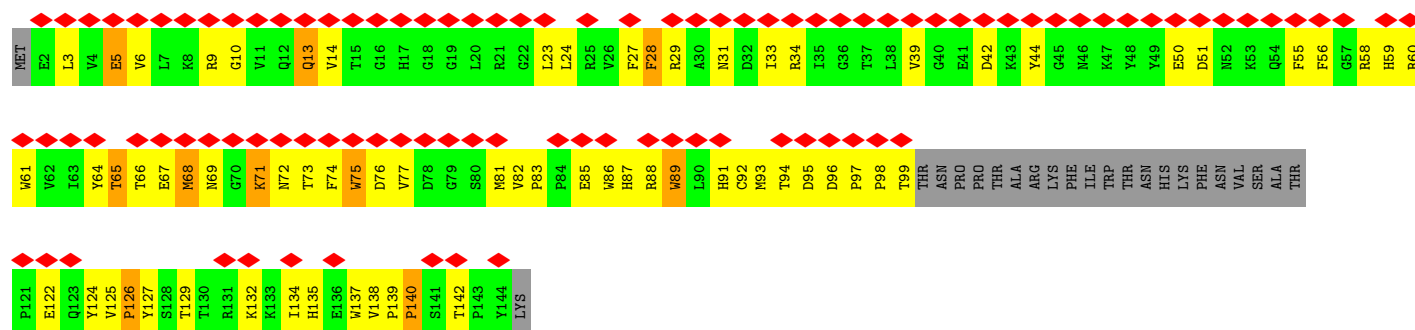


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

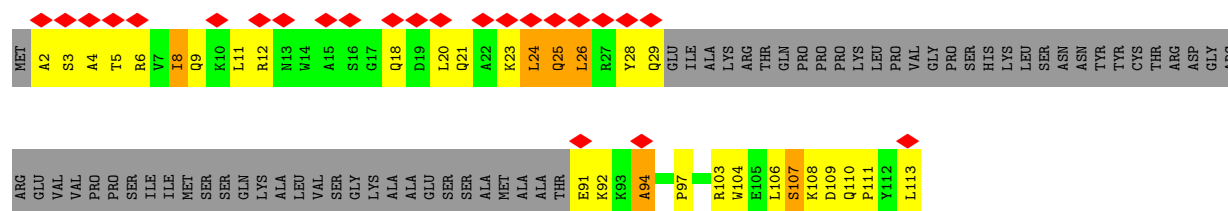
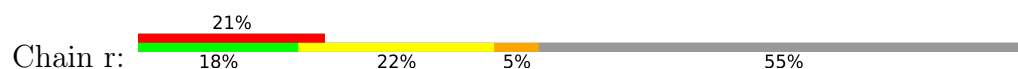




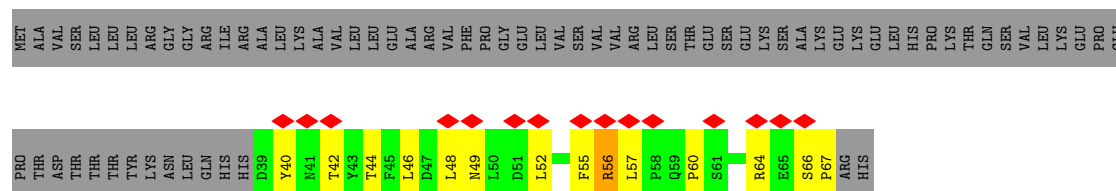
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



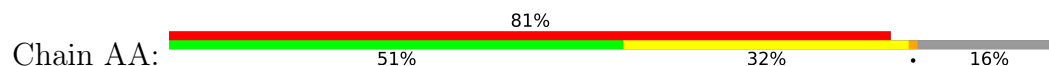
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



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

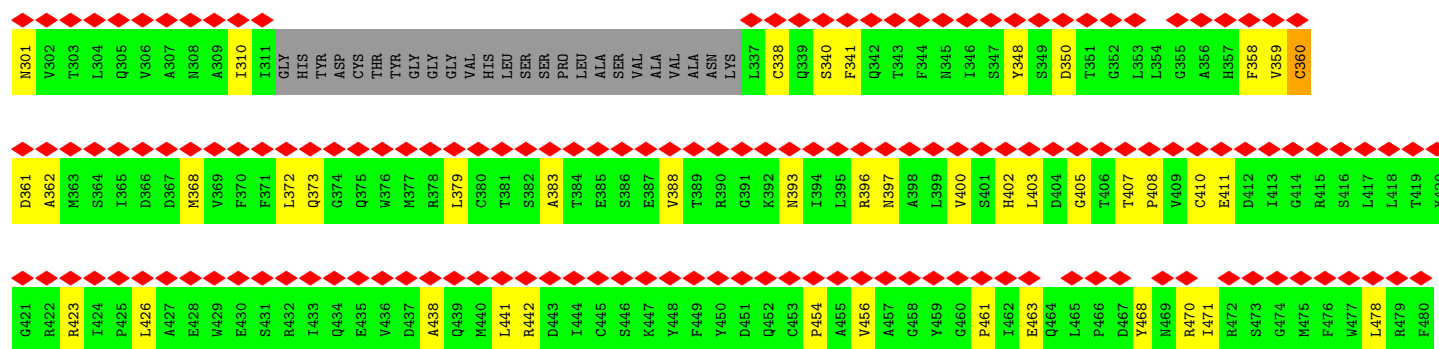


MET	ALA	ALA	SER	ALA	VAL	CYS	ARG	ALA	ALA	CYS	SER	GLY	THR	GLN	VAL	LEU	LEU	ARG	THR	ARG	SER	PRO	ALA	LEU	LEU	ARG	LEU	ALA	LEU	ARG	GLY	THR	ALA	THR	PHE	GLN	ALA	LEU	LEU	GLN	S44	V45	P46	E47	T48	Q49	V50	S51	I52	L53	D54	N55	G56	L57	R58	V59	A60						
S61	E62	Q63	S64	S65	H66	A67	T68	C69	T70	V71	G72	W73	W74	L75	D76	A77	G78	S79	R80	Y81	E82	T83	H84	R85	N86	N87	G88	A89	G90	Y91	L93	E94	H95	L96	A97	F98	K99	G100	T101	N102	N103	R104	P105	G106	N107	A108	L109	E110	K111	E112	V113	E114	S115	G117	A118	H119	L120						
N121	A122	Y123	S124	T125	R126	E127	H128	T129	A130	Y131	L132	I133	K134	A135	L136	S137	K138	D139	L140	P141	K142	V143	V144	E145	L146	L147	A148	D149	I150	V151	Q152	N153	S154	S155	L156	E157	D158	S159	Q160	I161	E162	K163	E164	R165	D166	V167	I168	L169	R170	E171	M172	Q173	E174	N175	I176	A177	S178	M179	Q180				
N181	V182	V183	F184	D185	Y186	L187	H188	A189	T190	A191	F192	Q193	G194	T195	P196	L197	Q199	A200	V201	E202	G203	P204	S205	E206	N207	V208	R209	R210	L211	S212	R213	T214	D215	L216	T217	D218	Y219	L220	N221	R222	H223	Y224	K225	A226	P227	R228	M229	V230	L231	A232	A233	A234	G235	G236	V237	E238	H239	Q240					
Q241	L242	L243	D244	L245	A246	Q247	K248	H249	L250	S251	S252	V253	S254	R255	VAL	TYR	GLU	ASP	ALA	VAL	PRO	GLY	THR	P267	C268	R269	F270	T271	G272	S273	E274	L275	R276	H277	R278	D279	D280	A281	L282	P283	L284	A285	H286	V287	A288	I289	V291	L290	E292	G293	P294	G295	W296	A297	N298	P299	D300						
N301	V302	T303	L304	Q305	V306	A307	N308	A309	I310	I311	G312	H313	Y314	ASP	CYS	THR	TYR	GLY	GLY	VAL	HIS	PRO	SER	PRO	ALA	LEU	SER	VAL	ALA	ASN	LYS	L337	C338	Q339	S340	F341	Q342	T343	F344	N345	I346	S347	Y348	S349	D350	T351	G352	L353	L354	G355	A356	H357	F358	V359	C360								
D361	A362	M363	S364	I365	D366	D367	M368	V369	F370	F371	L372	Q373	G374	Q375	W376	M377	R378	L379	C380	T381	S382	A383	D443	I444	C445	S446	E447	Y448	F449	R450	G451	D452	C453	P454	A455	V456	A457	G458	Y459	G460	P461	E462	L463	E463	D404	G464	Q464	G465	P466	D467	Y468	N469	R470	I471	D472	A473	G474	M475	F476	W477	L478	R479	PHE

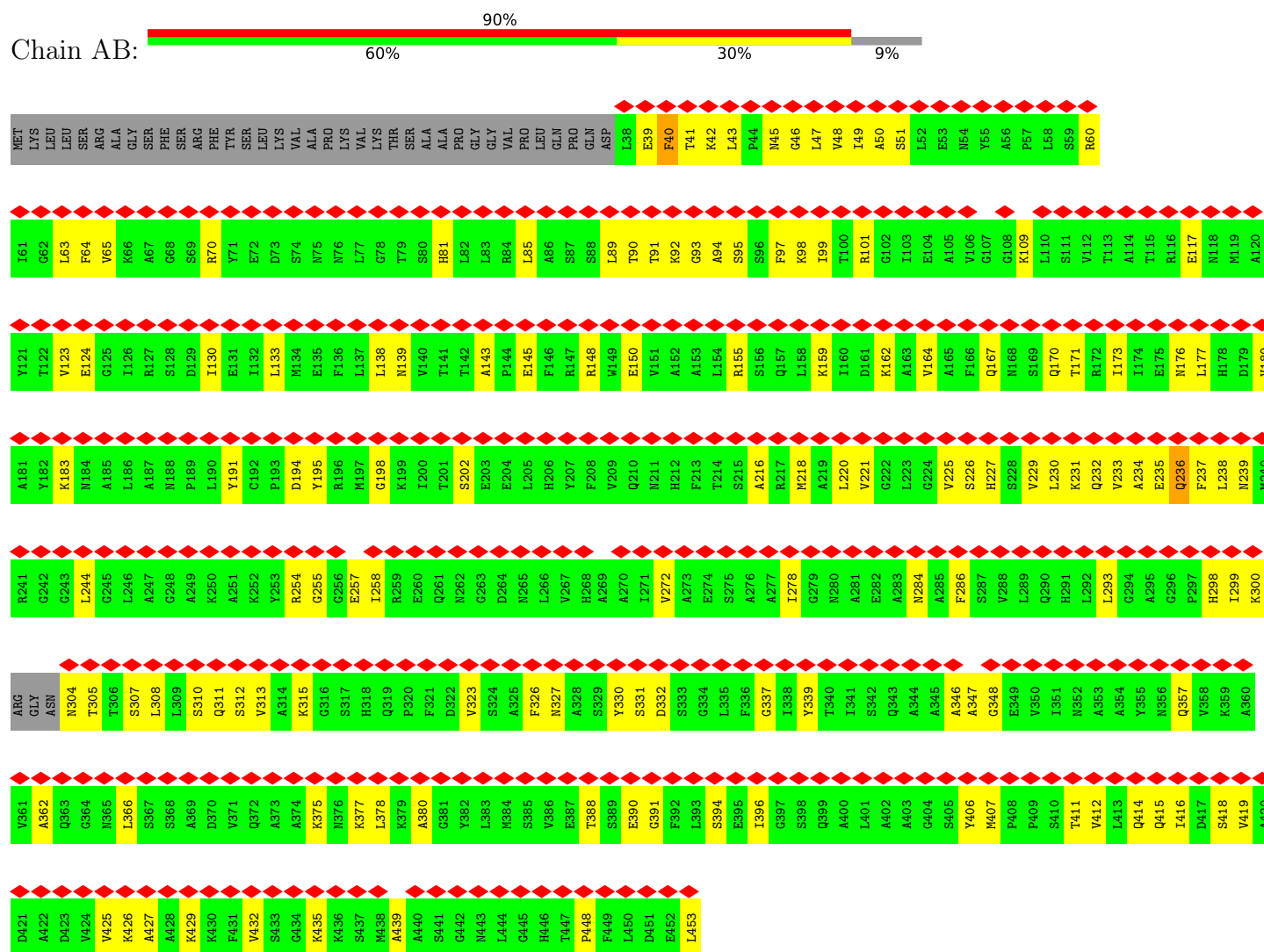
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



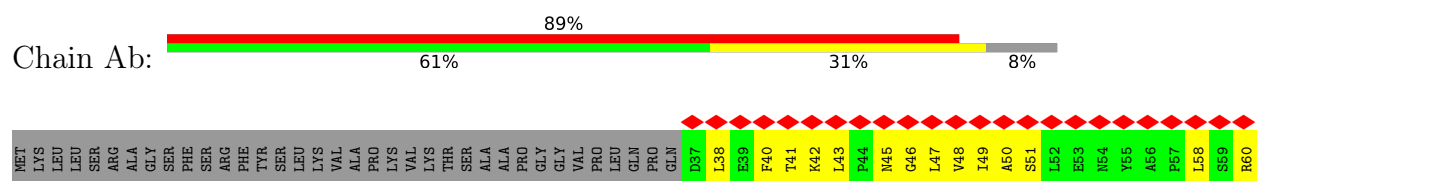
MET	ALA	ALA	SER	ALA	VAL	CYS	ARG	ALA	ALA	CYS	SER	GLY	THR	GLN	VAL	LEU	LEU	ARG	THR	ARG	SER	PRO	ALA	LEU	LEU	ARG	LEU	ALA	LEU	GLN	ALA	LEU	LEU	GLN	S44	V45	P46	E47	T48	Q49	V50	S51	I52	L53	D54	N55	G56	L57	R58	V59	A60								
S61	E62	Q63	S64	S65	H66	A67	T68	C69	T70	V71	G72	W73	W74	L75	D76	A77	G78	S79	R80	Y81	E82	T83	H84	R85	N86	N87	G88	A89	G90	Y91	L93	E94	H95	L96	A97	F98	K99	G100	T101	K102	N103	R104	P105	G106	N107	A108	L109	E110	K111	E112	V113	E114	S115	G117	A118	H119	L120		
N121	A122	Y123	S124	T125	R126	E127	H128	T129	A130	Y131	L132	I133	K134	A135	L136	S137	K138	D139	L140	P141	K142	V143	V144	E145	L146	L147	A148	D149	I150	V151	Q152	N153	S154	S155	L156	E157	D158	S159	Q160	T161	E162	K163	E164	R165	D166	V167	I168	L169	R170	E171	M172	Q173	E174	N175	I176	A177	S178	M179	Q180
N181	V182	V183	F184	D185	Y186	L187	H188	A189	T190	A191	F192	Q193	G194	T195	P196	L197	Q199	A200	V201	E202	G203	P204	S205	E206	N207	V208	R209	R210	L211	S212	R213	T214	D215	L216	T217	D218	Y219	L220	N221	R222	H223	Y224	K225	A226	P227	R228	M229	V230	L231	A232	A233	A234	G235	G236	V237	E238	H239	Q240	
Q241	L242	L243	D244	L245	A246	Q247	K248	H249	L250	S251	F252	V253	S254	ARG	VAL	TYR	GLU	GLU	ASP	ALA	VAL	PRO	GLY	LEU	THR	P267	C268	R269	F270	T271	G272	S273	E274	I275	R276	H277	R278	D279	D280	A281	L282	P283	L284	A285	H286	V287	A288	I289	A290	V291	E292	G293	P294	G295	W296	A297	N298	P299	D300

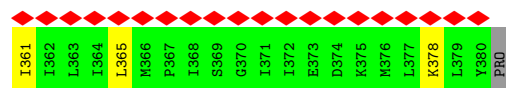


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

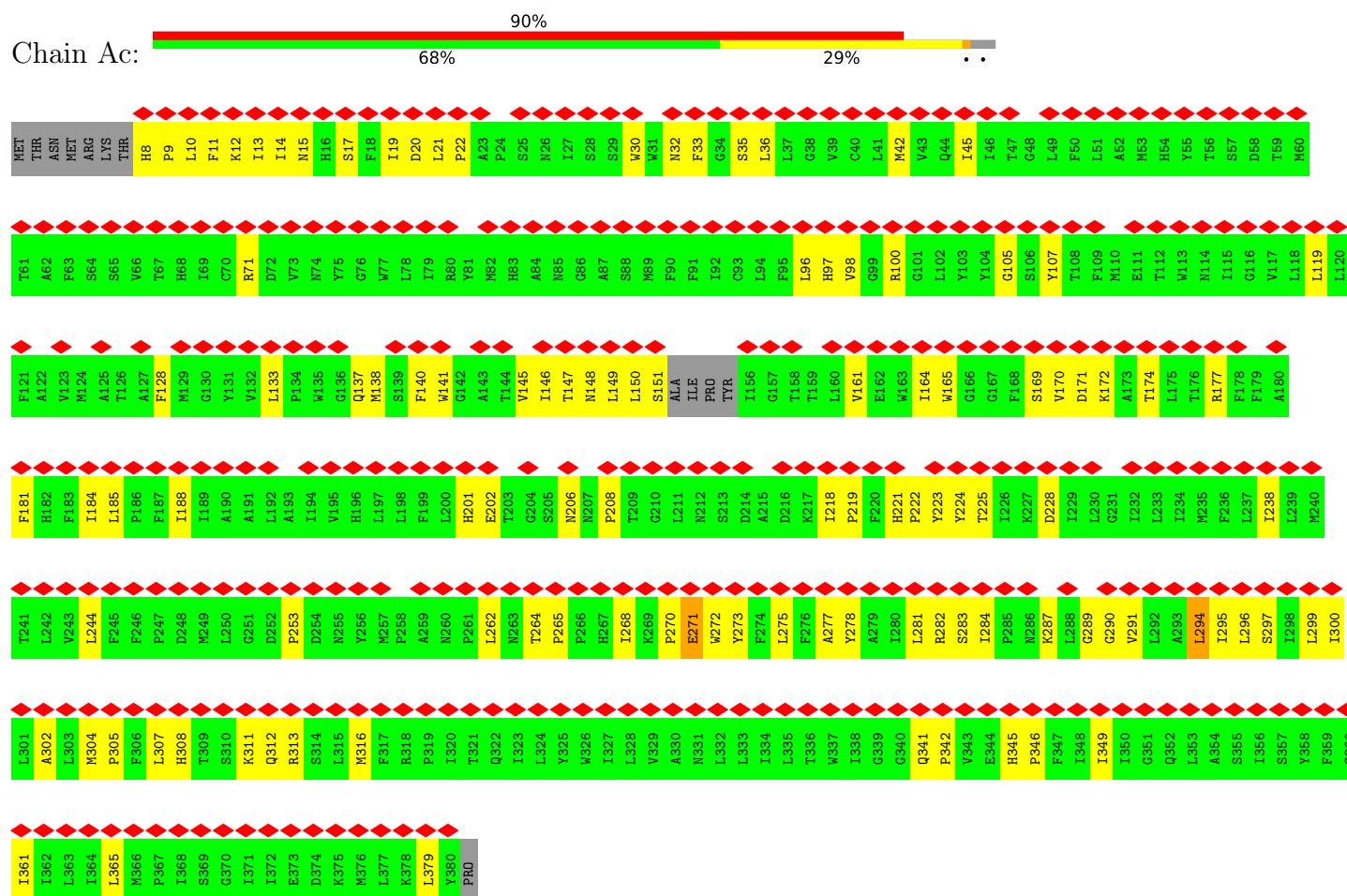


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

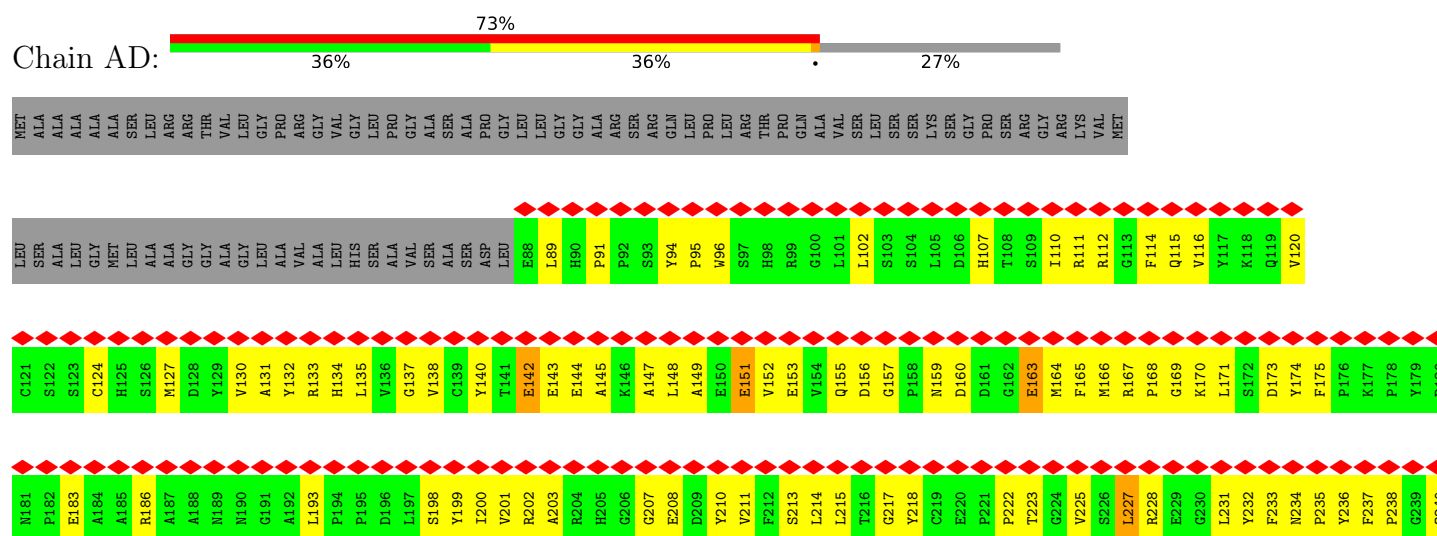


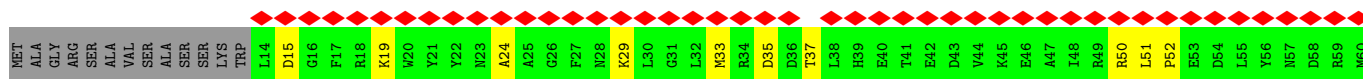


• Molecule 47: Cytochrome b



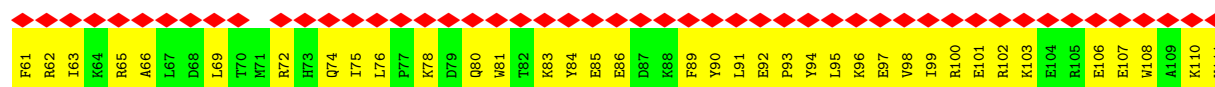
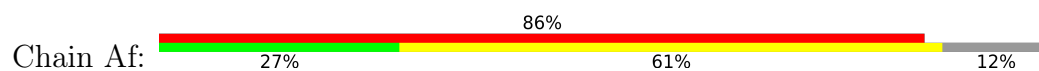
• Molecule 48: Cytochrome c1, heme protein, mitochondrial



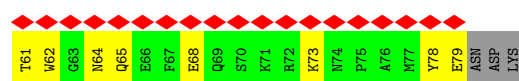
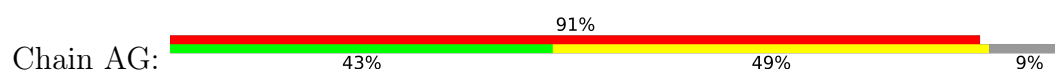




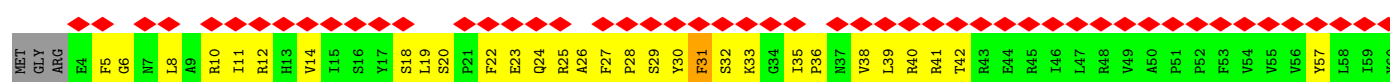
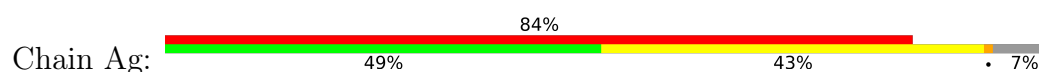
• Molecule 50: Cytochrome b-c1 complex subunit 7



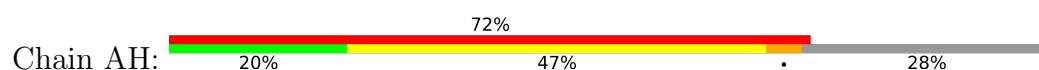
• Molecule 51: Cytochrome b-c1 complex subunit 8



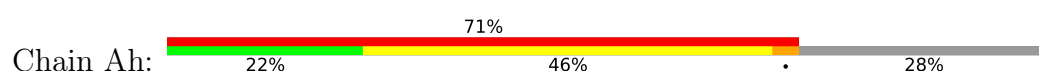
• Molecule 51: Cytochrome b-c1 complex subunit 8

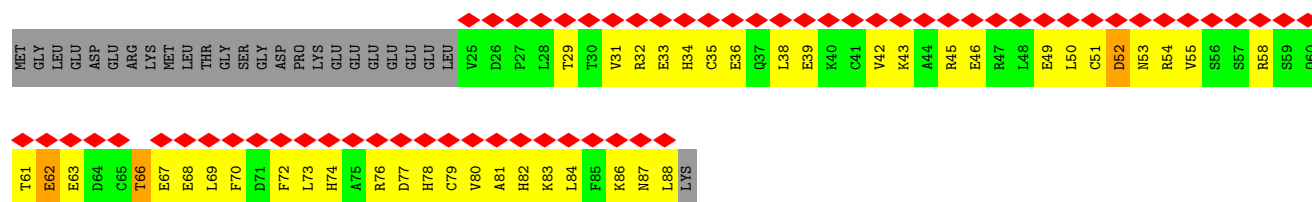


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



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





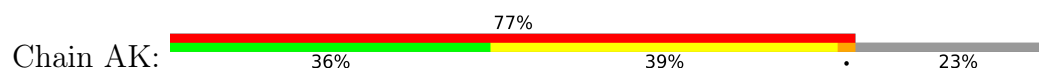
• Molecule 53: Cytochrome b-c1 complex subunit 9



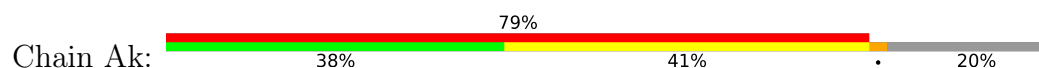
• Molecule 53: Cytochrome b-c1 complex subunit 9



• Molecule 54: Cytochrome b-c1 complex subunit 10



• Molecule 54: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0082	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, UQ6, FES, 3PE, ADP, NDP, SF4, UQ1, ZN, U10, CDL, PC1, FMN, UQ9, HEC, EH2

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	0.67	0/755	0.96	3/1029 (0.3%)
2	B	0.96	4/1278 (0.3%)	1.30	11/1730 (0.6%)
3	C	0.88	2/1687 (0.1%)	1.28	13/2297 (0.6%)
4	D	0.91	5/3532 (0.1%)	1.36	33/4782 (0.7%)
5	E	0.82	3/1675 (0.2%)	1.16	18/2282 (0.8%)
6	F	0.82	4/3347 (0.1%)	1.32	41/4522 (0.9%)
7	G	0.88	8/5374 (0.1%)	1.49	86/7281 (1.2%)
8	H	0.83	2/2607 (0.1%)	1.22	30/3561 (0.8%)
9	I	0.90	1/1418 (0.1%)	1.48	18/1915 (0.9%)
10	J	0.55	1/1205 (0.1%)	0.92	6/1633 (0.4%)
11	K	0.85	0/732	1.44	11/994 (1.1%)
12	L	0.97	6/4921 (0.1%)	1.56	108/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.56	85/5062 (1.7%)
14	N	1.00	3/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.86	6/2655 (0.2%)	1.21	27/3601 (0.7%)
16	P	0.79	4/2793 (0.1%)	1.17	23/3787 (0.6%)
17	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
18	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
19	S	0.94	2/678 (0.3%)	1.47	11/915 (1.2%)
20	T	1.03	1/613 (0.2%)	1.56	12/826 (1.5%)
20	U	0.96	1/712 (0.1%)	1.35	12/962 (1.2%)
21	V	0.86	0/937	1.47	14/1270 (1.1%)
22	W	0.73	0/993	0.95	3/1335 (0.2%)
23	X	0.72	0/1422	1.22	15/1921 (0.8%)
24	Y	0.85	0/1054	0.96	3/1429 (0.2%)
25	Z	0.81	1/1183 (0.1%)	1.23	11/1597 (0.7%)
26	a	0.88	0/561	1.38	8/755 (1.1%)
27	b	0.70	0/643	0.94	1/884 (0.1%)
28	c	0.69	0/400	1.24	8/544 (1.5%)
29	d	0.88	1/1028 (0.1%)	1.01	8/1387 (0.6%)
30	e	0.77	1/881 (0.1%)	1.01	4/1173 (0.3%)
31	f	0.59	0/451	0.75	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.87	3/863 (0.3%)	1.36	18/1175 (1.5%)
33	h	0.76	0/1197	1.22	7/1621 (0.4%)
34	i	0.85	0/790	1.38	16/1074 (1.5%)
35	j	0.75	0/599	1.23	8/820 (1.0%)
36	k	1.05	1/578 (0.2%)	1.56	18/782 (2.3%)
37	l	1.02	4/1359 (0.3%)	1.25	9/1855 (0.5%)
38	m	0.82	1/1079 (0.1%)	1.21	17/1463 (1.2%)
39	n	0.93	1/1589 (0.1%)	1.22	17/2152 (0.8%)
40	o	0.78	0/1063	1.14	7/1427 (0.5%)
41	p	0.72	1/1448 (0.1%)	1.01	13/1957 (0.7%)
42	q	1.04	2/1054 (0.2%)	1.53	19/1431 (1.3%)
43	r	1.16	3/426 (0.7%)	1.71	12/573 (2.1%)
44	s	0.45	0/244	1.10	2/331 (0.6%)
45	AA	0.42	0/3218	0.74	5/4362 (0.1%)
45	Aa	0.38	0/3191	0.69	2/4326 (0.0%)
46	AB	0.39	1/3146 (0.0%)	0.64	5/4252 (0.1%)
46	Ab	0.37	0/3178	0.62	0/4296
47	AC	0.46	1/3089 (0.0%)	0.69	6/4221 (0.1%)
47	Ac	0.47	1/3054 (0.0%)	0.65	1/4170 (0.0%)
48	AD	0.42	0/1955	0.78	6/2655 (0.2%)
48	Ad	0.43	0/1971	0.71	2/2677 (0.1%)
49	AE	0.63	0/1428	1.01	2/1934 (0.1%)
49	AI	0.48	0/331	0.94	0/451
49	Ae	0.62	0/1467	1.00	2/1985 (0.1%)
50	AF	0.38	0/875	0.57	1/1173 (0.1%)
50	Af	0.47	0/884	0.73	1/1184 (0.1%)
51	AG	0.49	0/653	0.89	2/883 (0.2%)
51	Ag	0.47	0/662	0.88	2/895 (0.2%)
52	AH	0.49	0/534	1.04	9/717 (1.3%)
52	Ah	0.57	0/534	1.04	5/717 (0.7%)
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.53	0/339	0.71	0/457
54	AK	0.49	0/368	0.77	1/504 (0.2%)
54	Ak	0.44	0/379	0.73	1/522 (0.2%)
All	All	0.77	87/97543 (0.1%)	1.17	914/132254 (0.7%)

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	227	ALA	C-O	15.85	1.42	1.24
18	R	89	PRO	N-CD	-15.14	1.26	1.47
12	L	265	PRO	N-CD	13.82	1.67	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	AC	271	GLU	C-N	13.68	1.52	1.34
36	k	50	PRO	N-CD	-13.63	1.28	1.47
47	Ac	271	GLU	C-N	13.58	1.51	1.34
42	q	139	PRO	N-CD	-13.51	1.28	1.47
14	N	255	PRO	N-CD	-13.45	1.28	1.47
30	e	91	LYS	C-N	12.91	1.51	1.33
16	P	371	PRO	N-CD	12.90	1.65	1.47
7	G	532	PRO	N-CD	-12.58	1.30	1.47
15	O	315	PRO	N-CD	-12.15	1.30	1.47
20	T	141	PRO	N-CD	11.77	1.64	1.47
15	O	210	PRO	N-CD	-11.31	1.31	1.47
6	F	295	PRO	N-CD	-11.19	1.32	1.47
12	L	234	PRO	N-CD	11.18	1.63	1.47
8	H	42	PRO	N-CD	10.84	1.62	1.47
13	M	370	PRO	N-CD	-10.63	1.32	1.47
43	r	91	GLU	N-CA	10.01	1.65	1.46
6	F	227	PRO	N-CD	9.93	1.61	1.47
16	P	290	PRO	N-CD	9.61	1.61	1.47
32	g	78	PRO	N-CD	-9.61	1.34	1.47
5	E	44	PRO	N-CD	-9.54	1.34	1.47
7	G	275	PRO	N-CD	-9.46	1.34	1.47
29	d	15	PRO	N-CD	-9.37	1.34	1.47
6	F	319	PRO	N-CD	9.06	1.60	1.47
9	I	107	PRO	N-CD	8.54	1.59	1.47
16	P	204	SER	C-O	-8.53	1.14	1.23
13	M	20	PRO	N-CD	8.52	1.59	1.47
4	D	163	PRO	N-CD	-8.26	1.36	1.47
12	L	212	PRO	N-CD	-8.26	1.36	1.47
39	n	155	PRO	N-CD	8.19	1.59	1.47
25	Z	73	PRO	N-CD	8.10	1.59	1.47
19	S	63	PRO	N-CD	-7.95	1.36	1.47
18	R	39	ASP	CA-C	7.93	1.64	1.53
4	D	352	PRO	N-CD	-7.86	1.36	1.47
17	Q	53	ILE	C-O	7.85	1.33	1.24
18	R	40	GLU	N-CA	7.84	1.56	1.46
2	B	88	SER	C-N	-7.65	1.20	1.33
43	r	111	PRO	N-CD	-7.46	1.37	1.47
2	B	96	GLY	CA-C	-7.44	1.47	1.52
37	l	115	ASN	C-N	-7.42	1.24	1.33
13	M	208	PRO	N-CD	7.23	1.57	1.47
37	l	104	PRO	N-CD	-7.16	1.37	1.47
14	N	238	PRO	N-CD	-6.91	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	541	PRO	N-CD	-6.82	1.38	1.47
15	O	206	TYR	C-N	6.82	1.42	1.33
7	G	203	ASP	CA-C	6.64	1.62	1.52
32	g	113	GLN	CA-C	6.64	1.61	1.52
46	AB	40	PHE	CA-C	6.62	1.61	1.53
10	J	136	GLU	CA-C	-6.55	1.44	1.52
7	G	600	GLU	CA-C	6.45	1.61	1.52
15	O	205	ILE	C-N	6.40	1.42	1.33
3	C	66	GLU	C-N	6.38	1.42	1.33
12	L	384	PRO	N-CD	6.31	1.56	1.47
2	B	153	PRO	N-CD	-6.30	1.39	1.47
7	G	127	ASP	CA-C	6.26	1.62	1.52
4	D	266	ARG	C-O	-6.23	1.16	1.24
6	F	384	PRO	N-CD	-6.17	1.39	1.47
41	p	10	TYR	CA-C	-6.14	1.46	1.52
2	B	110	PRO	C-O	-6.10	1.16	1.24
7	G	76	ARG	CA-C	6.09	1.61	1.53
38	m	72	ARG	CA-C	6.06	1.60	1.52
32	g	137	SER	C-O	-6.04	1.16	1.24
12	L	112	PRO	N-CD	6.02	1.56	1.47
43	r	25	GLN	CA-C	5.92	1.60	1.52
5	E	93	PRO	N-CD	-5.87	1.39	1.47
8	H	291	LYS	C-O	-5.81	1.16	1.24
18	R	59	PHE	CA-C	-5.81	1.45	1.52
37	l	45	PRO	N-CD	-5.74	1.39	1.47
14	N	333	SER	C-O	-5.72	1.17	1.23
15	O	87	PRO	N-CD	-5.70	1.39	1.47
13	M	454	ILE	CA-C	5.69	1.60	1.52
16	P	204	SER	CA-C	-5.69	1.46	1.53
13	M	252	PRO	N-CD	-5.53	1.40	1.47
19	S	95	LEU	CA-C	5.44	1.59	1.52
4	D	392	PRO	C-O	-5.42	1.20	1.24
20	U	140	CYS	C-O	-5.41	1.17	1.24
7	G	683	PRO	N-CD	-5.39	1.40	1.47
15	O	103	PRO	N-CD	-5.36	1.40	1.47
42	q	126	PRO	N-CD	5.33	1.55	1.47
4	D	266	ARG	CA-C	-5.24	1.45	1.52
13	M	424	ILE	CA-C	-5.14	1.45	1.52
37	l	111	MET	C-O	-5.10	1.17	1.24
12	L	56	HIS	CA-C	-5.06	1.46	1.52
13	M	159	PRO	N-CD	5.04	1.54	1.47
3	C	61	GLY	C-N	-5.01	1.27	1.33

All (914) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.30	132.46	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.59	130.04	111.02
13	M	370	PRO	N-CA-C	14.56	128.46	110.70
43	r	91	GLU	N-CA-CB	14.52	135.18	110.50
14	N	255	PRO	N-CA-C	14.41	128.28	110.70
15	O	118	TYR	N-CA-C	13.89	125.94	111.07
42	q	139	PRO	N-CA-CB	-13.57	95.59	103.19
7	G	251	ILE	N-CA-C	13.28	126.76	108.17
52	Ah	66	THR	N-CA-C	-13.03	97.16	111.36
9	I	164	VAL	N-CA-C	-12.77	100.19	112.83
7	G	77	MET	N-CA-C	-12.55	97.36	113.17
7	G	500	ILE	N-CA-C	-12.54	98.74	110.53
26	a	3	PHE	CB-CA-C	-12.41	89.59	110.68
16	P	106	LEU	N-CA-C	12.21	128.73	109.07
13	M	424	ILE	N-CA-C	-11.65	94.03	109.30
7	G	204	MET	N-CA-C	-11.63	91.45	109.25
6	F	288	VAL	N-CA-C	11.61	121.56	110.42
6	F	449	ARG	N-CA-C	-11.60	98.71	111.36
13	M	104	ILE	N-CA-C	-11.57	99.08	110.30
34	i	14	GLN	N-CA-C	11.54	123.86	111.28
12	L	194	ASN	N-CA-C	11.51	125.45	109.11
6	F	334	THR	N-CA-CB	11.47	127.25	109.82
13	M	311	GLY	N-CA-C	-11.38	99.31	112.50
7	G	599	THR	N-CA-C	11.34	126.21	112.38
37	l	116	ARG	N-CA-C	11.33	123.32	110.97
17	Q	60	ASP	N-CA-C	-11.33	90.32	109.24
48	AD	144	GLU	N-CA-C	-11.28	99.01	111.07
12	L	278	LEU	N-CA-C	-11.26	98.98	111.14
11	K	83	ASN	N-CA-C	-11.21	100.14	114.04
14	N	244	ILE	N-CA-C	-11.20	99.41	110.72
20	U	79	ILE	N-CA-C	-11.04	102.30	112.90
21	V	57	ASP	N-CA-C	-11.03	99.27	111.07
12	L	582	GLY	N-CA-C	-10.82	99.49	114.64
12	L	231	PRO	N-CA-C	10.75	127.82	113.84
33	h	101	ILE	N-CA-C	-10.64	98.52	108.95
12	L	556	ILE	N-CA-C	10.63	121.29	110.23
9	I	77	LEU	N-CA-C	-10.44	99.70	111.71
2	B	195	PRO	N-CA-C	-10.42	97.99	110.70
45	AA	360	CYS	N-CA-C	10.40	121.97	108.24
20	T	139	MET	N-CA-C	-10.38	97.49	113.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	276	CYS	N-CA-C	-10.38	99.97	111.28
5	E	68	ASN	N-CA-C	-10.37	99.98	111.07
15	O	210	PRO	N-CA-CB	-10.35	94.62	103.32
7	G	280	ASP	N-CA-C	10.31	122.52	111.28
15	O	96	THR	N-CA-C	-10.31	100.13	111.36
44	s	55	PHE	N-CA-C	10.22	125.75	112.26
16	P	366	ILE	N-CA-C	10.22	121.04	110.62
4	D	337	MET	N-CA-C	-10.21	100.15	111.07
4	D	140	ASP	CB-CA-C	-10.19	98.07	111.42
37	l	170	ARG	N-CA-C	-10.18	101.51	113.21
7	G	414	PHE	N-CA-C	-10.17	101.38	113.88
9	I	161	ALA	N-CA-C	10.10	122.29	111.28
20	T	135	ALA	N-CA-C	-10.07	100.30	111.28
26	a	4	GLU	N-CA-C	10.04	124.79	112.54
13	M	117	MET	N-CA-C	-10.03	100.35	111.28
20	T	133	ILE	N-CA-C	9.92	119.86	110.53
9	I	166	ALA	N-CA-C	-9.87	100.79	113.12
7	G	325	ARG	N-CA-C	-9.82	100.27	110.97
5	E	64	ALA	N-CA-C	-9.75	99.41	111.11
13	M	423	MET	N-CA-C	-9.72	96.94	110.35
36	k	50	PRO	CA-N-CD	9.72	125.61	112.00
7	G	654	VAL	N-CA-C	9.71	123.23	111.09
42	q	138	VAL	CA-C-N	-9.68	112.59	119.66
42	q	138	VAL	C-N-CA	-9.68	112.59	119.66
14	N	286	ALA	N-CA-C	-9.66	100.75	111.28
16	P	371	PRO	N-CA-CB	9.66	111.86	103.36
14	N	255	PRO	CA-N-CD	9.65	125.50	112.00
13	M	83	HIS	N-CA-C	-9.64	97.24	110.35
22	W	87	ILE	N-CA-C	-9.63	101.17	110.42
10	J	136	GLU	CA-C-N	-9.58	110.00	120.44
10	J	136	GLU	C-N-CA	-9.58	110.00	120.44
26	a	2	TRP	N-CA-C	-9.56	101.61	113.28
6	F	418	GLN	N-CA-C	-9.56	100.81	111.14
34	i	12	LEU	N-CA-C	-9.54	101.20	113.12
8	H	91	MET	N-CA-C	-9.52	96.49	110.20
23	X	70	PHE	N-CA-C	-9.49	99.72	111.11
12	L	375	ILE	N-CA-C	-9.49	101.31	110.42
8	H	52	ALA	N-CA-C	-9.46	100.94	111.07
13	M	104	ILE	N-CA-CB	9.45	120.92	110.62
4	D	427	PRO	N-CA-C	-9.45	95.66	110.50
18	R	38	TYR	N-CA-C	-9.43	96.37	110.24
41	p	56	HIS	N-CA-C	9.42	121.55	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	112	LEU	N-CA-C	-9.41	100.97	111.14
7	G	694	PHE	N-CA-C	9.38	121.50	111.28
42	q	139	PRO	CA-N-CD	9.37	125.12	112.00
14	N	228	ASN	N-CA-C	-9.35	101.07	111.07
36	k	60	MET	N-CA-C	9.34	121.15	110.97
12	L	40	ILE	N-CA-C	-9.29	101.33	110.72
36	k	56	ALA	N-CA-C	9.29	121.49	111.36
7	G	692	LYS	N-CA-C	-9.28	100.53	112.23
16	P	367	GLU	N-CA-C	9.28	122.59	111.82
16	P	369	THR	N-CA-CB	9.24	123.47	110.17
12	L	394	LEU	N-CA-C	-9.23	101.19	111.07
25	Z	69	ILE	N-CA-C	-9.20	100.70	110.36
12	L	483	PRO	N-CA-C	-9.16	96.81	111.38
7	G	640	ASP	N-CA-C	-9.16	101.38	111.36
5	E	85	ALA	N-CA-C	-9.15	101.38	111.36
38	m	48	LEU	N-CA-C	9.15	123.99	113.01
14	N	87	GLN	N-CA-C	9.14	123.30	109.41
6	F	103	ASN	N-CA-C	-9.13	101.06	113.30
13	M	442	ILE	N-CA-CB	9.12	117.57	110.45
28	c	64	GLU	N-CA-C	-9.11	101.32	111.07
12	L	467	VAL	N-CA-C	9.07	119.13	110.42
26	a	57	VAL	N-CA-C	-9.03	105.14	113.71
12	L	524	THR	N-CA-C	9.00	122.26	111.82
41	p	115	GLN	N-CA-C	-8.98	102.83	113.88
11	K	70	GLU	N-CA-C	-8.97	100.34	111.11
6	F	411	SER	N-CA-C	-8.96	101.48	111.07
12	L	344	GLY	N-CA-C	-8.92	102.16	112.50
12	L	406	ALA	N-CA-C	-8.87	101.70	111.36
7	G	133	GLN	N-CA-CB	8.81	121.55	110.45
15	O	183	CYS	N-CA-C	-8.80	100.55	111.11
14	N	233	LEU	N-CA-C	-8.78	101.72	111.28
7	G	212	LYS	N-CA-C	-8.75	94.63	108.90
13	M	255	LYS	N-CA-C	-8.75	101.71	111.07
14	N	81	LEU	N-CA-C	-8.73	94.40	108.55
40	o	72	ASP	N-CA-C	-8.71	99.03	110.53
39	n	70	GLU	N-CA-C	-8.71	101.76	111.07
22	W	20	VAL	N-CA-C	8.66	120.75	108.36
9	I	154	TYR	N-CA-CB	-8.66	99.24	111.62
13	M	248	ILE	N-CA-C	-8.62	102.15	110.42
14	N	255	PRO	N-CA-CB	-8.61	94.73	103.08
32	g	80	VAL	N-CA-C	-8.60	102.03	110.72
15	O	315	PRO	CA-N-CD	8.56	123.98	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	3	PHE	CA-CB-CG	8.55	122.36	113.80
19	S	18	GLU	N-CA-C	8.55	123.34	109.40
19	S	86	GLU	N-CA-C	-8.52	102.08	111.36
3	C	70	LYS	N-CA-C	8.50	121.62	111.33
14	N	109	ALA	CA-C-N	-8.50	110.68	120.12
14	N	109	ALA	C-N-CA	-8.50	110.68	120.12
2	B	100	CYS	N-CA-C	-8.48	102.69	113.72
12	L	212	PRO	N-CA-C	8.47	125.59	113.47
16	P	373	LYS	N-CA-C	8.47	121.87	110.35
20	U	74	LEU	N-CA-C	8.43	120.78	110.41
14	N	272	LYS	N-CA-C	-8.43	102.10	111.28
12	L	281	GLY	N-CA-C	-8.42	102.73	112.50
14	N	221	LEU	N-CA-C	-8.40	101.16	111.33
3	C	108	LYS	N-CA-C	8.40	120.06	111.07
12	L	287	PHE	N-CA-C	-8.36	102.13	111.07
23	X	99	HIS	N-CA-C	-8.36	102.25	111.36
7	G	532	PRO	CA-N-CD	8.35	123.69	112.00
17	Q	54	THR	N-CA-C	8.34	123.30	109.46
39	n	19	LEU	N-CA-C	-8.32	103.26	113.41
7	G	558	GLN	N-CA-C	-8.29	102.20	111.07
14	N	218	ALA	N-CA-C	-8.26	98.92	111.56
8	H	196	ALA	N-CA-C	8.25	128.04	109.81
12	L	151	SER	N-CA-C	-8.24	102.38	111.36
36	k	50	PRO	N-CA-CB	-8.23	93.54	102.76
13	M	274	SER	N-CA-C	8.21	120.23	111.28
3	C	196	PRO	N-CA-C	8.19	124.92	113.53
13	M	26	ASN	N-CA-C	-8.18	102.31	111.14
7	G	691	ILE	N-CA-C	8.17	123.66	111.89
7	G	484	ASP	N-CA-C	8.17	121.10	111.71
12	L	88	LEU	N-CA-C	-8.16	102.33	111.14
12	L	169	LEU	N-CA-C	-8.15	102.48	111.36
21	V	86	LYS	N-CA-C	-8.14	102.35	111.14
6	F	411	SER	N-CA-CB	8.12	121.78	110.01
14	N	32	GLY	N-CA-C	-8.09	103.12	112.50
7	G	534	VAL	N-CA-C	-8.09	104.71	111.91
29	d	15	PRO	N-CA-CB	-8.08	96.32	103.35
7	G	62	ARG	N-CA-C	8.07	121.56	108.32
9	I	201	ILE	N-CA-C	-8.07	102.57	110.72
39	n	170	ILE	N-CA-C	-8.05	103.04	111.58
36	k	38	VAL	N-CA-C	-8.05	102.59	110.72
30	e	91	LYS	CA-C-N	-8.03	109.04	122.29
30	e	91	LYS	C-N-CA	-8.03	109.04	122.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	500	ILE	N-CA-CB	8.01	120.82	110.57
13	M	385	LEU	N-CA-C	-8.00	102.56	111.28
12	L	276	THR	N-CA-CB	8.00	121.61	110.01
2	B	110	PRO	N-CA-C	7.99	124.44	113.65
13	M	141	GLU	N-CA-C	7.99	122.87	113.20
19	S	76	THR	N-CA-C	7.99	121.93	108.90
52	AH	52	ASP	N-CA-C	-7.98	102.66	111.36
45	Aa	360	CYS	N-CA-C	7.96	120.99	109.14
28	c	45	GLY	N-CA-C	7.95	123.66	113.24
8	H	271	LEU	N-CA-C	-7.94	102.56	111.14
42	q	67	GLU	CB-CA-C	-7.93	99.62	112.06
7	G	651	PRO	CB-CA-C	-7.92	98.49	111.56
21	V	6	LYS	N-CA-C	-7.89	100.11	110.53
1	A	9	ILE	N-CA-C	-7.88	102.58	110.62
13	M	205	ILE	N-CA-C	7.88	117.98	110.42
7	G	270	VAL	N-CA-CB	-7.86	100.65	110.31
12	L	265	PRO	N-CA-CB	7.84	111.70	103.15
13	M	330	ALA	N-CA-C	-7.83	102.69	111.14
38	m	50	GLN	N-CA-C	-7.83	102.74	114.64
12	L	415	ALA	N-CA-C	-7.82	102.76	111.28
9	I	74	LEU	N-CA-C	-7.80	102.78	111.28
12	L	111	ASP	N-CA-C	-7.79	100.27	109.93
9	I	160	GLU	N-CA-C	7.79	124.14	111.37
11	K	51	SER	N-CA-C	-7.79	102.86	113.30
12	L	265	PRO	CA-N-CD	-7.79	101.09	112.00
4	D	141	TYR	CA-C-N	7.76	130.19	120.72
4	D	141	TYR	C-N-CA	7.76	130.19	120.72
14	N	336	THR	N-CA-C	-7.76	103.33	114.12
13	M	85	LYS	N-CA-C	-7.71	101.53	113.02
42	q	44	TYR	N-CA-C	-7.69	98.89	110.28
42	q	89	TRP	N-CA-C	-7.69	102.83	111.14
12	L	265	PRO	N-CA-C	-7.68	101.33	113.78
52	Ah	68	GLU	N-CA-C	7.68	120.33	111.11
6	F	334	THR	N-CA-C	-7.68	101.65	111.02
18	R	47	ARG	N-CA-C	7.65	120.58	111.33
5	E	68	ASN	N-CA-CB	7.63	121.07	110.01
18	R	74	HIS	N-CA-C	7.60	121.22	110.50
7	G	569	GLN	N-CA-C	7.59	121.98	108.24
15	O	210	PRO	CA-N-CD	7.57	122.60	112.00
20	T	141	PRO	N-CA-C	-7.56	103.02	113.53
23	X	140	ASN	CA-C-N	-7.56	112.95	120.21
23	X	140	ASN	C-N-CA	-7.56	112.95	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	124	VAL	N-CA-C	-7.56	103.09	110.72
9	I	119	CYS	N-CA-C	-7.55	103.13	111.36
25	Z	73	PRO	N-CA-C	-7.54	103.05	113.53
2	B	183	ARG	N-CA-C	-7.54	104.32	113.97
8	H	223	PHE	CB-CA-C	-7.53	99.06	110.88
20	U	147	TYR	N-CA-C	-7.52	103.02	111.14
9	I	158	CYS	N-CA-C	-7.52	103.08	111.28
4	D	361	ALA	N-CA-C	-7.52	103.21	112.38
40	o	81	LYS	N-CA-C	-7.50	104.66	113.88
12	L	245	ALA	N-CA-C	7.49	119.09	111.07
46	AB	40	PHE	CA-C-O	7.49	128.63	121.67
30	e	46	GLY	N-CA-C	-7.48	104.94	114.37
6	F	295	PRO	CA-N-CD	7.48	122.47	112.00
12	L	138	PHE	N-CA-C	-7.47	103.13	111.28
11	K	14	LEU	N-CA-C	-7.45	103.23	111.36
35	j	82	GLY	N-CA-C	-7.45	103.47	112.48
7	G	277	MET	N-CA-C	7.45	120.54	109.59
6	F	125	CYS	N-CA-C	-7.44	103.77	112.92
6	F	430	GLY	N-CA-C	7.42	121.63	112.73
12	L	392	LYS	N-CA-C	7.41	119.00	111.07
12	L	605	ASN	N-CA-CB	7.40	121.20	110.47
4	D	350	LYS	CB-CA-C	-7.39	100.98	111.85
21	V	57	ASP	N-CA-CB	7.39	120.72	110.01
12	L	123	LEU	N-CA-C	-7.38	103.31	111.36
7	G	510	TRP	N-CA-CB	7.38	120.84	109.85
47	AC	202	GLU	N-CA-C	-7.38	103.26	111.82
13	M	250	LEU	N-CA-C	-7.37	103.58	112.58
12	L	21	ILE	N-CA-CB	7.37	121.64	110.58
37	l	97	LEU	N-CA-C	-7.36	103.90	113.17
18	R	39	ASP	N-CA-C	7.35	121.25	110.59
42	q	24	LEU	N-CA-C	-7.35	103.27	111.28
7	G	303	THR	N-CA-C	7.35	122.95	113.18
39	n	29	SER	N-CA-C	-7.33	104.85	114.31
47	Ac	202	GLU	N-CA-C	-7.33	103.32	111.82
20	T	105	MET	N-CA-C	7.33	119.34	111.36
19	S	94	VAL	N-CA-C	7.32	117.44	110.42
13	M	455	THR	N-CA-C	-7.31	100.40	110.35
3	C	195	HIS	CB-CA-C	7.29	117.38	110.17
12	L	28	LYS	N-CA-C	-7.29	103.34	111.28
49	AE	221	GLY	N-CA-C	7.27	126.85	113.76
49	Ae	221	GLY	N-CA-C	7.27	126.85	113.76
40	o	12	ASP	N-CA-C	7.27	121.33	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	72	ARG	N-CA-C	7.26	122.43	113.50
7	G	661	GLU	N-CA-C	7.25	118.88	110.97
21	V	68	LEU	N-CA-C	-7.25	103.37	111.28
7	G	374	THR	CB-CA-C	-7.25	99.82	111.28
12	L	19	ILE	N-CA-C	7.23	117.36	110.42
13	M	289	SER	N-CA-C	-7.23	103.33	111.07
47	AC	8	HIS	CA-C-N	7.23	126.93	119.56
47	AC	8	HIS	C-N-CA	7.23	126.93	119.56
7	G	384	ASN	N-CA-C	-7.22	103.44	111.82
39	n	30	TRP	N-CA-C	-7.21	104.11	113.12
11	K	81	VAL	N-CA-C	7.19	117.95	110.62
36	k	73	ILE	N-CA-C	-7.19	103.28	110.62
41	p	168	LYS	N-CA-C	-7.16	104.17	113.12
6	F	295	PRO	N-CA-CB	-7.14	96.77	103.19
8	H	50	ALA	N-CA-C	7.13	118.70	111.07
7	G	497	VAL	N-CA-C	-7.13	103.35	110.62
13	M	244	ILE	N-CA-C	7.13	117.89	110.62
12	L	554	ASP	N-CA-CB	7.13	121.25	110.42
13	M	34	ILE	N-CA-C	-7.13	103.35	110.62
8	H	176	LEU	CA-C-N	-7.12	113.47	120.52
8	H	176	LEU	C-N-CA	-7.12	113.47	120.52
4	D	99	LEU	N-CA-C	7.11	121.11	109.24
6	F	269	ARG	N-CA-C	7.09	118.66	111.07
21	V	95	LEU	N-CA-C	-7.08	103.56	111.28
17	Q	162	ALA	N-CA-C	7.08	119.00	111.28
35	j	65	MET	N-CA-C	-7.06	103.51	111.07
23	X	153	VAL	N-CA-C	7.06	118.03	107.80
47	AC	17	SER	N-CA-C	7.04	122.03	113.38
39	n	102	TRP	N-CA-C	-7.03	105.05	112.93
44	s	56	ARG	N-CA-C	7.03	120.65	108.76
11	K	48	SER	N-CA-C	-7.03	103.62	111.28
13	M	325	LEU	N-CA-C	-7.03	103.55	111.07
12	L	319	MET	N-CA-C	-7.02	104.71	112.72
49	Ae	218	THR	N-CA-C	-7.02	102.76	111.75
42	q	77	VAL	N-CA-C	-7.01	99.67	109.21
7	G	217	GLU	N-CA-C	-7.01	101.79	110.41
13	M	365	ALA	N-CA-C	-7.01	103.72	111.36
2	B	166	ASN	N-CA-C	-7.01	103.33	110.97
6	F	246	GLU	N-CA-C	-7.01	103.64	111.28
7	G	150	ARG	N-CA-C	7.00	119.57	109.14
13	M	213	HIS	CB-CA-C	-6.98	96.84	110.11
6	F	455	GLN	N-CA-C	6.98	118.54	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	471	ASN	N-CA-C	6.98	118.97	111.36
14	N	132	THR	N-CA-C	6.96	122.89	113.97
12	L	100	ILE	N-CA-C	6.96	119.75	111.05
10	J	125	MET	N-CA-C	-6.95	101.80	111.39
49	AE	218	THR	N-CA-C	-6.95	102.85	111.75
13	M	264	LEU	N-CA-C	-6.95	103.64	111.07
6	F	418	GLN	N-CA-CB	6.95	120.14	110.07
6	F	428	GLY	N-CA-C	-6.94	103.88	112.77
34	i	9	LYS	N-CA-C	-6.94	104.80	112.72
45	AA	368	MET	N-CA-C	-6.94	102.78	111.11
7	G	582	VAL	N-CA-C	6.94	118.47	108.48
12	L	546	LEU	N-CA-C	6.94	119.49	111.02
25	Z	34	SER	N-CA-C	-6.94	103.65	111.07
6	F	103	ASN	N-CA-CB	6.94	121.08	110.61
20	T	145	VAL	N-CA-C	-6.93	103.72	110.72
13	M	91	LEU	N-CA-C	-6.92	103.84	112.90
7	G	294	TYR	N-CA-C	-6.91	104.66	113.23
12	L	86	SER	N-CA-C	6.90	118.46	111.07
18	R	45	ARG	N-CA-C	-6.90	104.73	113.01
13	M	235	LEU	N-CA-C	6.90	119.39	111.11
34	i	11	ARG	N-CA-C	-6.88	104.89	113.28
36	k	59	TYR	N-CA-CB	-6.87	98.86	110.41
12	L	26	LEU	N-CA-C	6.87	119.61	111.71
7	G	300	GLN	N-CA-CB	6.86	122.44	112.08
52	Ah	52	ASP	N-CA-C	-6.86	103.73	111.07
46	AB	41	THR	N-CA-C	-6.86	100.29	110.23
13	M	276	CYS	N-CA-CB	6.85	120.19	110.12
39	n	117	ASP	N-CA-C	-6.84	103.88	111.82
13	M	442	ILE	N-CA-C	-6.84	104.14	112.35
11	K	83	ASN	N-CA-CB	6.84	120.93	110.81
6	F	329	LYS	N-CA-C	6.84	119.60	111.33
38	m	127	ILE	N-CA-C	-6.83	106.14	112.43
25	Z	28	ARG	N-CA-C	6.83	119.65	108.52
12	L	547	LYS	N-CA-C	6.82	118.72	111.28
18	R	56	ASN	N-CA-C	6.81	120.00	108.90
32	g	78	PRO	CA-N-CD	6.80	121.52	112.00
7	G	133	GLN	N-CA-C	-6.79	101.24	110.68
7	G	268	GLY	N-CA-C	6.78	124.73	115.30
13	M	165	ILE	N-CA-C	-6.77	102.62	111.09
11	K	70	GLU	N-CA-CB	6.77	120.02	109.94
13	M	248	ILE	N-CA-CB	6.75	118.45	110.55
7	G	434	SER	N-CA-C	-6.75	100.97	110.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	374	ASN	N-CA-C	-6.75	103.85	111.07
8	H	8	THR	N-CA-C	-6.75	101.18	110.35
52	AH	81	ALA	N-CA-C	6.74	119.20	111.11
15	O	93	TYR	N-CA-C	-6.74	104.01	111.36
6	F	244	ASN	N-CA-C	-6.74	101.00	110.50
21	V	114	TRP	N-CA-CB	6.74	120.34	110.30
5	E	140	MET	N-CA-C	-6.73	103.87	111.07
37	l	86	ARG	N-CA-C	-6.71	99.59	110.20
12	L	95	PHE	N-CA-C	-6.70	103.90	111.07
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
21	V	8	THR	N-CA-C	6.70	119.03	108.79
43	r	11	LEU	N-CA-C	-6.69	104.07	111.36
16	P	371	PRO	CA-N-CD	-6.69	102.64	112.00
20	U	140	CYS	CA-C-N	-6.69	114.01	120.83
20	U	140	CYS	C-N-CA	-6.69	114.01	120.83
11	K	76	ALA	N-CA-C	-6.67	104.09	111.36
12	L	499	LEU	N-CA-C	-6.67	103.70	110.97
13	M	410	MET	N-CA-C	-6.67	103.93	111.07
15	O	315	PRO	N-CA-CB	-6.67	95.99	103.33
35	j	53	SER	N-CA-C	6.67	119.40	111.33
10	J	132	GLY	N-CA-C	-6.66	100.98	110.91
6	F	344	GLN	N-CA-C	-6.66	103.95	111.07
23	X	129	THR	N-CA-C	6.66	120.89	110.17
15	O	175	ASN	N-CA-C	-6.65	104.10	111.82
20	U	150	ASP	CB-CA-C	6.65	121.83	110.79
34	i	8	GLU	N-CA-C	-6.64	104.76	114.39
13	M	143	LEU	N-CA-C	-6.63	103.97	111.07
6	F	196	PHE	N-CA-C	6.63	119.95	109.81
7	G	640	ASP	N-CA-CB	6.63	119.97	110.16
32	g	76	SER	N-CA-C	6.63	118.16	111.07
3	C	69	PRO	N-CA-C	-6.63	104.32	113.53
36	k	49	ASP	CA-C-N	-6.63	113.38	120.47
36	k	49	ASP	C-N-CA	-6.63	113.38	120.47
7	G	287	SER	N-CA-C	6.62	119.27	110.53
14	N	228	ASN	N-CA-CB	6.62	119.61	110.01
4	D	184	ILE	N-CA-C	-6.62	103.87	110.62
21	V	86	LYS	N-CA-CB	6.62	119.67	110.07
39	n	115	TYR	N-CA-CB	6.62	122.15	110.37
7	G	601	GLY	N-CA-C	6.62	124.83	115.30
13	M	161	LEU	N-CA-C	-6.61	103.99	111.07
20	U	102	SER	N-CA-C	6.61	119.62	107.99
16	P	116	ILE	N-CA-C	-6.61	104.05	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AD	142	GLU	N-CA-C	6.60	119.03	111.11
6	F	228	PRO	N-CA-C	-6.60	98.87	112.47
13	M	303	ILE	N-CA-C	-6.60	104.06	110.72
8	H	208	VAL	N-CA-CB	-6.60	104.14	111.66
3	C	125	PHE	N-CA-CB	-6.59	100.68	110.17
15	O	140	LEU	N-CA-C	-6.59	104.02	111.07
5	E	44	PRO	CA-N-CD	6.58	121.21	112.00
7	G	435	PRO	N-CA-C	-6.58	100.18	110.50
17	Q	141	ASN	N-CA-CB	6.57	120.77	110.46
6	F	336	LEU	N-CA-CB	-6.56	101.00	111.43
8	H	182	ALA	N-CA-C	-6.55	104.06	111.07
20	T	141	PRO	N-CA-CB	6.55	110.53	103.33
38	m	51	TYR	N-CA-C	-6.54	105.60	113.97
8	H	267	SER	N-CA-C	-6.54	104.23	111.36
12	L	130	ILE	N-CA-C	-6.53	103.96	110.62
4	D	388	GLY	N-CA-C	6.53	119.65	110.38
8	H	223	PHE	N-CA-C	-6.53	104.09	111.07
12	L	329	ILE	N-CA-C	-6.52	104.16	110.42
19	S	16	LEU	N-CA-C	-6.51	98.28	108.90
15	O	114	LEU	N-CA-C	-6.51	104.26	111.36
43	r	24	LEU	N-CA-C	6.51	119.68	110.50
15	O	118	TYR	N-CA-CB	-6.51	100.58	110.01
23	X	98	ARG	N-CA-C	6.50	120.47	112.54
12	L	232	TRP	N-CA-C	6.50	120.47	112.54
12	L	423	SER	N-CA-C	-6.50	104.12	111.07
25	Z	65	LEU	N-CA-C	-6.49	104.29	111.36
36	k	57	TRP	N-CA-C	-6.48	104.63	112.54
36	k	46	GLY	N-CA-C	-6.48	106.98	114.69
42	q	75	TRP	N-CA-C	6.48	121.45	112.45
7	G	361	VAL	N-CA-C	-6.47	105.02	111.88
41	p	54	ARG	N-CA-C	-6.47	103.73	111.69
7	G	605	GLN	N-CA-C	6.47	119.06	108.52
14	N	315	THR	N-CA-C	-6.46	104.16	111.07
15	O	320	GLY	N-CA-C	-6.46	96.57	111.04
20	T	141	PRO	CA-N-CD	-6.45	102.97	112.00
24	Y	96	GLY	N-CA-C	-6.45	104.51	112.77
11	K	11	ALA	N-CA-C	-6.45	104.17	111.07
7	G	250	SER	N-CA-C	6.44	116.78	108.34
7	G	275	PRO	CB-CA-C	-6.44	102.54	110.98
3	C	125	PHE	N-CA-C	6.44	119.58	110.50
45	AA	215	ASP	N-CA-C	-6.44	103.95	110.97
18	R	81	GLY	N-CA-C	-6.44	106.84	115.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	49	GLU	N-CA-C	-6.44	104.26	111.28
6	F	78	GLY	N-CA-C	-6.43	104.54	112.77
4	D	140	ASP	N-CA-C	-6.43	96.50	107.23
45	Aa	215	ASP	N-CA-C	-6.42	103.97	110.97
28	c	72	ARG	N-CA-C	-6.42	104.20	111.07
13	M	32	PHE	N-CA-C	-6.41	104.21	111.07
8	H	177	PRO	N-CA-C	-6.41	101.58	111.13
36	k	42	LEU	N-CA-C	-6.41	103.55	111.75
7	G	275	PRO	CA-N-CD	6.40	120.97	112.00
12	L	325	ALA	N-CA-C	-6.40	104.30	111.28
6	F	370	LEU	N-CA-C	-6.39	104.39	111.36
42	q	28	PHE	N-CA-C	6.39	117.91	111.07
12	L	439	PRO	N-CA-C	6.39	122.41	113.53
32	g	112	MET	N-CA-C	6.38	120.85	113.38
12	L	70	THR	N-CA-C	-6.38	103.85	111.69
29	d	15	PRO	CA-N-CD	6.37	120.92	112.00
13	M	317	ILE	N-CA-C	-6.37	104.55	110.53
7	G	273	ILE	N-CA-C	-6.36	98.36	107.77
37	l	119	THR	N-CA-C	-6.36	98.17	108.41
9	I	205	ILE	N-CA-C	-6.35	104.31	110.72
7	G	95	PRO	N-CA-C	-6.35	101.21	110.80
17	Q	59	LEU	N-CA-C	-6.34	100.79	110.30
5	E	141	LEU	N-CA-C	-6.33	101.74	110.35
43	r	8	ILE	N-CA-C	-6.33	104.33	110.72
8	H	271	LEU	N-CA-CB	6.33	119.24	110.07
6	F	416	SER	N-CA-C	6.32	117.84	111.07
15	O	98	THR	N-CA-C	6.32	120.58	109.96
21	V	71	LEU	N-CA-C	6.31	118.16	111.28
12	L	234	PRO	CA-N-CD	-6.31	103.17	112.00
32	g	123	LEU	N-CA-CB	6.31	119.15	110.01
12	L	387	THR	N-CA-C	6.30	118.96	111.71
34	i	32	GLU	CA-C-N	-6.30	111.97	119.84
34	i	32	GLU	C-N-CA	-6.30	111.97	119.84
21	V	91	ALA	N-CA-C	-6.29	104.42	111.28
16	P	315	THR	N-CA-C	6.29	118.98	109.23
12	L	337	ALA	N-CA-C	-6.29	104.42	111.28
6	F	415	ILE	N-CA-C	-6.29	104.37	110.72
4	D	73	LYS	N-CA-C	6.28	118.50	109.14
23	X	99	HIS	N-CA-CB	6.28	119.46	110.16
12	L	490	ALA	N-CA-C	-6.28	104.36	111.07
26	a	26	ILE	N-CA-C	-6.27	104.54	113.07
14	N	89	GLN	N-CA-C	6.27	120.49	112.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	176	CYS	N-CA-C	6.27	119.57	110.42
37	I	105	ILE	CA-C-O	-6.26	115.14	121.59
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
6	F	409	ILE	N-CA-C	6.26	116.43	110.42
5	E	64	ALA	N-CA-CB	6.25	119.26	109.94
4	D	141	TYR	N-CA-C	6.25	120.91	113.16
15	O	113	SER	N-CA-C	6.25	118.60	108.41
52	AH	88	LEU	N-CA-CB	6.25	121.12	110.50
13	M	26	ASN	N-CA-CB	6.24	119.11	110.07
8	H	101	GLY	N-CA-C	6.24	120.19	112.64
28	c	47	SER	N-CA-CB	6.24	120.80	110.33
4	D	233	HIS	N-CA-C	6.23	119.00	111.40
35	j	78	ASP	N-CA-C	-6.23	102.82	110.61
14	N	91	ASN	N-CA-CB	6.23	119.12	109.97
43	r	26	LEU	N-CA-CB	-6.22	101.08	110.35
14	N	337	LEU	CA-C-N	-6.22	113.72	119.82
14	N	337	LEU	C-N-CA	-6.22	113.72	119.82
36	k	59	TYR	N-CA-C	6.22	120.70	113.18
2	B	113	ASP	N-CA-CB	6.21	119.47	109.28
8	H	52	ALA	N-CA-CB	6.21	119.01	110.01
17	Q	141	ASN	N-CA-C	-6.20	105.72	113.28
42	q	69	ASN	N-CA-CB	6.19	121.32	111.66
48	AD	144	GLU	N-CA-CB	6.19	118.98	110.01
14	N	276	LEU	N-CA-C	-6.19	105.38	113.17
39	n	63	LEU	N-CA-C	-6.18	104.09	111.69
8	H	269	THR	N-CA-C	6.18	118.02	111.28
40	o	110	GLN	N-CA-C	-6.18	104.62	111.36
25	Z	69	ILE	N-CA-CB	6.17	117.36	110.51
4	D	291	VAL	N-CA-C	-6.17	103.38	111.09
6	F	212	LEU	N-CA-C	-6.16	104.56	111.28
8	H	276	SER	N-CA-C	6.16	118.97	111.82
16	P	368	GLU	N-CA-CB	6.16	119.79	110.30
13	M	121	LEU	N-CA-C	-6.16	104.65	111.36
41	p	127	LYS	N-CA-C	-6.15	104.12	111.69
16	P	118	LYS	N-CA-C	6.14	118.95	111.82
12	L	98	TRP	N-CA-C	-6.14	104.67	111.36
14	N	47	LYS	N-CA-C	-6.14	104.70	111.82
7	G	418	ILE	N-CA-C	-6.14	103.45	112.04
12	L	361	ASN	CB-CA-C	-6.13	102.84	111.80
7	G	420	LYS	N-CA-C	6.13	118.75	111.33
32	g	109	ASP	CA-CB-CG	6.13	118.73	112.60
14	N	216	PHE	N-CA-C	6.12	118.04	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	46	ASN	N-CA-C	-6.12	105.84	113.55
6	F	272	GLY	N-CA-C	6.12	122.39	111.01
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
36	k	30	ILE	N-CA-C	6.10	118.72	111.09
33	h	142	ILE	N-CA-C	-6.10	104.56	110.42
13	M	4	ILE	N-CA-C	-6.09	104.04	112.50
13	M	3	LYS	N-CA-C	-6.09	105.98	113.41
19	S	87	VAL	N-CA-C	-6.08	104.42	110.62
12	L	287	PHE	N-CA-CB	6.08	118.82	110.01
19	S	61	VAL	N-CA-C	-6.08	99.73	108.42
25	Z	65	LEU	N-CA-CB	6.08	119.15	110.16
28	c	47	SER	N-CA-C	-6.07	104.60	112.68
12	L	140	LEU	N-CA-C	-6.07	104.67	111.28
13	M	57	SER	N-CA-C	6.06	119.08	109.50
14	N	91	ASN	N-CA-C	-6.06	101.31	110.28
33	h	101	ILE	N-CA-CB	6.06	115.72	110.08
10	J	135	LEU	N-CA-C	6.05	118.39	108.52
51	AG	31	PHE	N-CA-C	-6.05	105.93	113.38
52	AH	83	LYS	N-CA-CB	6.05	121.19	111.20
8	H	185	TRP	N-CA-C	-6.05	104.04	112.45
32	g	123	LEU	N-CA-C	-6.05	104.60	111.07
38	m	72	ARG	CA-C-O	6.05	125.79	119.14
8	H	24	GLU	N-CA-C	-6.04	104.05	112.45
7	G	638	THR	N-CA-C	-6.04	100.12	109.24
16	P	370	LYS	N-CA-C	6.04	119.29	108.47
15	O	160	GLU	CB-CA-C	-6.04	109.59	116.54
38	m	52	ASN	N-CA-C	-6.04	105.22	112.59
50	AF	95	LEU	N-CA-C	-6.04	104.61	111.07
7	G	508	ALA	N-CA-C	6.04	117.86	111.28
15	O	234	LEU	N-CA-C	-6.03	104.79	111.36
13	M	213	HIS	N-CA-C	6.02	120.48	113.20
9	I	66	LEU	N-CA-C	-6.02	104.29	111.69
7	G	353	ALA	N-CA-C	-6.01	104.65	112.23
7	G	532	PRO	N-CA-CB	-6.01	97.06	103.38
13	M	370	PRO	CA-N-CD	6.01	120.42	112.00
12	L	454	ILE	N-CA-C	-6.01	104.49	110.62
38	m	22	GLU	N-CA-C	-6.00	104.65	111.07
41	p	8	ASP	N-CA-C	6.00	120.67	113.23
51	Ag	31	PHE	N-CA-C	-6.00	106.00	113.38
13	M	396	MET	N-CA-C	-5.98	105.96	113.20
43	r	108	LYS	N-CA-C	5.98	117.88	111.36
2	B	196	PRO	N-CA-C	-5.98	101.82	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	AB	244	LEU	N-CA-C	-5.97	105.99	113.28
8	H	7	LEU	N-CA-C	-5.97	104.40	111.03
14	N	295	ARG	N-CA-C	-5.97	104.78	111.28
4	D	72	LEU	N-CA-C	5.96	117.38	108.31
32	g	78	PRO	N-CA-C	5.96	121.82	113.53
13	M	88	ASN	N-CA-C	5.96	120.17	113.02
15	O	183	CYS	N-CA-CB	5.96	118.81	109.94
5	E	66	VAL	N-CA-C	5.95	116.61	110.36
12	L	247	LEU	N-CA-CB	5.95	120.69	110.34
12	L	112	PRO	CB-CA-C	-5.94	103.01	111.68
39	n	27	LEU	N-CA-C	-5.94	106.00	113.72
12	L	88	LEU	N-CA-CB	5.93	118.67	110.07
13	M	300	SER	N-CA-C	-5.92	107.04	114.56
36	k	82	ALA	N-CA-C	-5.92	104.83	111.28
7	G	480	ALA	N-CA-C	-5.92	104.91	111.36
12	L	278	LEU	N-CA-CB	5.91	118.64	110.07
13	M	222	GLU	N-CA-C	5.91	120.33	113.18
54	AK	38	TRP	N-CA-C	-5.91	101.44	110.30
4	D	352	PRO	N-CA-CB	-5.91	97.35	103.08
18	R	34	THR	N-CA-C	-5.90	106.72	112.97
14	N	16	GLY	CA-C-N	-5.89	112.43	118.85
14	N	16	GLY	C-N-CA	-5.89	112.43	118.85
43	r	92	LYS	N-CA-CB	-5.89	101.69	110.17
13	M	253	LEU	N-CA-C	5.89	117.70	111.28
15	O	181	LYS	N-CA-C	5.88	117.36	111.07
52	Ah	52	ASP	N-CA-CB	5.88	118.54	110.01
12	L	387	THR	CB-CA-C	-5.88	99.76	110.63
15	O	205	ILE	O-C-N	5.87	129.04	122.75
51	Ag	6	GLY	N-CA-C	-5.87	105.37	112.48
20	U	75	THR	N-CA-CB	5.87	121.77	111.55
15	O	130	ARG	N-CA-C	-5.87	104.88	111.28
15	O	262	GLU	N-CA-C	-5.87	104.89	111.28
9	I	116	CYS	N-CA-C	-5.86	105.62	112.89
20	U	143	GLU	N-CA-C	-5.86	104.25	111.75
36	k	80	GLY	N-CA-C	-5.86	105.70	112.50
12	L	248	HIS	CB-CA-C	5.86	120.81	110.85
42	q	5	GLU	N-CA-C	-5.86	104.98	111.36
3	C	209	LEU	N-CA-CB	-5.85	100.64	110.83
7	G	639	LEU	N-CA-C	5.85	118.61	111.82
16	P	122	HIS	N-CA-C	5.85	120.12	112.92
8	H	208	VAL	N-CA-C	5.85	116.10	107.15
12	L	234	PRO	N-CA-CB	5.85	109.49	103.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	94	ASP	N-CA-CB	-5.85	105.17	111.66
42	q	65	THR	N-CA-C	5.85	119.21	110.14
14	N	15	LEU	N-CA-C	-5.85	105.64	112.89
7	G	672	ALA	N-CA-C	-5.84	104.91	111.28
19	S	86	GLU	N-CA-CB	5.84	118.81	110.16
34	i	10	LEU	N-CA-C	-5.84	107.15	114.56
16	P	330	THR	CB-CA-C	-5.84	109.83	116.54
34	i	105	PHE	CA-C-N	-5.83	113.69	119.99
34	i	105	PHE	C-N-CA	-5.83	113.69	119.99
30	e	91	LYS	O-C-N	5.83	129.44	122.27
5	E	223	CYS	CB-CA-C	-5.83	109.31	117.23
29	d	53	VAL	N-CA-C	5.82	116.47	110.36
16	P	367	GLU	CB-CA-C	-5.82	99.50	110.67
48	Ad	159	ASN	CB-CA-C	-5.82	109.85	116.54
21	V	19	THR	N-CA-CB	5.81	120.72	110.37
17	Q	164	PHE	N-CA-CB	5.81	119.83	110.42
13	M	272	THR	N-CA-C	-5.80	105.03	111.36
38	m	116	ILE	N-CA-C	-5.80	104.85	110.42
13	M	424	ILE	O-C-N	5.80	128.41	122.79
23	X	36	CYS	CB-CA-C	-5.80	102.53	111.74
20	U	101	ASN	N-CA-C	-5.79	106.07	113.02
4	D	414	ASP	N-CA-C	-5.79	101.39	110.36
35	j	73	PHE	N-CA-C	-5.79	104.88	111.07
12	L	428	TYR	N-CA-C	-5.78	104.89	111.14
14	N	321	LYS	N-CA-C	5.78	118.53	110.20
39	n	52	LYS	N-CA-C	-5.78	105.90	113.12
25	Z	44	ILE	N-CA-C	-5.78	104.87	110.42
26	a	3	PHE	N-CA-CB	5.78	118.73	110.06
7	G	275	PRO	N-CA-CB	-5.77	97.96	103.33
52	Ah	62	GLU	N-CA-C	-5.77	106.14	112.72
6	F	393	ASN	N-CA-C	-5.76	104.90	111.07
29	d	62	LEU	N-CA-C	5.76	117.56	111.28
32	g	78	PRO	N-CA-CB	-5.75	97.00	103.33
23	X	97	PHE	N-CA-C	5.73	118.47	111.82
12	L	419	THR	N-CA-C	-5.73	105.03	111.28
52	AH	87	ASN	N-CA-C	5.73	118.46	111.82
12	L	467	VAL	N-CA-CB	-5.72	103.85	110.55
13	M	124	ALA	N-CA-C	-5.72	105.13	111.36
7	G	289	LYS	N-CA-C	5.71	117.51	111.28
13	M	279	GLN	N-CA-C	-5.71	98.58	108.69
16	P	272	LEU	N-CA-C	-5.71	101.83	110.28
12	L	342	CYS	N-CA-CB	5.71	118.29	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	66	ALA	N-CA-C	-5.71	105.14	111.36
12	L	495	VAL	N-CA-C	5.71	115.90	110.42
18	R	35	GLY	N-CA-C	5.70	121.81	113.48
12	L	177	ILE	N-CA-C	-5.70	104.81	110.62
19	S	73	GLN	N-CA-C	-5.70	100.42	109.59
12	L	605	ASN	N-CA-C	-5.69	106.19	113.02
40	o	71	ARG	N-CA-C	-5.69	104.46	111.40
47	AC	17	SER	N-CA-CB	-5.69	102.05	110.53
12	L	214	MET	N-CA-C	-5.69	105.16	111.36
5	E	137	THR	CA-C-N	-5.68	113.06	118.97
5	E	137	THR	C-N-CA	-5.68	113.06	118.97
32	g	67	LYS	N-CA-C	-5.68	102.05	110.46
42	q	140	PRO	N-CA-C	-5.67	102.23	110.80
12	L	371	SER	N-CA-C	-5.67	105.01	111.14
6	F	457	HIS	N-CA-CB	-5.67	100.86	110.50
18	R	52	GLN	N-CA-C	5.67	118.01	110.53
13	M	214	LEU	N-CA-C	-5.66	105.64	112.54
14	N	232	LEU	N-CA-C	-5.66	106.60	112.93
12	L	20	LEU	N-CA-C	5.65	119.89	112.89
4	D	352	PRO	N-CA-C	5.65	117.59	110.70
34	i	14	GLN	N-CA-CB	-5.65	101.82	110.12
37	l	49	ALA	N-CA-C	-5.65	106.55	113.50
52	AH	52	ASP	N-CA-CB	5.65	118.52	110.16
19	S	63	PRO	CA-N-CD	5.64	119.90	112.00
38	m	104	VAL	N-CA-C	-5.64	105.60	111.58
38	m	31	ARG	N-CA-C	-5.64	106.53	113.41
45	AA	338	CYS	CA-CB-SG	-5.64	101.44	114.40
2	B	135	GLY	N-CA-C	5.63	118.61	111.85
2	B	112	TYR	N-CA-C	5.63	122.80	110.80
2	B	201	LEU	N-CA-C	-5.63	105.14	111.28
13	M	19	SER	N-CA-C	5.62	117.65	109.84
16	P	119	ALA	N-CA-C	-5.62	105.07	111.14
41	p	115	GLN	N-CA-CB	5.62	118.06	110.59
7	G	599	THR	CA-C-N	-5.61	114.19	122.83
7	G	599	THR	C-N-CA	-5.61	114.19	122.83
12	L	151	SER	N-CA-CB	5.61	118.46	110.16
5	E	183	PRO	N-CA-C	-5.61	102.12	111.26
17	Q	124	MET	CA-C-N	-5.61	115.02	122.98
17	Q	124	MET	C-N-CA	-5.61	115.02	122.98
9	I	191	LEU	N-CA-C	-5.60	105.25	111.36
15	O	220	LYS	N-CA-C	5.60	117.39	111.28
4	D	72	LEU	CB-CA-C	-5.60	110.10	116.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	268	GLU	CB-CA-C	-5.59	110.11	116.54
32	g	140	PHE	N-CA-CB	5.59	118.32	109.71
12	L	445	GLU	CB-CA-C	-5.59	101.96	111.02
25	Z	64	ASP	N-CA-C	5.59	119.82	112.89
12	L	155	ILE	N-CA-C	-5.59	105.28	110.53
32	g	107	VAL	N-CA-C	-5.59	102.87	108.96
42	q	68	MET	N-CA-C	5.58	119.35	112.54
5	E	119	THR	N-CA-C	-5.58	105.97	112.89
7	G	530	TYR	N-CA-C	-5.58	102.02	110.28
34	i	74	HIS	CA-C-N	-5.58	115.76	122.35
34	i	74	HIS	C-N-CA	-5.58	115.76	122.35
38	m	60	ILE	N-CA-C	-5.58	101.99	109.30
7	G	615	LEU	N-CA-C	-5.58	106.24	113.16
35	j	80	VAL	CB-CA-C	-5.57	106.15	111.44
29	d	5	ARG	CA-C-N	-5.57	114.22	119.90
29	d	5	ARG	C-N-CA	-5.57	114.22	119.90
34	i	84	TYR	N-CA-C	-5.56	105.22	111.28
14	N	251	LEU	N-CA-C	-5.54	105.24	111.28
24	Y	13	GLU	N-CA-C	5.54	117.76	111.11
26	a	25	TYR	N-CA-C	-5.54	107.77	114.75
12	L	152	PHE	N-CA-C	-5.54	105.14	111.07
38	m	46	GLU	N-CA-C	-5.54	106.52	113.72
41	p	120	ASN	N-CA-C	-5.53	105.15	113.89
12	L	234	PRO	N-CA-C	-5.53	105.56	113.47
28	c	64	GLU	N-CA-CB	5.52	118.02	110.01
43	r	94	ALA	N-CA-C	-5.52	101.68	109.96
7	G	127	ASP	CA-C-O	5.52	129.01	121.89
32	g	113	GLN	CA-C-O	5.51	126.17	119.11
42	q	142	THR	N-CA-CB	5.51	119.77	109.68
18	R	89	PRO	N-CA-CB	-5.51	98.31	103.27
12	L	370	SER	N-CA-C	-5.51	105.36	111.36
40	o	74	PHE	CA-C-N	-5.51	113.94	119.56
40	o	74	PHE	C-N-CA	-5.51	113.94	119.56
16	P	86	CYS	N-CA-C	-5.50	103.12	110.55
13	M	370	PRO	N-CA-CB	-5.50	97.75	103.08
12	L	394	LEU	N-CA-CB	5.49	117.97	110.01
14	N	36	SER	N-CA-C	-5.49	105.29	111.28
42	q	71	LYS	N-CA-C	5.49	119.97	113.16
4	D	132	ALA	N-CA-C	-5.48	106.59	113.72
4	D	163	PRO	N-CA-CB	-5.48	97.76	103.08
13	M	223	ALA	N-CA-CB	5.48	118.11	110.11
13	M	355	MET	N-CA-C	-5.48	104.70	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	465	GLY	N-CA-C	-5.47	105.77	112.77
13	M	73	LEU	N-CA-C	-5.47	105.31	112.75
20	T	135	ALA	N-CA-CB	5.47	118.16	110.12
39	n	136	GLU	CB-CA-C	5.47	121.30	110.42
4	D	231	GLY	N-CA-C	-5.46	103.05	110.43
12	L	194	ASN	CB-CA-C	-5.46	103.36	111.72
13	M	174	LEU	N-CA-C	-5.46	106.40	112.57
28	c	31	VAL	N-CA-C	-5.46	105.01	110.30
7	G	682	ASP	CA-C-N	-5.45	114.15	119.76
7	G	682	ASP	C-N-CA	-5.45	114.15	119.76
7	G	404	GLY	N-CA-C	5.44	121.42	113.48
34	i	77	ILE	CB-CA-C	-5.44	108.58	114.35
15	O	154	GLY	N-CA-C	-5.44	107.52	114.37
32	g	137	SER	N-CA-CB	-5.44	101.28	110.41
46	AB	236	GLN	N-CA-C	-5.44	105.91	112.54
48	AD	163	GLU	N-CA-C	5.44	118.13	109.81
12	L	413	LEU	N-CA-C	5.43	117.20	111.28
4	D	200	PHE	CA-CB-CG	5.43	119.23	113.80
35	j	64	LEU	N-CA-C	-5.43	105.44	111.36
43	r	111	PRO	N-CA-C	-5.42	106.46	113.57
7	G	420	LYS	N-CA-CB	-5.41	101.94	110.06
41	p	94	ARG	N-CA-C	5.41	116.86	111.07
7	G	150	ARG	N-CA-CB	-5.41	102.86	111.62
25	Z	55	GLN	N-CA-C	-5.41	105.39	111.28
33	h	173	THR	O-C-N	5.41	125.77	121.55
14	N	108	LEU	N-CA-C	5.41	118.05	109.24
13	M	234	ILE	N-CA-C	5.40	116.28	111.90
14	N	89	GLN	N-CA-CB	-5.40	100.46	110.18
6	F	180	GLY	N-CA-C	-5.40	108.19	115.21
12	L	21	ILE	N-CA-C	-5.40	105.27	110.72
23	X	27	ALA	N-CA-C	-5.40	105.05	111.69
14	N	62	THR	N-CA-C	-5.39	105.30	111.07
16	P	374	THR	N-CA-C	5.39	117.52	108.73
7	G	556	THR	N-CA-C	-5.39	101.57	109.81
46	AB	40	PHE	CB-CA-C	-5.38	103.78	112.07
4	D	201	PHE	N-CA-C	-5.37	105.50	111.36
45	AA	399	LEU	N-CA-C	-5.37	106.42	112.87
6	F	199	ARG	N-CA-C	5.37	117.49	109.59
2	B	101	ALA	N-CA-C	-5.37	105.43	111.28
18	R	88	HIS	CB-CA-C	5.37	117.29	109.08
25	Z	50	MET	N-CA-C	-5.37	105.43	111.28
12	L	386	LEU	N-CA-C	-5.36	100.97	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	494	SER	N-CA-C	-5.36	105.35	111.14
4	D	141	TYR	N-CA-CB	-5.36	102.24	110.44
12	L	543	ASN	N-CA-C	-5.36	105.44	111.28
5	E	74	GLN	N-CA-C	-5.35	107.40	114.04
13	M	53	SER	N-CA-C	5.35	115.60	108.38
36	k	48	ARG	N-CA-C	-5.35	98.85	108.48
13	M	117	MET	N-CA-CB	5.35	117.98	110.12
17	Q	163	ASN	CB-CA-C	-5.34	99.32	109.95
12	L	550	LEU	CA-C-O	-5.34	115.28	120.89
23	X	145	ARG	CB-CA-C	-5.34	110.44	116.63
7	G	510	TRP	N-CA-C	-5.34	101.95	109.96
4	D	109	CYS	N-CA-C	5.34	118.42	107.69
20	U	141	PRO	N-CA-C	-5.34	109.13	114.68
12	L	311	GLY	N-CA-C	-5.33	106.33	112.73
48	Ad	227	LEU	N-CA-CB	-5.33	102.11	110.69
14	N	218	ALA	N-CA-CB	5.33	118.45	110.14
20	T	92	LYS	N-CA-C	-5.33	106.37	112.92
17	Q	164	PHE	N-CA-C	-5.32	106.77	113.20
21	V	84	ALA	N-CA-C	5.31	116.75	111.07
52	AH	82	HIS	CA-C-O	5.31	125.95	119.05
13	M	343	ILE	N-CA-C	5.30	116.03	110.62
5	E	44	PRO	N-CA-CB	-5.30	97.66	103.39
13	M	409	TYR	N-CA-C	-5.30	105.67	111.82
39	n	104	LEU	N-CA-C	-5.30	106.84	113.15
12	L	231	PRO	CB-CA-C	-5.30	104.33	111.85
13	M	25	THR	CB-CA-C	-5.30	100.50	110.67
48	AD	227	LEU	N-CA-CB	-5.30	102.16	110.69
5	E	143	ASP	N-CA-C	5.29	118.93	111.52
13	M	167	ILE	N-CA-C	5.29	117.67	111.05
9	I	160	GLU	N-CA-CB	-5.29	100.73	109.72
12	L	415	ALA	N-CA-CB	5.28	117.89	110.12
8	H	305	ILE	N-CA-C	-5.28	105.98	111.58
32	g	68	ASN	N-CA-CB	5.28	119.05	111.51
8	H	46	LEU	N-CA-C	-5.27	106.62	113.16
4	D	363	VAL	N-CA-C	5.27	116.34	111.81
4	D	391	VAL	CA-C-N	-5.26	115.87	119.66
4	D	391	VAL	C-N-CA	-5.26	115.87	119.66
23	X	33	GLY	N-CA-C	-5.26	107.79	114.16
12	L	183	ILE	N-CA-C	-5.26	105.25	110.62
47	AC	16	HIS	N-CA-C	5.26	117.76	111.71
39	n	36	LYS	N-CA-C	-5.26	105.55	111.28
13	M	212	VAL	CB-CA-C	-5.26	105.16	112.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	72	ILE	N-CA-C	-5.25	108.38	113.53
8	H	146	MET	N-CA-C	-5.25	105.45	111.07
8	H	103	LEU	N-CA-C	-5.25	105.45	111.07
13	M	294	MET	N-CA-C	-5.25	106.89	113.72
33	h	129	PRO	N-CA-C	-5.25	106.69	113.57
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
39	n	12	HIS	N-CA-C	-5.25	105.00	111.40
7	G	277	MET	N-CA-CB	-5.24	101.64	109.71
16	P	68	TYR	N-CA-C	5.24	117.07	111.36
52	AH	86	LYS	N-CA-C	5.24	117.67	111.33
7	G	435	PRO	CB-CA-C	-5.23	105.86	111.56
14	N	335	MET	CB-CA-C	-5.23	104.37	111.95
12	L	190	SER	N-CA-C	-5.23	106.75	113.23
41	p	13	PRO	O-C-N	5.23	123.61	121.15
12	L	375	ILE	N-CA-CB	5.23	116.66	110.55
13	M	20	PRO	N-CA-C	-5.22	106.27	113.53
15	O	264	GLU	N-CA-C	-5.22	107.27	113.38
43	r	25	GLN	N-CA-C	5.22	118.91	112.54
13	M	98	MET	N-CA-C	-5.22	105.49	111.07
35	j	76	ASP	CB-CA-C	-5.21	104.64	112.09
12	L	386	LEU	CA-C-O	-5.21	115.88	121.45
3	C	164	TRP	N-CA-C	5.20	117.03	111.36
12	L	217	LEU	N-CA-C	-5.20	105.61	111.28
10	J	124	LEU	N-CA-C	-5.20	101.39	109.14
7	G	600	GLU	CB-CA-C	-5.20	103.00	111.06
12	L	485	PHE	N-CA-CB	5.20	117.54	110.01
38	m	17	THR	N-CA-C	-5.19	103.67	110.53
19	S	85	ASP	N-CA-C	5.19	117.84	111.82
39	n	26	HIS	N-CA-C	-5.19	106.54	112.92
12	L	137	MET	N-CA-C	5.19	119.23	113.01
43	r	111	PRO	CA-N-CD	5.19	119.26	112.00
13	M	317	ILE	N-CA-CB	5.17	117.19	110.57
29	d	37	LEU	N-CA-C	-5.17	105.64	111.28
43	r	107	SER	N-CA-C	-5.17	102.20	109.96
41	p	167	ARG	CB-CA-C	5.17	117.19	109.13
15	O	206	TYR	CA-C-N	-5.17	115.01	122.45
15	O	206	TYR	C-N-CA	-5.17	115.01	122.45
4	D	391	VAL	N-CA-C	5.17	113.83	109.02
16	P	204	SER	CA-C-O	-5.16	115.05	121.50
51	AG	6	GLY	N-CA-C	-5.16	108.94	115.08
14	N	90	THR	N-CA-C	5.15	117.56	110.35
7	G	172	ILE	N-CA-C	-5.15	98.62	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	332	HIS	N-CA-C	-5.15	105.66	111.28
14	N	222	ASN	N-CA-C	-5.15	106.24	112.88
12	L	497	GLY	N-CA-C	-5.14	106.53	112.50
14	N	225	MET	N-CA-C	-5.14	106.59	112.92
3	C	156	VAL	N-CA-C	-5.14	104.08	111.17
6	F	271	SER	N-CA-C	-5.13	99.92	108.34
28	c	60	GLN	N-CA-C	-5.13	105.58	111.07
41	p	43	TRP	CA-C-N	-5.13	113.63	118.97
41	p	43	TRP	C-N-CA	-5.13	113.63	118.97
13	M	86	LYS	N-CA-C	-5.13	106.26	112.88
38	m	61	GLU	N-CA-C	5.13	119.62	112.90
7	G	569	GLN	CB-CA-C	-5.13	104.26	112.05
9	I	95	PRO	N-CA-C	5.13	121.24	113.81
7	G	713	ALA	N-CA-C	-5.12	105.59	111.07
27	b	82	LYS	N-CA-C	-5.12	103.77	110.53
8	H	196	ALA	CA-C-N	-5.12	113.48	119.32
8	H	196	ALA	C-N-CA	-5.12	113.48	119.32
12	L	284	THR	N-CA-C	-5.12	105.78	111.36
37	l	168	LEU	N-CA-C	-5.12	105.61	111.14
6	F	337	MET	CB-CA-C	-5.11	103.10	111.68
12	L	396	ILE	O-C-N	5.11	126.91	121.91
13	M	32	PHE	N-CA-CB	5.11	117.41	110.01
54	Ak	18	ILE	CB-CA-C	-5.10	108.85	113.70
1	A	2	ASN	CA-C-N	-5.10	113.05	120.29
1	A	2	ASN	C-N-CA	-5.10	113.05	120.29
8	H	277	TYR	N-CA-C	5.10	117.91	110.10
36	k	44	ALA	N-CA-C	-5.10	105.72	111.28
13	M	30	TYR	N-CA-C	5.10	116.84	111.28
14	N	292	PHE	CA-CB-CG	5.10	118.90	113.80
33	h	158	ARG	N-CA-C	-5.10	105.63	111.14
38	m	47	TYR	N-CA-C	-5.10	105.90	112.68
12	L	249	SER	N-CA-C	5.09	116.64	111.14
6	F	293	SER	CB-CA-C	-5.09	104.37	111.80
3	C	109	SER	N-CA-C	5.08	118.10	109.76
13	M	234	ILE	CB-CA-C	5.08	116.18	111.30
34	i	16	ARG	N-CA-C	-5.08	105.74	111.28
13	M	330	ALA	N-CA-CB	5.08	117.44	110.07
38	m	26	SER	N-CA-C	-5.07	102.79	109.84
32	g	137	SER	N-CA-C	5.07	119.32	113.18
16	P	376	ASN	CB-CA-C	-5.07	102.23	110.85
23	X	112	LEU	N-CA-CB	5.07	117.42	110.07
5	E	181	ASN	N-CA-C	-5.06	99.54	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	169	HIS	CB-CA-C	5.06	118.73	110.17
42	q	13	GLN	N-CA-C	-5.06	105.65	111.07
14	N	42	PRO	CB-CA-C	-5.06	105.02	113.06
48	AD	151	GLU	N-CA-C	-5.06	105.77	111.28
7	G	203	ASP	CA-C-O	5.05	127.18	121.32
37	l	45	PRO	N-CA-C	5.05	120.47	113.65
24	Y	72	PHE	N-CA-C	-5.05	105.67	111.07
14	N	217	MET	N-CA-C	-5.05	106.95	113.01
7	G	280	ASP	N-CA-CB	-5.05	102.70	110.12
7	G	393	GLY	N-CA-C	-5.05	107.79	115.66
33	h	161	ARG	N-CA-C	-5.04	105.47	110.97
52	AH	87	ASN	CB-CA-C	-5.04	100.99	110.67
9	I	160	GLU	CB-CA-C	5.04	119.20	110.84
16	P	136	THR	N-CA-CB	-5.04	102.77	110.42
18	R	43	TYR	N-CA-CB	-5.04	103.20	110.70
32	g	124	VAL	N-CA-CB	5.04	118.13	110.58
3	C	208	GLU	CA-C-O	-5.03	115.71	121.40
13	M	56	PHE	N-CA-C	5.03	116.72	108.52
11	K	48	SER	N-CA-CB	5.03	117.51	110.12
13	M	267	TRP	N-CA-C	-5.03	105.88	111.36
20	T	140	CYS	CB-CA-C	-5.03	104.12	109.85
20	U	81	ASP	N-CA-C	-5.02	106.32	112.90
22	W	112	GLU	N-CA-C	5.02	116.83	111.36
12	L	384	PRO	N-CA-CB	5.01	107.71	103.35
14	N	64	ALA	N-CA-C	5.01	116.44	111.07
50	Af	80	GLN	N-CA-C	-5.01	106.42	112.54
13	M	229	MET	N-CA-C	-5.01	105.71	111.07
12	L	142	ILE	N-CA-C	-5.01	105.51	110.62
14	N	282	MET	N-CA-C	-5.01	105.71	111.07
3	C	221	GLU	N-CA-C	-5.00	102.45	108.25
13	M	281	ASP	N-CA-CB	5.00	118.57	110.17
29	d	60	ARG	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	737	0	800	113	0
2	B	1247	0	1256	144	0
3	C	1641	0	1596	118	0
4	D	3443	0	3389	337	0
5	E	1635	0	1626	171	0
6	F	3273	0	3231	311	0
7	G	5287	0	5323	528	0
8	H	2531	0	2619	350	0
9	I	1389	0	1352	137	0
10	J	1178	0	1204	214	0
11	K	721	0	753	91	0
12	L	4798	0	4986	584	0
13	M	3630	0	3854	500	0
14	N	2694	0	2896	345	0
15	O	2588	0	2539	250	0
16	P	2720	0	2740	227	0
17	Q	957	0	949	84	0
18	R	660	0	639	77	0
19	S	667	0	683	91	0
20	T	604	0	596	87	0
20	U	700	0	691	70	0
21	V	915	0	954	82	0
22	W	970	0	991	67	0
23	X	1385	0	1370	156	0
24	Y	1030	0	1015	80	0
25	Z	1152	0	1148	126	0
26	a	548	0	562	63	0
27	b	620	0	617	83	0
28	c	389	0	385	34	0
29	d	996	0	1001	71	0
30	e	859	0	849	121	0
31	f	439	0	433	35	0
32	g	835	0	772	67	0
33	h	1162	0	1163	121	0
34	i	765	0	769	60	0
35	j	574	0	522	91	0
36	k	560	0	560	47	0
37	l	1304	0	1193	95	0
38	m	1050	0	1061	114	0
39	n	1534	0	1463	135	0
40	o	1038	0	1030	105	0
41	p	1415	0	1385	106	0
42	q	1020	0	976	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	r	418	0	434	50	0
44	s	238	0	225	24	0
45	AA	3157	0	3075	173	0
45	Aa	3131	0	3052	136	0
46	AB	3097	0	3108	127	0
46	Ab	3128	0	3135	141	0
47	AC	2988	0	3045	146	0
47	Ac	2956	0	3012	123	0
48	AD	1896	0	1845	151	0
48	Ad	1912	0	1860	149	0
49	AE	1397	0	1376	192	0
49	AI	328	0	346	46	0
49	Ae	1436	0	1414	183	0
50	AF	855	0	841	39	0
50	Af	864	0	854	78	0
51	AG	634	0	637	53	0
51	Ag	643	0	643	51	0
52	AH	527	0	507	66	0
52	Ah	527	0	505	58	0
53	AJ	332	0	324	26	0
53	Aj	332	0	324	31	0
54	AK	355	0	351	23	0
54	Ak	365	0	358	32	0
55	B	8	0	0	3	0
55	F	8	0	0	6	0
55	G	16	0	0	2	0
55	I	16	0	0	5	0
56	B	18	0	18	3	0
57	B	35	0	44	6	0
57	I	43	0	60	8	0
58	Ac	58	0	64	3	0
58	Ag	51	0	82	0	0
58	D	38	0	50	6	0
58	H	97	0	151	18	0
58	J	46	0	66	1	0
58	L	133	0	194	18	0
58	M	86	0	123	15	0
58	i	40	0	54	11	0
58	m	41	0	56	9	0
59	E	4	0	0	4	0
59	G	4	0	0	5	0
60	F	31	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	H	35	0	43	28	0
62	Aa	46	0	36	1	0
62	Ag	98	0	84	3	0
62	L	73	0	90	12	0
62	M	82	0	114	12	0
62	Y	71	0	86	5	0
62	d	65	0	74	8	0
62	h	68	0	83	13	0
62	q	57	0	58	22	0
63	L	1	0	0	0	0
63	R	1	0	0	0	0
64	O	27	0	12	3	0
65	P	48	0	26	5	0
66	W	32	0	0	4	0
66	n	32	0	0	1	0
67	AC	86	0	60	31	0
67	Ac	86	0	60	9	0
68	AC	28	0	31	29	0
68	Ac	23	0	23	10	0
69	AD	43	0	31	13	0
69	Ad	43	0	31	12	0
70	Ac	23	0	23	11	0
All	All	97017	0	97158	7400	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 38.

All (7400) 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)
48:AD:124:CYS:SG	69:AD:401:HEC:HAC	1.53	1.48
48:Ad:124:CYS:SG	69:Ad:401:HEC:HAC	1.53	1.47
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
67:Ac:403:HEM:CBA	68:Ac:406:UQ6:H4M2	1.64	1.27
10:J:134:MET:HE3	27:b:51:TYR:CD1	1.69	1.27
67:Ac:403:HEM:HBA1	68:Ac:406:UQ6:C4M	1.68	1.22
12:L:141:PHE:CE2	13:M:370:PRO:HG3	1.75	1.21
11:K:66:PHE:HZ	14:N:35:PHE:CZ	1.56	1.21
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.20
10:J:133:VAL:HG21	25:Z:68:ARG:NH2	1.55	1.20
1:A:83:LYS:CE	10:J:146:SER:HB2	1.70	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:90:TYR:CE2	20:U:92:LYS:HB2	1.76	1.20
12:L:437:PHE:CE1	12:L:441:ILE:HG12	1.77	1.19
21:V:44:TYR:CE1	21:V:48:THR:HG21	1.77	1.18
12:L:358:LYS:HG3	39:n:80:TYR:CZ	1.79	1.17
12:L:466:PHE:CZ	35:j:72:ARG:NH2	2.14	1.16
13:M:369:LEU:HD23	13:M:371:PRO:HD2	1.18	1.16
47:AC:21:LEU:HD21	68:AC:403:UQ6:H3M2	1.24	1.15
34:i:74:HIS:O	34:i:78:PRO:HG2	1.46	1.14
10:J:134:MET:CE	27:b:51:TYR:CD1	2.30	1.14
12:L:247:LEU:CD1	12:L:248:HIS:CD2	2.31	1.14
45:AA:403:LEU:HG	45:AA:404:ASP:H	0.99	1.14
52:Ah:84:LEU:O	52:Ah:88:LEU:HG	1.47	1.14
11:K:66:PHE:CZ	14:N:35:PHE:CZ	2.35	1.13
8:H:52:ALA:HB2	61:H:401:UQ9:H23	1.26	1.13
8:H:224:PHE:CE2	61:H:401:UQ9:H17A	1.84	1.12
18:R:38:TYR:HE2	42:q:127:TYR:HB2	1.04	1.12
4:D:72:LEU:HD11	14:N:50:PRO:CG	1.79	1.12
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.22	1.12
12:L:437:PHE:HE1	12:L:441:ILE:HG12	0.97	1.12
47:AC:287:LYS:HG3	49:Ae:219:HIS:CD2	1.85	1.12
14:N:215:MET:CE	14:N:248:LEU:HD21	1.79	1.12
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.47	1.12
18:R:38:TYR:CE2	42:q:127:TYR:HB2	1.85	1.11
46:Ab:38:LEU:HD12	46:Ab:38:LEU:O	1.51	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
48:AD:155:GLN:HA	48:AD:166:MET:HA	1.25	1.11
12:L:229:LEU:HD12	12:L:229:LEU:O	1.51	1.10
12:L:365:ILE:HD12	12:L:366:MET:HG3	1.32	1.10
20:U:90:TYR:OH	20:U:92:LYS:HD2	1.48	1.10
45:AA:360:CYS:SG	45:AA:361:ASP:N	2.12	1.10
48:Ad:124:CYS:SG	69:Ad:401:HEC:CAC	2.40	1.10
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
12:L:121:LEU:HD22	12:L:246:LEU:HD21	1.32	1.09
12:L:594:ASN:ND2	14:N:110:PRO:HB2	1.66	1.09
12:L:553:LEU:HD11	38:m:93:ALA:HB3	1.34	1.09
13:M:127:ILE:CD1	14:N:256:PRO:HG3	1.82	1.09
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.88	1.09
9:I:53:ALA:HB1	27:b:14:ALA:HB2	1.27	1.09
45:AA:276:ARG:HG3	45:AA:462:ILE:HD12	1.13	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:41:ILE:HG23	33:h:179:ILE:HD11	1.36	1.08
37:l:184:TYR:HB3	40:o:34:ARG:HD2	1.34	1.08
48:AD:124:CYS:SG	69:AD:401:HEC:CAC	2.40	1.08
10:J:123:TRP:CE3	30:e:73:MET:HG2	1.88	1.08
12:L:466:PHE:HB2	35:j:68:TRP:CZ2	1.89	1.08
36:k:34:PRO:HG2	36:k:59:TYR:CE1	1.88	1.08
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
14:N:307:THR:HB	15:O:319:ILE:HD11	1.36	1.07
1:A:83:LYS:HE2	10:J:146:SER:HB2	1.29	1.07
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.11	1.07
9:I:54:THR:HG22	27:b:13:TRP:HE1	1.02	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
49:Ae:204:ARG:HB3	49:Ae:260:VAL:HG21	1.35	1.07
23:X:4:ILE:HG22	23:X:5:VAL:H	0.96	1.06
12:L:466:PHE:CB	35:j:68:TRP:HZ2	1.68	1.06
3:C:149:LEU:HD11	22:W:80:ARG:NH2	1.70	1.06
12:L:16:LEU:HD23	12:L:126:ILE:HD13	1.30	1.06
19:S:23:LEU:HD12	19:S:23:LEU:O	1.54	1.06
47:AC:287:LYS:NZ	49:Ae:219:HIS:HA	1.69	1.06
4:D:47:PHE:HB3	14:N:227:ILE:HD11	1.32	1.06
4:D:279:THR:HG23	21:V:13:GLY:HA3	1.34	1.06
6:F:270:ASN:OD1	6:F:270:ASN:O	1.70	1.06
20:T:138:LEU:HD12	20:T:138:LEU:O	1.55	1.06
19:S:79:LEU:HA	19:S:82:LEU:HD12	1.38	1.05
12:L:141:PHE:HB2	12:L:182:PHE:CE2	1.92	1.05
21:V:44:TYR:CE1	21:V:48:THR:CG2	2.39	1.05
45:AA:276:ARG:HG3	45:AA:462:ILE:CD1	1.86	1.05
48:Ad:223:THR:HG21	52:Ah:52:ASP:HA	1.29	1.05
10:J:22:LYS:NZ	11:K:22:PHE:HA	1.72	1.04
12:L:364:LYS:HE2	36:k:67:ILE:CD1	1.86	1.04
43:r:2:ALA:N	43:r:26:LEU:HD12	1.70	1.04
2:B:149:TYR:HA	2:B:152:MET:HE2	1.35	1.04
12:L:466:PHE:HB2	35:j:68:TRP:HZ2	1.17	1.04
12:L:466:PHE:CE1	35:j:72:ARG:CZ	2.40	1.04
48:AD:215:LEU:HD11	69:AD:401:HEC:CMB	1.87	1.04
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.04
14:N:307:THR:HB	15:O:319:ILE:CD1	1.87	1.04
37:l:38:PRO:HB2	38:m:75:ASN:HD22	1.20	1.04
49:AE:204:ARG:HB3	49:AE:260:VAL:HG21	1.35	1.04
45:AA:396:ARG:HA	45:AA:399:LEU:HD23	1.39	1.04
12:L:466:PHE:CE1	35:j:72:ARG:NH2	2.25	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:149:LEU:HA	49:Ae:220:LEU:HD22	1.39	1.04
48:Ad:215:LEU:HD11	69:Ad:401:HEC:CMB	1.87	1.04
13:M:249:ILE:O	13:M:250:LEU:HG	1.58	1.03
14:N:233:LEU:HD23	14:N:241:LEU:HD12	1.36	1.03
35:j:97:LEU:HB3	40:o:104:ARG:HB2	1.05	1.03
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.57	1.03
48:AD:215:LEU:HD11	69:AD:401:HEC:HMB1	1.34	1.03
9:I:53:ALA:CB	27:b:14:ALA:HB2	1.88	1.03
12:L:131:LEU:HD12	12:L:140:LEU:HD12	1.36	1.03
40:o:69:CYS:O	40:o:80:CYS:SG	2.17	1.02
48:Ad:215:LEU:HD11	69:Ad:401:HEC:HMB1	1.34	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
10:J:169:ILE:HD11	11:K:77:LEU:HD23	1.40	1.02
47:AC:21:LEU:CD2	68:AC:403:UQ6:H3M2	1.88	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.01
13:M:179:LEU:HB3	13:M:249:ILE:HD11	1.42	1.01
10:J:135:LEU:HG	11:K:54:MET:HE1	1.40	1.01
12:L:141:PHE:CE2	13:M:375:LEU:HD21	1.96	1.01
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.01
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.01
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.42	1.01
15:O:323:GLN:HE22	32:g:54:GLN:HB3	1.21	1.01
10:J:154:VAL:HG22	14:N:35:PHE:HZ	1.21	1.01
12:L:228:GLY:O	12:L:229:LEU:HG	1.61	1.01
21:V:72:LEU:HD11	21:V:80:VAL:HG21	1.40	1.01
45:AA:342:GLN:HE21	45:AA:357:HIS:HB3	1.20	1.01
10:J:154:VAL:HG22	14:N:35:PHE:CZ	1.95	1.00
12:L:222:GLY:HA2	12:L:229:LEU:HD11	1.40	1.00
25:Z:110:VAL:HG11	30:e:72:THR:CG2	1.90	1.00
13:M:172:GLY:O	13:M:173:THR:HG23	1.61	1.00
35:j:97:LEU:HB3	40:o:104:ARG:CB	1.91	1.00
42:q:66:THR:HG22	42:q:74:PHE:HB2	1.39	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
37:l:91:GLN:HE21	39:n:2:ALA:HB1	1.26	1.00
50:Af:27:PHE:HB2	50:Af:32:LEU:HB2	1.41	1.00
5:E:203:ILE:HG23	5:E:213:PRO:HG2	1.43	0.99
21:V:44:TYR:CZ	21:V:48:THR:HG21	1.97	0.99
23:X:53:PRO:HD3	25:Z:116:TRP:CD1	1.96	0.99
45:Aa:341:PHE:HD2	45:Aa:368:MET:CE	1.74	0.99
12:L:358:LYS:CG	39:n:80:TYR:CZ	2.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:90:ASP:OD2	26:a:62:VAL:HG11	1.59	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
13:M:196:TRP:CD1	13:M:250:LEU:HD13	1.96	0.99
14:N:232:LEU:HD23	14:N:307:THR:HG23	1.39	0.99
26:a:64:LYS:HE2	26:a:66:LEU:HD12	1.43	0.99
30:e:95:PRO:HD2	30:e:98:HIS:HD1	1.28	0.99
47:AC:37:LEU:HB3	67:AC:402:HEM:HMB1	1.43	0.99
8:H:52:ALA:CB	61:H:401:UQ9:H23	1.93	0.98
5:E:134:CYS:HG	59:E:301:FES:FE1	0.78	0.98
10:J:9:SER:CB	11:K:7:ASN:HD22	1.76	0.98
13:M:143:LEU:HD21	14:N:303:THR:CG2	1.94	0.98
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.98
8:H:30:TYR:CE1	26:a:1:MET:O	2.16	0.98
37:l:158:PRO:HD3	40:o:22:ILE:HB	1.45	0.98
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.44	0.98
12:L:141:PHE:HB2	12:L:182:PHE:HE2	1.27	0.98
12:L:553:LEU:HD11	38:m:93:ALA:CB	1.94	0.98
13:M:275:ILE:HD11	13:M:288:TYR:CG	1.98	0.98
13:M:458:THR:CG2	41:p:148:ALA:HB1	1.93	0.98
22:W:55:LEU:HB3	22:W:107:MET:CE	1.94	0.98
2:B:82:ILE:HG23	8:H:57:MET:SD	2.03	0.97
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.43	0.97
23:X:135:ARG:HH12	23:X:138:PRO:HD3	1.23	0.97
7:G:611:THR:HG21	17:Q:105:GLU:HA	1.47	0.97
23:X:4:ILE:HG22	23:X:5:VAL:N	1.77	0.97
6:F:379:CYS:SG	55:F:502:SF4:FE1	1.56	0.97
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.45	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
9:I:54:THR:CG2	27:b:13:TRP:HE1	1.77	0.96
46:Ab:278:ILE:HG22	46:Ab:330:TYR:C	1.88	0.96
12:L:216:LEU:HD22	12:L:259:LEU:HD21	1.44	0.96
6:F:382:CYS:HG	55:F:502:SF4:FE2	0.79	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.96
12:L:141:PHE:CE2	13:M:375:LEU:CD2	2.48	0.96
12:L:174:TYR:HD2	12:L:232:TRP:CD1	1.82	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
4:D:72:LEU:HD11	14:N:50:PRO:HG2	1.44	0.96
10:J:169:ILE:HG13	14:N:45:ILE:HD11	1.47	0.96
15:O:347:VAL:HG11	28:c:29:PHE:HA	1.47	0.96
12:L:174:TYR:CD2	12:L:232:TRP:HD1	1.83	0.96
16:P:376:ASN:OD1	16:P:377:TYR:N	1.98	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HE2	10:J:146:SER:CB	1.94	0.96
13:M:250:LEU:HD12	13:M:250:LEU:O	1.65	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
12:L:363:THR:HG23	12:L:431:THR:HB	1.48	0.96
12:L:174:TYR:HD2	12:L:232:TRP:HD1	1.02	0.95
12:L:550:LEU:HD12	13:M:275:ILE:HB	1.43	0.95
10:J:123:TRP:CZ3	30:e:73:MET:HG2	2.01	0.95
13:M:173:THR:HG21	33:h:147:ALA:HB2	1.48	0.95
20:U:90:TYR:HE2	20:U:92:LYS:HB2	1.24	0.95
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.95
10:J:164:PHE:CE2	14:N:8:ILE:HG13	2.01	0.95
12:L:319:MET:HE1	12:L:399:ILE:HA	1.47	0.95
12:L:364:LYS:HE2	36:k:67:ILE:HD11	1.47	0.95
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.95
9:I:54:THR:HG22	27:b:13:TRP:NE1	1.80	0.95
14:N:31:VAL:O	14:N:35:PHE:CD2	2.18	0.95
6:F:63:TYR:HB3	6:F:256:ARG:HE	1.29	0.95
48:Ad:249:TYR:CE1	48:Ad:252:VAL:HG23	2.02	0.95
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.95
12:L:247:LEU:HD12	12:L:248:HIS:CD2	1.98	0.95
10:J:123:TRP:CH2	30:e:73:MET:HA	2.02	0.94
13:M:4:ILE:HG22	13:M:107:ILE:HD13	1.47	0.94
51:Ag:19:LEU:HD23	51:Ag:24:GLN:HB3	1.49	0.94
5:E:189:ASP:CG	6:F:163:TYR:HB3	1.92	0.94
3:C:85:ILE:CD1	3:C:140:ILE:HD11	1.98	0.94
13:M:216:LEU:HG	13:M:220:HIS:CE1	2.02	0.94
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.94
7:G:78:CYS:SG	59:G:803:FES:FE2	1.59	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
19:S:16:LEU:HD11	19:S:51:LEU:HD11	1.46	0.94
33:h:57:VAL:HG22	39:n:104:LEU:HD11	1.49	0.94
12:L:362:ILE:HD12	12:L:430:VAL:HG12	1.50	0.94
13:M:369:LEU:CD2	13:M:371:PRO:HD2	1.97	0.94
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.48	0.94
10:J:151:MET:HE1	14:N:28:LEU:HD13	1.47	0.94
12:L:246:LEU:HD12	12:L:247:LEU:N	1.81	0.94
4:D:67:ASN:HB2	15:O:193:LEU:CD2	1.97	0.94
13:M:1:MET:HG3	13:M:4:ILE:HD13	1.50	0.94
9:I:162:CYS:SG	55:I:303:SF4:FE4	1.60	0.93
10:J:133:VAL:HG21	25:Z:68:ARG:CZ	1.98	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:458:THR:HG22	41:p:148:ALA:HB1	1.50	0.93
20:U:140:CYS:HB2	20:U:143:GLU:HG2	1.49	0.93
48:AD:249:TYR:CE1	48:AD:252:VAL:HG23	2.02	0.93
49:AI:64:LEU:HA	49:AI:78:PHE:HA	1.49	0.93
3:C:98:PHE:HA	21:V:90:LEU:HD11	1.47	0.93
12:L:247:LEU:HD11	12:L:248:HIS:NE2	1.83	0.93
51:AG:19:LEU:HD23	51:AG:24:GLN:HB3	1.49	0.93
12:L:274:LEU:HA	12:L:277:MET:HE3	1.49	0.93
12:L:141:PHE:HE2	13:M:375:LEU:CD2	1.81	0.93
13:M:453:LEU:CD1	13:M:454:ILE:HG23	1.99	0.93
9:I:113:CYS:SG	55:I:303:SF4:FE3	1.60	0.93
49:AE:218:THR:HG21	49:AE:256:LEU:O	1.68	0.93
12:L:41:LYS:HG3	12:L:98:TRP:CZ2	2.04	0.93
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.34	0.92
15:O:314:LEU:CD1	15:O:315:PRO:HD2	2.00	0.92
13:M:143:LEU:HD21	14:N:303:THR:HG21	1.48	0.92
10:J:133:VAL:CG2	25:Z:68:ARG:CZ	2.47	0.92
48:AD:131:ALA:HA	48:AD:174:TYR:HA	1.51	0.92
7:G:176:CYS:SG	55:G:802:SF4:FE4	1.59	0.92
7:G:617:ARG:HH11	22:W:129:HIS:HA	1.35	0.92
49:Ae:218:THR:HG21	49:Ae:256:LEU:O	1.68	0.91
22:W:55:LEU:HB3	22:W:107:MET:HE1	1.52	0.91
10:J:169:ILE:HD11	11:K:77:LEU:CD2	1.99	0.91
23:X:4:ILE:CG2	23:X:5:VAL:H	1.82	0.91
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.91
12:L:245:ALA:O	12:L:249:SER:HB3	1.70	0.91
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.91
10:J:59:TYR:HA	10:J:63:MET:HB3	1.51	0.91
10:J:135:LEU:HG	11:K:54:MET:CE	2.00	0.91
12:L:202:MET:HE3	12:L:265:PRO:HG3	1.53	0.91
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.00	0.91
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.52	0.91
4:D:72:LEU:CD1	14:N:50:PRO:CG	2.49	0.91
6:F:225:LEU:HB2	17:Q:160:TYR:CE2	2.06	0.91
45:Aa:402:HIS:CD2	45:Aa:403:LEU:HD12	2.06	0.91
5:E:179:CYS:SG	59:E:301:FES:FE2	1.63	0.90
13:M:162:ILE:HG23	14:N:271:MET:HE3	1.52	0.90
35:j:97:LEU:CB	40:o:104:ARG:HB2	1.99	0.90
10:J:62:GLY:HA2	10:J:65:VAL:HB	1.53	0.90
10:J:71:THR:HG22	11:K:27:MET:HG2	1.53	0.90
16:P:221:ARG:HD3	16:P:286:ARG:HD3	1.51	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:106:ILE:HG12	15:O:111:SER:HA	1.50	0.90
9:I:80:GLU:HG3	26:a:1:MET:SD	2.11	0.90
10:J:134:MET:HE3	27:b:51:TYR:CE1	2.06	0.90
10:J:165:ILE:HG23	14:N:42:PRO:HG3	1.53	0.90
47:AC:287:LYS:HZ2	49:Ae:219:HIS:HA	1.35	0.90
4:D:72:LEU:CD1	14:N:50:PRO:HG2	2.00	0.90
7:G:362:ASP:HB2	19:S:71:PHE:CE1	2.06	0.90
13:M:127:ILE:CD1	14:N:256:PRO:CG	2.49	0.90
47:AC:197:LEU:HD12	68:AC:403:UQ6:H1M2	1.53	0.90
5:E:39:VAL:HG22	7:G:205:GLN:HE22	1.34	0.90
4:D:67:ASN:HB2	15:O:193:LEU:HD23	1.54	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
12:L:358:LYS:HG3	39:n:80:TYR:OH	1.72	0.90
13:M:231:LEU:HD12	13:M:235:LEU:CD1	2.00	0.90
15:O:314:LEU:CG	15:O:315:PRO:HD2	2.02	0.90
15:O:347:VAL:O	15:O:347:VAL:HG12	1.71	0.90
45:AA:403:LEU:HG	45:AA:404:ASP:N	1.82	0.90
4:D:280:ALA:CB	21:V:11:LEU:HG	2.00	0.90
7:G:36:VAL:HG11	7:G:56:VAL:HG11	1.52	0.90
12:L:141:PHE:HE2	13:M:375:LEU:HD22	1.35	0.90
10:J:164:PHE:HE2	14:N:8:ILE:HG13	1.34	0.89
12:L:123:LEU:HD22	12:L:150:MET:SD	2.12	0.89
42:q:76:ASP:OD1	42:q:76:ASP:O	1.90	0.89
13:M:2:LEU:HA	13:M:5:ILE:HG12	1.53	0.89
10:J:124:LEU:HD23	10:J:125:MET:N	1.87	0.89
13:M:453:LEU:HD12	13:M:454:ILE:N	1.88	0.89
9:I:67:ILE:HG23	57:I:301:PC1:H381	1.53	0.89
13:M:142:ARG:HH21	14:N:303:THR:HG22	1.37	0.89
13:M:380:PHE:HA	13:M:383:MET:HE2	1.55	0.89
21:V:72:LEU:HD12	21:V:72:LEU:O	1.73	0.89
25:Z:86:ILE:HG23	25:Z:128:ARG:HE	1.38	0.89
10:J:59:TYR:CE1	11:K:64:LEU:HD22	2.07	0.89
19:S:16:LEU:HD22	19:S:19:ILE:HD11	1.53	0.89
4:D:270:ASN:HB3	8:H:284:GLN:NE2	1.87	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
58:L:701:3PE:H321	58:L:701:3PE:H361	1.55	0.88
13:M:50:LYS:HE2	13:M:52:PHE:HE1	1.36	0.88
20:T:79:ILE:HB	20:T:145:VAL:HG13	1.55	0.88
1:A:67:LEU:HD11	11:K:68:ALA:CB	2.03	0.88
6:F:379:CYS:HG	55:F:502:SF4:FE1	0.88	0.88
46:AB:51:SER:HB2	46:AB:230:LEU:HD12	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LYS:HZ3	11:K:22:PHE:HA	1.39	0.88
13:M:8:SER:HA	13:M:11:LEU:HD13	1.54	0.88
49:AI:64:LEU:HD13	46:Ab:174:ILE:HG21	1.55	0.88
1:A:55:PHE:CZ	8:H:282:TYR:HE2	1.92	0.88
6:F:41:ILE:HG21	6:F:250:VAL:HG12	1.54	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
7:G:64:CYS:HG	59:G:803:FES:FE1	0.71	0.88
39:n:101:GLU:O	39:n:122:ARG:NH2	2.06	0.88
48:Ad:131:ALA:HA	48:Ad:174:TYR:HA	1.55	0.88
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.88
22:W:32:LYS:NZ	66:W:201:EHZ:C19	2.37	0.88
10:J:123:TRP:CZ3	30:e:73:MET:CG	2.57	0.88
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.56	0.88
13:M:173:THR:CG2	33:h:147:ALA:HB2	2.03	0.88
3:C:102:HIS:HE1	21:V:48:THR:HG22	1.35	0.88
13:M:310:MET:SD	13:M:455:THR:HB	2.13	0.88
12:L:362:ILE:HD12	12:L:430:VAL:CG1	2.03	0.88
15:O:275:TYR:CE1	21:V:23:ARG:NH1	2.41	0.88
30:e:17:HIS:CD2	30:e:18:PHE:HD1	1.92	0.88
1:A:67:LEU:HD11	11:K:68:ALA:HB1	1.56	0.87
1:A:83:LYS:NZ	10:J:146:SER:HB2	1.88	0.87
6:F:55:GLY:HA2	6:F:58:ARG:HD2	1.54	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
8:H:52:ALA:HB2	61:H:401:UQ9:C23	2.04	0.87
45:Aa:341:PHE:CD2	45:Aa:368:MET:CE	2.56	0.87
52:Ah:51:CYS:HA	52:Ah:54:ARG:HB3	1.56	0.87
13:M:447:LEU:HD11	13:M:454:ILE:HG21	1.55	0.87
7:G:78:CYS:HG	59:G:803:FES:FE2	0.57	0.87
12:L:428:TYR:HA	12:L:432:MET:HG2	1.56	0.87
13:M:368:ALA:HB1	13:M:375:LEU:HD13	1.56	0.87
45:Aa:102:LYS:HZ1	45:Aa:153:ASN:HA	1.38	0.87
12:L:496:LEU:HD12	12:L:497:GLY:N	1.90	0.87
10:J:9:SER:OG	11:K:7:ASN:ND2	2.08	0.87
13:M:102:LEU:HD13	13:M:230:ILE:HG12	1.57	0.87
16:P:221:ARG:HD3	16:P:286:ARG:CD	2.05	0.87
18:R:51:ARG:HH21	42:q:125:VAL:HG12	1.38	0.87
2:B:121:PHE:HB2	56:B:302:UQ1:H8	1.54	0.87
43:r:2:ALA:N	43:r:26:LEU:CD1	2.37	0.87
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.10	0.87
48:AD:290:LEU:HD23	53:AJ:44:TYR:HB2	1.54	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:402:HIS:HD2	45:Aa:403:LEU:CD1	1.87	0.87
12:L:594:ASN:CG	14:N:110:PRO:HB2	2.00	0.86
51:AG:29:SER:HB2	51:AG:32:SER:HB2	1.56	0.86
3:C:217:ARG:HH12	22:W:112:GLU:HB2	1.38	0.86
16:P:122:HIS:HB2	18:R:46:VAL:HG12	1.55	0.86
18:R:32:THR:HG22	18:R:36:GLN:H	1.40	0.86
20:T:138:LEU:HD13	20:T:144:ILE:HG12	1.56	0.86
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.54	0.86
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.03	0.86
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.56	0.86
12:L:79:SER:HB2	12:L:135:ASN:HB2	1.55	0.86
13:M:1:MET:HE1	13:M:111:SER:HB2	1.58	0.86
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.86
37:l:157:GLY:HA2	40:o:22:ILE:HG13	1.57	0.86
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.56	0.86
13:M:127:ILE:HD12	14:N:256:PRO:HG3	1.56	0.86
16:P:344:PRO:HB2	16:P:347:LEU:HD13	1.55	0.86
40:o:15:VAL:HG23	40:o:16:GLU:OE2	1.76	0.86
7:G:617:ARG:NH1	22:W:129:HIS:HA	1.90	0.86
3:C:217:ARG:NH1	22:W:112:GLU:HB2	1.91	0.86
15:O:314:LEU:HG	15:O:315:PRO:HD2	1.58	0.86
6:F:425:CYS:HG	55:F:502:SF4:FE4	0.58	0.86
19:S:16:LEU:HD12	19:S:16:LEU:O	1.76	0.86
45:Aa:403:LEU:HD22	45:Aa:426:LEU:HD21	1.57	0.86
15:O:347:VAL:CG1	28:c:29:PHE:HA	2.06	0.85
32:g:145:ILE:HG23	41:p:160:LYS:HE2	1.57	0.85
49:AE:174:LEU:HD11	49:AE:273:VAL:HG11	1.56	0.85
5:E:147:ILE:HG23	5:E:200:ILE:HG12	1.57	0.85
37:l:167:TYR:HD2	37:l:168:LEU:HD12	1.41	0.85
57:B:303:PC1:H322	57:B:303:PC1:H232	1.55	0.85
12:L:417:SER:HB3	12:L:493:ILE:HG13	1.58	0.85
2:B:116:ARG:HA	8:H:37:PRO:HA	1.56	0.85
12:L:455:LYS:NZ	35:j:57:GLN:OE1	2.10	0.85
57:B:303:PC1:H142	8:H:39:ILE:HD11	1.55	0.85
25:Z:110:VAL:HG11	30:e:72:THR:HG23	1.57	0.85
12:L:54:PHE:O	12:L:58:ASN:N	2.10	0.85
49:AE:238:CYS:SG	47:Ac:268:ILE:HD13	2.17	0.85
51:Ag:29:SER:HB2	51:Ag:32:SER:HB2	1.57	0.85
21:V:56:LEU:HD12	21:V:57:ASP:N	1.92	0.85
37:l:89:TRP:CZ2	39:n:86:PRO:HD2	2.11	0.85
45:AA:52:ILE:HA	45:AA:58:ARG:HA	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ILE:HG12	8:H:57:MET:CE	2.06	0.85
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.06	0.85
9:I:78:PHE:HB3	43:r:8:ILE:CG2	2.07	0.85
12:L:437:PHE:HE1	12:L:441:ILE:CG1	1.85	0.85
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.59	0.85
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.59	0.85
42:q:42:ASP:OD2	42:q:83:PRO:HG2	1.77	0.85
45:AA:255:ARG:O	45:AA:255:ARG:HG3	1.75	0.85
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.42	0.84
12:L:247:LEU:HD11	12:L:248:HIS:CD2	2.11	0.84
10:J:133:VAL:CG2	25:Z:68:ARG:NH2	2.39	0.84
11:K:66:PHE:HZ	14:N:35:PHE:HZ	1.25	0.84
47:Ac:294:LEU:HD11	70:Ac:405:U10:H1M3	1.58	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.95	0.84
12:L:128:MET:HG2	12:L:251:THR:HB	1.59	0.84
12:L:594:ASN:HD21	14:N:110:PRO:HB2	1.43	0.84
23:X:49:GLU:HG3	23:X:138:PRO:HG2	1.58	0.84
12:L:445:GLU:HB2	12:L:450:LEU:HD23	1.59	0.84
15:O:314:LEU:HD12	15:O:315:PRO:HD2	1.56	0.84
30:e:14:LEU:HD12	30:e:15:ASP:HB2	1.57	0.84
49:Ae:152:ILE:HB	49:Ae:169:TRP:CD1	2.12	0.84
4:D:137:ASP:OD1	4:D:148:GLU:CD	2.20	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.84
13:M:447:LEU:HD11	13:M:454:ILE:CG2	2.06	0.84
45:Aa:49:GLN:HE21	45:Aa:239:HIS:HB2	1.43	0.84
3:C:114:THR:HG22	4:D:421:ARG:NH1	1.93	0.84
37:l:167:TYR:CD2	37:l:168:LEU:HD12	2.13	0.84
49:AE:123:VAL:HG13	53:AJ:29:ALA:HA	1.59	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
14:N:215:MET:SD	14:N:248:LEU:HD21	2.18	0.84
20:T:110:LEU:HG	20:T:114:ASP:HB2	1.59	0.84
22:W:55:LEU:HD22	22:W:107:MET:HE2	1.58	0.84
21:V:75:GLY:HA2	43:r:103:ARG:HD2	1.59	0.84
47:AC:150:LEU:HB3	47:AC:160:LEU:HD23	1.60	0.84
12:L:20:LEU:HD12	12:L:21:ILE:N	1.92	0.84
13:M:196:TRP:NE1	13:M:250:LEU:HD13	1.92	0.84
49:AI:65:VAL:HB	49:AI:77:ARG:HB2	1.56	0.84
49:Ae:123:VAL:HG13	53:AJ:29:ALA:HA	1.59	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
14:N:273:ASN:ND2	24:Y:143:VAL:HA	1.92	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Ab:142:THR:HG21	46:Ab:238:LEU:H	1.42	0.83
2:B:152:MET:HB3	2:B:153:PRO:HD2	1.57	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
2:B:92:PRO:HD2	2:B:121:PHE:H	1.44	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
10:J:9:SER:HB2	11:K:7:ASN:HD22	1.42	0.83
10:J:22:LYS:HD2	11:K:23:ARG:HG3	1.61	0.83
13:M:373:ILE:HG12	13:M:454:ILE:HD11	1.60	0.83
16:P:275:HIS:HA	16:P:278:LYS:HE2	1.60	0.83
27:b:67:PRO:HD3	27:b:74:LEU:HB2	1.60	0.83
7:G:176:CYS:HG	55:G:802:SF4:FE4	0.55	0.83
30:e:87:MET:HE3	30:e:93:THR:HA	1.60	0.83
7:G:674:LEU:HD11	19:S:46:LYS:HE2	1.60	0.83
10:J:122:ASP:O	10:J:123:TRP:HD1	1.61	0.83
12:L:16:LEU:HD23	12:L:126:ILE:CD1	2.08	0.83
45:AA:360:CYS:SG	45:AA:364:SER:HB2	2.18	0.83
16:P:94:LEU:HA	16:P:97:MET:HE2	1.59	0.83
4:D:254:ARG:HH11	43:r:25:GLN:HB2	1.44	0.83
13:M:361:MET:HB3	13:M:441:MET:HE3	1.60	0.83
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.83
15:O:63:ASP:OD1	15:O:161:ARG:HA	1.79	0.83
19:S:48:HIS:CE1	19:S:95:LEU:HD22	2.13	0.83
24:Y:38:GLY:HA2	62:Y:201:CDL:H532	1.58	0.83
15:O:124:ASN:O	32:g:51:MET:HE3	1.79	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
12:L:131:LEU:CD1	12:L:140:LEU:HD12	2.09	0.82
37:l:91:GLN:NE2	39:n:2:ALA:HB1	1.94	0.82
12:L:432:MET:HG3	12:L:432:MET:O	1.78	0.82
13:M:269:MET:HE1	13:M:396:MET:HA	1.61	0.82
14:N:335:MET:HG3	14:N:335:MET:O	1.79	0.82
45:AA:276:ARG:CG	45:AA:462:ILE:HD12	2.04	0.82
45:Aa:195:THR:HG21	45:Aa:269:ARG:H	1.45	0.82
46:Ab:51:SER:HB2	46:Ab:230:LEU:HD12	1.61	0.82
45:AA:102:LYS:NZ	45:AA:153:ASN:HA	1.94	0.82
45:Aa:280:ASP:H	51:Ag:12:ARG:HG2	1.43	0.82
16:P:122:HIS:CB	18:R:46:VAL:HG12	2.08	0.82
42:q:85:GLU:HG2	42:q:98:PRO:HB3	1.59	0.82
45:AA:119:HIS:ND1	46:AB:298:HIS:HA	1.94	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
46:AB:89:LEU:HD22	46:AB:150:GLU:HB3	1.62	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:134:MET:CE	27:b:51:TYR:CE1	2.61	0.82
12:L:493:ILE:HD12	12:L:496:LEU:HD21	1.61	0.82
43:r:4:ALA:HB1	43:r:9:GLN:HB2	1.60	0.82
49:AI:78:PHE:HZ	46:Ab:168:ASN:HD21	1.26	0.82
45:Aa:102:LYS:NZ	45:Aa:153:ASN:HA	1.94	0.82
6:F:278:ILE:HD11	6:F:299:LEU:HD21	1.61	0.82
12:L:222:GLY:HA2	12:L:229:LEU:CD1	2.08	0.82
45:Aa:341:PHE:CE2	45:Aa:372:LEU:HD13	2.15	0.82
5:E:174:GLU:OE2	6:F:373:PHE:CD1	2.33	0.82
7:G:64:CYS:SG	59:G:803:FES:FE1	1.72	0.82
12:L:141:PHE:CE2	13:M:370:PRO:CG	2.61	0.82
3:C:85:ILE:HG13	3:C:140:ILE:HD11	1.60	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.42	0.82
16:P:221:ARG:CD	16:P:286:ARG:HD3	2.10	0.81
23:X:142:TYR:HB2	25:Z:115:ARG:HH11	1.45	0.81
30:e:41:ILE:CG2	33:h:179:ILE:HD11	2.10	0.81
45:AA:313:HIS:HD1	45:AA:341:PHE:HD1	1.28	0.81
12:L:16:LEU:CD2	12:L:126:ILE:HD13	2.10	0.81
17:Q:146:ASP:OD1	17:Q:146:ASP:O	1.97	0.81
19:S:36:PHE:HZ	19:S:44:LEU:HD11	1.45	0.81
22:W:55:LEU:CD2	22:W:107:MET:HE2	2.09	0.81
36:k:34:PRO:HD2	36:k:59:TYR:CD1	2.16	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
52:Ah:83:LYS:HA	52:Ah:86:LYS:HD3	1.60	0.81
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.60	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
16:P:141:PHE:HD2	16:P:179:LYS:HD2	1.43	0.81
42:q:71:LYS:O	42:q:72:ASN:OD1	1.99	0.81
45:AA:403:LEU:CG	45:AA:404:ASP:H	1.82	0.81
48:Ad:290:LEU:HD23	53:Aj:44:TYR:HB2	1.63	0.81
30:e:45:HIS:CD2	33:h:176:LYS:HD3	2.15	0.81
12:L:229:LEU:O	12:L:229:LEU:CD1	2.28	0.81
14:N:277:ILE:HG23	14:N:278:MET:N	1.95	0.81
20:T:93:ILE:HG21	20:T:110:LEU:HD22	1.63	0.81
13:M:172:GLY:O	13:M:173:THR:CG2	2.28	0.81
36:k:30:ILE:HD11	36:k:39:GLN:HB2	1.61	0.81
4:D:72:LEU:HD11	14:N:50:PRO:CB	2.09	0.80
14:N:307:THR:HG22	14:N:308:ASN:H	1.47	0.80
33:h:163:ARG:HG2	33:h:165:ASP:HB2	1.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:287:LYS:HG3	49:Ae:219:HIS:HD2	1.43	0.80
47:Ac:150:LEU:HD13	47:Ac:164:ILE:HD12	1.61	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
13:M:263:LEU:HD11	38:m:102:TYR:HD1	1.45	0.80
14:N:200:LEU:HD21	14:N:265:ILE:HG12	1.62	0.80
25:Z:98:MET:HE1	30:e:78:ASP:OD2	1.81	0.80
7:G:432:ILE:HG23	7:G:451:ILE:HD11	1.63	0.80
13:M:216:LEU:HD12	13:M:236:LEU:HD21	1.60	0.80
14:N:277:ILE:CG2	14:N:278:MET:H	1.93	0.80
8:H:97:ASN:HD22	26:a:38:VAL:HG13	1.46	0.80
9:I:162:CYS:HG	55:I:303:SF4:FE4	0.50	0.80
13:M:453:LEU:HD12	13:M:454:ILE:HG23	1.63	0.80
48:AD:156:ASP:HB3	48:AD:165:PHE:CE1	2.16	0.80
54:Ak:41:ILE:HA	54:Ak:44:TRP:CD1	2.17	0.80
8:H:187:ILE:HD12	58:H:403:3PE:H242	1.62	0.80
3:C:85:ILE:CG1	3:C:140:ILE:HD11	2.12	0.80
14:N:275:CYS:SG	24:Y:139:PRO:HG2	2.22	0.80
16:P:163:ARG:HD2	16:P:253:THR:HA	1.62	0.80
35:j:99:ILE:HA	40:o:108:LEU:HD21	1.63	0.80
41:p:6:ASP:HB3	41:p:9:VAL:HG22	1.61	0.80
2:B:99:CYS:HB3	4:D:141:TYR:CE2	2.16	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
21:V:95:LEU:HA	21:V:100:TRP:HH2	1.46	0.80
45:Aa:341:PHE:CZ	45:Aa:372:LEU:HD13	2.17	0.80
37:l:38:PRO:HB2	38:m:75:ASN:ND2	1.94	0.80
45:AA:102:LYS:HZ1	45:AA:153:ASN:HA	1.46	0.80
9:I:113:CYS:HG	55:I:303:SF4:FE3	0.49	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
7:G:334:GLU:OE1	19:S:71:PHE:HE1	1.64	0.80
15:O:117:PHE:CE1	15:O:173:MET:HE3	2.17	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.79
47:AC:21:LEU:HD21	68:AC:403:UQ6:C3M	2.09	0.79
15:O:199:LEU:HD11	15:O:294:LEU:HD22	1.64	0.79
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.79
12:L:507:LEU:HD12	12:L:510:LYS:HD3	1.63	0.79
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.62	0.79
35:j:97:LEU:O	40:o:104:ARG:NH1	2.15	0.79
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
20:U:76:LEU:HD12	20:U:156:GLU:HB2	1.62	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
12:L:516:ALA:HB2	39:n:30:TRP:CH2	2.18	0.79
13:M:122:PHE:CZ	13:M:206:LYS:HD3	2.18	0.79
49:AI:64:LEU:HA	49:AI:78:PHE:CA	2.11	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
12:L:130:ILE:HG23	12:L:139:GLN:HE21	1.46	0.79
23:X:120:PRO:CB	23:X:125:LEU:HD11	2.13	0.79
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.96	0.79
6:F:425:CYS:SG	55:F:502:SF4:FE4	1.74	0.79
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.79
12:L:552:LEU:HD21	38:m:90:GLY:HA2	1.65	0.79
13:M:367:LEU:HD21	13:M:408:MET:HE2	1.64	0.79
30:e:30:ALA:HB2	33:h:184:LYS:HG3	1.65	0.79
12:L:446:ASN:ND2	35:j:51:THR:HG21	1.98	0.79
14:N:338:PRO:HG3	62:d:201:CDL:H592	1.65	0.79
23:X:132:LYS:HB2	27:b:59:ASP:HB3	1.64	0.79
39:n:20:TYR:CE2	39:n:24:LEU:HD11	2.18	0.79
12:L:131:LEU:HD12	12:L:140:LEU:CD1	2.12	0.79
12:L:475:THR:HA	40:o:55:GLN:NE2	1.97	0.79
67:AC:402:HEM:HAA2	68:AC:403:UQ6:C5	2.12	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:51:ASP:OD2	61:H:401:UQ9:H15B	1.80	0.78
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.63	0.78
16:P:208:GLY:H	16:P:211:ASP:HB3	1.48	0.78
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.78
14:N:123:PRO:HG2	14:N:126:MET:HG2	1.64	0.78
15:O:117:PHE:HE1	15:O:173:MET:CE	1.96	0.78
23:X:50:GLU:HG2	23:X:138:PRO:HG3	1.66	0.78
51:AG:19:LEU:HD11	51:AG:23:GLU:HG2	1.65	0.78
48:Ad:156:ASP:HB3	48:Ad:165:PHE:CE1	2.18	0.78
53:Aj:30:LEU:HA	54:Ak:34:TRP:CD1	2.16	0.78
2:B:82:ILE:HA	8:H:57:MET:HE1	1.64	0.78
13:M:248:ILE:HG13	13:M:249:ILE:HD12	1.64	0.78
62:M:503:CDL:H122	29:d:47:MET:HE1	1.63	0.78
20:T:87:LEU:HD21	20:T:104:PHE:HZ	1.47	0.78
33:h:159:LEU:HB3	33:h:163:ARG:HH12	1.47	0.78
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.64	0.78
8:H:114:TYR:OH	10:J:33:ILE:CD1	2.32	0.78
12:L:3:ILE:H	12:L:3:ILE:HD12	1.48	0.78
12:L:466:PHE:CB	35:j:68:TRP:CZ2	2.56	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:20:ARG:HG3	19:S:54:LEU:HB2	1.64	0.78
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.61	0.78
13:M:231:LEU:HD12	13:M:235:LEU:HD13	1.64	0.78
13:M:370:PRO:HA	13:M:375:LEU:CD2	2.13	0.78
23:X:168:PHE:O	23:X:170:TRP:CD1	2.37	0.78
34:i:81:PHE:HB3	58:i:201:3PE:H242	1.64	0.78
48:AD:156:ASP:HB2	48:AD:167:ARG:HG2	1.63	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.65	0.78
12:L:534:HIS:O	12:L:538:PRO:HG3	1.83	0.78
13:M:9:LEU:HD23	13:M:104:ILE:HD13	1.65	0.78
20:T:87:LEU:HD22	20:T:104:PHE:CE1	2.19	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.78
9:I:68:ARG:NH2	25:Z:26:PRO:HD2	1.97	0.78
15:O:314:LEU:HD12	15:O:315:PRO:CD	2.13	0.78
30:e:89:GLU:HB2	30:e:91:LYS:HG2	1.65	0.78
37:l:44:THR:OG1	37:l:45:PRO:HD2	1.83	0.78
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.78
11:K:42:ILE:O	11:K:46:VAL:HG23	1.84	0.78
13:M:319:HIS:HA	13:M:322:THR:HG22	1.66	0.78
40:o:7:ARG:HA	40:o:11:TRP:CD1	2.19	0.78
12:L:136:ASN:HA	12:L:197:GLU:HA	1.66	0.78
14:N:215:MET:CE	14:N:248:LEU:CD2	2.62	0.78
46:AB:40:PHE:O	46:AB:40:PHE:CD1	2.36	0.78
47:AC:37:LEU:HB3	67:AC:402:HEM:CMB	2.14	0.78
7:G:272:ARG:HD2	7:G:274:LEU:HD23	1.63	0.78
13:M:127:ILE:HD11	14:N:256:PRO:CG	2.13	0.78
49:AE:191:GLU:HB2	49:AE:194:GLN:HB2	1.66	0.78
4:D:254:ARG:HE	43:r:25:GLN:NE2	1.82	0.77
12:L:466:PHE:HE1	35:j:72:ARG:CZ	1.94	0.77
52:AH:79:CYS:HA	52:AH:82:HIS:NE2	1.99	0.77
51:Ag:19:LEU:HD11	51:Ag:23:GLU:HG2	1.66	0.77
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.77
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	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
47:AC:197:LEU:HD11	68:AC:403:UQ6:C6	2.13	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
23:X:20:VAL:HG22	23:X:24:VAL:HG21	1.65	0.77
45:AA:341:PHE:CE2	45:AA:372:LEU:HD13	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.49	0.77
10:J:134:MET:HE3	27:b:51:TYR:CG	2.18	0.77
13:M:204:LEU:HD22	13:M:209:LEU:HD12	1.65	0.77
15:O:305:LEU:HD12	15:O:305:LEU:O	1.83	0.77
23:X:135:ARG:NH1	23:X:138:PRO:HD3	1.98	0.77
26:a:3:PHE:HE2	62:q:201:CDL:HA4	1.47	0.77
30:e:17:HIS:CD2	30:e:18:PHE:CD1	2.72	0.77
47:AC:149:LEU:HA	49:Ae:220:LEU:CD2	2.13	0.77
14:N:170:LEU:HD11	14:N:288:LEU:HG	1.65	0.77
18:R:95:LEU:HD21	18:R:111:PHE:HB3	1.66	0.77
23:X:86:TRP:CZ2	26:a:64:LYS:HB3	2.18	0.77
45:AA:276:ARG:CG	45:AA:462:ILE:CD1	2.61	0.77
45:Aa:402:HIS:HD2	45:Aa:403:LEU:HD12	1.46	0.77
7:G:667:GLN:HE21	19:S:38:VAL:HA	1.49	0.77
8:H:116:ILE:HG13	8:H:117:LEU:N	1.99	0.77
58:i:201:3PE:H362	58:i:201:3PE:H2A1	1.66	0.77
37:l:169:GLU:C	37:l:171:GLY:H	1.92	0.77
47:Ac:147:THR:HG22	47:Ac:161:VAL:HG13	1.66	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
42:q:56:PHE:HA	42:q:59:HIS:HD2	1.50	0.77
49:Ae:89:SER:HA	49:Ae:92:ARG:HB2	1.66	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
20:T:83:VAL:CG2	20:T:126:PHE:HZ	1.97	0.77
7:G:664:TYR:OH	19:S:23:LEU:HD11	1.84	0.77
13:M:208:PRO:HG2	13:M:216:LEU:HD13	1.67	0.77
14:N:31:VAL:O	14:N:35:PHE:HD2	1.68	0.77
14:N:45:ILE:O	14:N:45:ILE:HG13	1.83	0.77
25:Z:144:THR:HA	26:a:45:TRP:HZ3	1.50	0.77
49:Ae:173:PRO:HG2	49:Ae:223:VAL:HG22	1.67	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
13:M:98:MET:CE	13:M:128:PRO:HA	2.14	0.77
13:M:453:LEU:HD11	13:M:454:ILE:HG23	1.66	0.77
14:N:232:LEU:CD2	14:N:307:THR:HG23	2.15	0.77
23:X:124:GLN:O	23:X:125:LEU:HD12	1.85	0.77
37:l:113:ILE:HG23	37:l:115:ASN:H	1.50	0.77
49:AI:43:LEU:HD12	46:Ab:163:ALA:HB3	1.65	0.77
7:G:454:ASP:HA	7:G:459:ARG:HH21	1.48	0.76
12:L:598:ILE:HD11	14:N:153:ILE:HG12	1.66	0.76
13:M:171:VAL:HG11	13:M:179:LEU:HD21	1.65	0.76
49:AE:173:PRO:HG2	49:AE:223:VAL:HG22	1.67	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:419:THR:HA	12:L:422:TYR:CE2	2.20	0.76
13:M:175:ASN:HD22	33:h:143:GLU:HG2	1.50	0.76
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.65	0.76
35:j:97:LEU:O	40:o:104:ARG:HG3	1.85	0.76
46:AB:63:LEU:HD11	46:AB:238:LEU:HD21	1.65	0.76
20:U:86:VAL:HB	20:U:122:MET:HE1	1.67	0.76
42:q:96:ASP:OD1	42:q:97:PRO:HD2	1.85	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
13:M:42:LEU:HG	13:M:67:ILE:HD11	1.68	0.76
13:M:60:PRO:O	13:M:64:PRO:HD3	1.85	0.76
62:M:503:CDL:H742	62:M:503:CDL:H151	1.68	0.76
15:O:275:TYR:HE1	21:V:23:ARG:NH1	1.82	0.76
17:Q:81:VAL:HG21	17:Q:150:LYS:HG3	1.65	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
13:M:231:LEU:HD12	13:M:235:LEU:HD12	1.67	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
7:G:655:ARG:NH1	19:S:59:SER:HB3	2.01	0.76
10:J:29:GLY:N	11:K:31:LEU:HD21	2.00	0.76
10:J:124:LEU:HD23	10:J:125:MET:H	1.50	0.76
51:Ag:78:TYR:OH	52:Ah:62:GLU:HB2	1.85	0.76
12:L:496:LEU:HD12	12:L:496:LEU:C	2.09	0.76
37:l:158:PRO:HD3	40:o:22:ILE:CB	2.16	0.76
46:AB:407:MET:HG2	46:AB:411:THR:OG1	1.85	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.85	0.76
12:L:516:ALA:HB2	39:n:30:TRP:HH2	1.49	0.76
12:L:556:ILE:HG21	38:m:80:PHE:CE1	2.21	0.76
14:N:211:LEU:HD23	14:N:333:SER:HB2	1.68	0.76
20:T:119:ILE:HD12	20:T:138:LEU:HD11	1.67	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.65	0.76
10:J:59:TYR:HE1	11:K:64:LEU:HD22	1.49	0.76
16:P:143:ASP:HA	16:P:147:ASN:HB2	1.67	0.76
34:i:94:PRO:HG3	41:p:10:TYR:CE2	2.20	0.76
4:D:270:ASN:HB3	8:H:284:GLN:HE22	1.51	0.76
12:L:232:TRP:CZ3	12:L:233:LEU:CD2	2.69	0.76
16:P:214:LEU:HG	16:P:353:LEU:HD21	1.68	0.76
67:Ac:403:HEM:HBA1	68:Ac:406:UQ6:H4M2	0.81	0.76
49:Ae:191:GLU:HB2	49:Ae:194:GLN:HB2	1.66	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
9:I:64:THR:HG22	57:I:301:PC1:H231	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:605:ASN:OD1	12:L:605:ASN:O	2.03	0.75
14:N:215:MET:HE2	14:N:248:LEU:HD21	1.67	0.75
47:AC:197:LEU:HD11	68:AC:403:UQ6:C7	2.15	0.75
48:Ad:111:ARG:HB2	48:Ad:139:CYS:HB3	1.66	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
46:Ab:407:MET:HG2	46:Ab:411:THR:OG1	1.85	0.75
49:Ae:152:ILE:HG23	49:Ae:154:ILE:HD11	1.68	0.75
20:T:93:ILE:HG23	20:T:110:LEU:HD13	1.66	0.75
38:m:125:PHE:HE1	41:p:133:THR:HG22	1.51	0.75
39:n:20:TYR:CZ	39:n:24:LEU:HD11	2.21	0.75
45:AA:341:PHE:HD2	45:AA:368:MET:HE3	1.51	0.75
50:Af:46:GLU:HB3	50:Af:49:ARG:HH21	1.50	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
12:L:23:MET:HE1	62:L:703:CDL:H192	1.67	0.75
12:L:387:THR:HG23	12:L:461:SER:O	1.85	0.75
14:N:275:CYS:SG	24:Y:139:PRO:CG	2.75	0.75
1:A:63:LEU:HG	10:J:66:VAL:HG21	1.67	0.75
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.50	0.75
9:I:184:LEU:HD23	17:Q:112:MET:HG3	1.68	0.75
48:AD:227:LEU:HD12	48:AD:227:LEU:O	1.87	0.75
14:N:227:ILE:HA	14:N:230:ILE:HG22	1.66	0.75
18:R:104:CYS:SG	18:R:107:CYS:HB2	2.27	0.75
22:W:55:LEU:HB3	22:W:107:MET:HE2	1.66	0.75
62:L:703:CDL:H731	62:L:703:CDL:H542	1.68	0.75
14:N:307:THR:C	15:O:319:ILE:HG12	2.12	0.75
16:P:348:LYS:O	16:P:351:GLU:HG2	1.86	0.75
17:Q:167:ASN:O	17:Q:168:LYS:CD	2.35	0.75
45:AA:338:CYS:HB2	45:AA:364:SER:HB3	1.67	0.75
49:Ae:263:TYR:HB3	49:Ae:273:VAL:HG22	1.68	0.75
1:A:90:MET:HG2	10:J:152:MET:HE3	1.68	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.75
7:G:667:GLN:NE2	19:S:38:VAL:HA	2.00	0.75
10:J:88:ILE:HD11	11:K:23:ARG:HH12	1.51	0.75
12:L:393:ASP:OD1	12:L:394:LEU:N	2.19	0.75
12:L:553:LEU:HD21	38:m:93:ALA:C	2.11	0.75
14:N:277:ILE:HG23	14:N:278:MET:H	1.50	0.75
16:P:170:LEU:HA	16:P:202:ARG:HB3	1.68	0.75
48:Ad:227:LEU:HD12	48:Ad:227:LEU:O	1.87	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
8:H:317:TYR:OH	10:J:136:GLU:OE2	2.04	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:117:LEU:HA	40:o:120:ALA:HB3	1.69	0.75
46:Ab:38:LEU:HD12	46:Ab:38:LEU:C	2.10	0.75
2:B:112:TYR:OH	9:I:91:GLY:CA	2.31	0.74
4:D:371:MET:SD	4:D:381:HIS:CD2	2.79	0.74
13:M:388:TRP:CE2	38:m:109:ARG:HD2	2.22	0.74
15:O:117:PHE:CE1	15:O:128:SER:HB2	2.22	0.74
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.69	0.74
8:H:224:PHE:CD2	61:H:401:UQ9:C20	2.69	0.74
10:J:169:ILE:HG13	14:N:45:ILE:CD1	2.17	0.74
15:O:333:GLU:O	15:O:333:GLU:CD	2.30	0.74
24:Y:71:MET:HG3	24:Y:102:THR:HG21	1.68	0.74
4:D:280:ALA:HB1	21:V:11:LEU:HG	1.66	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
13:M:314:MET:HA	13:M:454:ILE:HD12	1.70	0.74
22:W:32:LYS:HZ3	66:W:201:EHZ:C19	1.98	0.74
27:b:35:ILE:HD12	27:b:35:ILE:O	1.88	0.74
35:j:92:TRP:CZ3	40:o:100:LYS:HA	2.22	0.74
45:AA:337:LEU:HD23	45:AA:368:MET:HA	1.67	0.74
12:L:362:ILE:HG23	12:L:366:MET:HE3	1.68	0.74
13:M:29:SER:HB3	32:g:91:PHE:CD2	2.22	0.74
13:M:29:SER:HB3	32:g:91:PHE:HD2	1.52	0.74
16:P:235:THR:OG1	16:P:273:LEU:HB3	1.87	0.74
38:m:45:ARG:HD2	39:n:150:MET:CE	2.17	0.74
46:AB:164:VAL:CG2	49:AI:34:VAL:HG23	2.17	0.74
49:AE:156:LEU:HB2	49:AE:269:ASP:HA	1.70	0.74
49:AE:206:LYS:HB2	49:AE:265:PHE:HE2	1.50	0.74
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.18	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
8:H:85:LEU:HD21	8:H:108:THR:HB	1.68	0.74
20:T:88:LYS:HG3	20:T:98:LEU:HD22	1.70	0.74
22:W:32:LYS:HZ2	66:W:201:EHZ:C19	2.01	0.74
48:AD:155:GLN:HB2	48:AD:166:MET:HG2	1.68	0.74
46:Ab:215:SER:HB2	46:Ab:242:GLY:HA2	1.68	0.74
2:B:93:MET:HE1	2:B:131:MET:HE2	1.68	0.74
4:D:249:LYS:HA	25:Z:19:ILE:HG23	1.68	0.74
13:M:310:MET:HG3	13:M:455:THR:HA	1.70	0.74
15:O:254:GLU:HG3	15:O:276:LEU:HD13	1.68	0.74
17:Q:61:ILE:O	17:Q:61:ILE:HD12	1.86	0.74
23:X:23:ALA:HB2	23:X:95:GLN:NE2	2.03	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.27	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:154:VAL:CG2	14:N:35:PHE:CZ	2.70	0.74
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.70	0.74
24:Y:76:THR:HG23	24:Y:95:GLY:HA3	1.70	0.74
7:G:608:VAL:HG23	17:Q:103:THR:OG1	1.88	0.74
12:L:14:LEU:HD21	34:i:74:HIS:O	1.87	0.74
52:AH:44:ALA:HA	52:AH:47:ARG:HD3	1.69	0.74
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.23	0.74
16:P:350:ILE:HB	16:P:366:ILE:HG23	1.70	0.74
20:T:117:GLU:HA	20:T:120:MET:HE3	1.67	0.74
10:J:123:TRP:CE3	30:e:73:MET:CG	2.68	0.74
13:M:200:MET:HE1	13:M:247:SER:HB2	1.69	0.74
1:A:73:LEU:O	1:A:76:PRO:HD2	1.88	0.73
10:J:24:SER:HB2	10:J:27:TYR:HD1	1.53	0.73
13:M:1:MET:HB2	13:M:52:PHE:CD2	2.23	0.73
15:O:217:ARG:O	15:O:220:LYS:HG2	1.89	0.73
20:T:94:ASP:HB3	20:T:98:LEU:HB2	1.68	0.73
20:T:103:HIS:CG	20:T:106:LYS:HD2	2.23	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.73
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.68	0.73
10:J:2:ASN:HB3	10:J:121:GLY:HA3	1.70	0.73
14:N:202:LEU:O	14:N:206:MET:HG2	1.87	0.73
50:Af:78:LYS:HA	50:Af:81:TRP:CD2	2.22	0.73
4:D:383:LYS:HD3	7:G:140:GLN:NE2	2.03	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.68	0.73
8:H:64:LEU:H	8:H:64:LEU:HD23	1.52	0.73
13:M:260:PRO:O	13:M:264:LEU:HG	1.88	0.73
15:O:117:PHE:HE1	15:O:173:MET:HE3	1.53	0.73
47:AC:268:ILE:HD12	49:Ae:238:CYS:SG	2.28	0.73
15:O:323:GLN:NE2	32:g:54:GLN:HB3	2.00	0.73
25:Z:93:GLU:O	25:Z:97:ILE:HG13	1.88	0.73
47:AC:147:THR:O	47:AC:161:VAL:HG22	1.88	0.73
2:B:147:LYS:HE3	2:B:151:GLN:HE21	1.51	0.73
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.73
12:L:20:LEU:HD12	12:L:20:LEU:C	2.13	0.73
62:L:703:CDL:H312	62:L:703:CDL:H351	1.69	0.73
13:M:167:ILE:HD11	13:M:195:LEU:HD21	1.70	0.73
21:V:54:GLU:HG2	21:V:58:MET:HE2	1.70	0.73
9:I:171:PRO:HB3	42:q:93:MET:HE1	1.69	0.73
12:L:232:TRP:CZ3	12:L:233:LEU:HD23	2.23	0.73
23:X:142:TYR:HB3	25:Z:115:ARG:HD3	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:AC:402:HEM:HAA2	68:AC:403:UQ6:C4	2.18	0.73
1:A:90:MET:CG	10:J:152:MET:HE3	2.18	0.73
10:J:57:LEU:HD12	10:J:58:ILE:HG12	1.69	0.73
12:L:579:ASN:OD1	12:L:579:ASN:O	2.06	0.73
13:M:216:LEU:HG	13:M:220:HIS:HE1	1.49	0.73
14:N:308:ASN:C	15:O:319:ILE:HG23	2.13	0.73
42:q:56:PHE:HA	42:q:59:HIS:CD2	2.24	0.73
42:q:68:MET:SD	42:q:81:MET:HB3	2.28	0.73
48:Ad:159:ASN:HB2	48:Ad:165:PHE:CE2	2.24	0.73
49:Ae:187:GLU:HB3	49:Ae:201:ASP:HB3	1.71	0.73
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.71	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
12:L:150:MET:HE1	62:L:703:CDL:H511	1.69	0.73
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.13	0.73
17:Q:167:ASN:O	17:Q:168:LYS:HD2	1.88	0.73
46:Ab:38:LEU:O	46:Ab:38:LEU:CD1	2.34	0.73
48:Ad:295:MET:HG2	53:Aj:36:PHE:CZ	2.23	0.73
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.73
5:E:128:LYS:HB3	5:E:167:LEU:HA	1.71	0.73
13:M:122:PHE:CD1	13:M:238:LEU:HG	2.23	0.73
21:V:72:LEU:HD11	21:V:80:VAL:CG2	2.19	0.73
50:AF:50:ARG:O	46:Ab:148:ARG:NH2	2.22	0.73
58:D:501:3PE:H232	12:L:567:SER:HA	1.71	0.72
10:J:123:TRP:CZ3	30:e:73:MET:HA	2.24	0.72
12:L:358:LYS:HG2	39:n:80:TYR:CE1	2.24	0.72
14:N:277:ILE:CG2	14:N:278:MET:N	2.52	0.72
6:F:42:PHE:HA	6:F:137:LYS:NZ	2.04	0.72
10:J:9:SER:CB	11:K:7:ASN:ND2	2.52	0.72
15:O:80:GLN:HG3	15:O:270:VAL:CG2	2.11	0.72
20:U:79:ILE:HD11	20:U:148:ILE:HG22	1.71	0.72
41:p:7:LYS:O	41:p:11:PRO:HA	1.89	0.72
45:Aa:403:LEU:HD22	45:Aa:426:LEU:CD2	2.19	0.72
6:F:127:ASP:HB3	6:F:245:VAL:HG21	1.70	0.72
12:L:136:ASN:HD21	62:h:201:CDL:H273	1.54	0.72
13:M:243:MET:HE1	13:M:302:MET:HE3	1.71	0.72
13:M:441:MET:SD	13:M:444:LEU:HD23	2.30	0.72
14:N:215:MET:SD	14:N:248:LEU:CD2	2.77	0.72
23:X:29:ALA:HB2	25:Z:71:LEU:HD11	1.70	0.72
25:Z:65:LEU:O	25:Z:69:ILE:HG12	1.89	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.70	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
12:L:141:PHE:CD2	13:M:370:PRO:HB3	2.24	0.72
16:P:317:ASP:HB3	16:P:321:ARG:NH2	2.04	0.72
36:k:34:PRO:HG2	36:k:59:TYR:HE1	1.54	0.72
45:Aa:196:PRO:O	45:Aa:199:GLN:HG2	1.89	0.72
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.72
9:I:93:LEU:O	42:q:93:MET:HG2	1.89	0.72
12:L:316:THR:CG2	12:L:325:ALA:HB2	2.19	0.72
15:O:176:GLN:HB2	15:O:178:TYR:HD2	1.55	0.72
52:AH:79:CYS:HA	52:AH:82:HIS:CD2	2.25	0.72
15:O:126:GLY:HA3	32:g:51:MET:HE1	1.71	0.72
19:S:69:TYR:CE2	19:S:75:LYS:HG3	2.24	0.72
42:q:56:PHE:HD1	42:q:59:HIS:HE2	1.35	0.72
46:AB:47:LEU:HD22	46:AB:238:LEU:HB3	1.72	0.72
46:Ab:63:LEU:HD11	46:Ab:238:LEU:HD21	1.70	0.72
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.72	0.72
12:L:141:PHE:HD2	13:M:370:PRO:HB3	1.53	0.72
62:M:503:CDL:H671	62:d:201:CDL:H151	1.69	0.72
21:V:12:VAL:HG13	21:V:13:GLY:N	2.04	0.72
25:Z:128:ARG:HA	30:e:98:HIS:HD2	1.55	0.72
34:i:74:HIS:O	34:i:78:PRO:CG	2.33	0.72
4:D:206:GLU:OE1	43:r:25:GLN:NE2	2.21	0.72
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.72
14:N:59:TYR:CE2	14:N:63:GLN:HG3	2.23	0.72
25:Z:110:VAL:CG1	30:e:72:THR:CG2	2.68	0.72
8:H:175:LEU:HD21	57:I:301:PC1:H2C2	1.71	0.72
12:L:247:LEU:HD12	12:L:248:HIS:N	2.03	0.72
16:P:166:HIS:HB3	16:P:200:ILE:HD13	1.71	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.72
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.25	0.72
12:L:299:LYS:HB2	12:L:354:GLN:HE21	1.55	0.72
13:M:373:ILE:CG1	13:M:454:ILE:HD11	2.19	0.72
47:AC:197:LEU:HD12	68:AC:403:UQ6:C1M	2.18	0.72
6:F:278:ILE:HD11	6:F:299:LEU:CD2	2.19	0.71
22:W:42:TRP:CH2	22:W:93:LEU:HA	2.25	0.71
49:AE:199:GLN:O	49:AE:248:ARG:HD3	1.90	0.71
5:E:151:LEU:HD12	5:E:204:ILE:HD11	1.72	0.71
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.71
8:H:224:PHE:CD2	61:H:401:UQ9:H20	2.25	0.71
13:M:395:LEU:HD21	38:m:101:TRP:CE2	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:31:ILE:HA	27:b:34:MET:HE2	1.71	0.71
4:D:67:ASN:HB3	4:D:69:VAL:HG12	1.71	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
52:AH:51:CYS:O	52:AH:55:VAL:HG23	1.90	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
8:H:114:TYR:OH	10:J:33:ILE:HD11	1.90	0.71
10:J:151:MET:HE1	14:N:28:LEU:CD1	2.19	0.71
12:L:441:ILE:HG21	35:j:48:PRO:HD3	1.71	0.71
13:M:106:LEU:HD13	13:M:234:ILE:HG22	1.72	0.71
14:N:146:TYR:CD1	14:N:147:PRO:HD3	2.26	0.71
49:AE:156:LEU:HG	49:AE:271:VAL:HG23	1.72	0.71
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
5:E:174:GLU:HG2	6:F:369:ARG:NH1	1.96	0.71
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.72	0.71
7:G:126:LEU:HD11	18:R:89:PRO:CB	2.20	0.71
15:O:336:GLY:H	15:O:344:ASN:ND2	1.89	0.71
47:Ac:294:LEU:CD1	70:Ac:405:U10:H1M3	2.20	0.71
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.71	0.71
13:M:313:THR:HG21	13:M:456:GLY:HA3	1.71	0.71
38:m:9:ALA:HB1	38:m:10:PRO:HD2	1.71	0.71
53:AJ:30:LEU:HA	54:AK:34:TRP:CD1	2.25	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
12:L:368:PHE:HB3	12:L:445:GLU:CD	2.15	0.71
20:U:144:ILE:O	20:U:148:ILE:HG12	1.91	0.71
23:X:93:ASN:OD1	23:X:94:MET:N	2.24	0.71
37:l:106:HIS:CD2	37:l:107:TRP:H	2.08	0.71
48:AD:222:PRO:HD2	48:AD:225:VAL:HG11	1.72	0.71
49:AE:178:HIS:HB2	49:AE:210:TRP:CZ3	2.26	0.71
49:AI:64:LEU:HD21	46:Ab:171:THR:HA	1.72	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
3:C:70:LYS:O	21:V:103:LEU:HD12	1.90	0.71
5:E:179:CYS:HG	59:E:301:FES:FE2	0.48	0.71
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.72	0.71
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:61:MET:HE3	8:H:63:PRO:HA	1.72	0.71
13:M:220:HIS:CE1	13:M:231:LEU:HD23	2.26	0.71
13:M:370:PRO:HA	13:M:375:LEU:HD23	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:8:PRO:HD3	23:X:54:ARG:HD3	1.71	0.71
47:AC:287:LYS:CG	49:Ae:219:HIS:CD2	2.70	0.71
48:AD:290:LEU:CD2	53:AJ:44:TYR:HB2	2.21	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
4:D:47:PHE:CB	14:N:227:ILE:HD11	2.16	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
20:U:102:SER:O	20:U:141:PRO:HD3	1.91	0.71
47:AC:150:LEU:CD1	47:AC:164:ILE:HD12	2.21	0.71
50:AF:88:LYS:HE3	50:AF:90:TYR:CD1	2.26	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.88	0.71
38:m:45:ARG:O	38:m:45:ARG:HG2	1.90	0.71
48:Ad:222:PRO:HD2	48:Ad:225:VAL:HG11	1.72	0.71
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.56	0.70
4:D:137:ASP:OD1	4:D:148:GLU:CG	2.39	0.70
4:D:261:MET:O	4:D:265:ASN:HB2	1.91	0.70
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.26	0.70
8:H:33:LEU:CD2	43:r:25:GLN:HG2	2.21	0.70
13:M:373:ILE:HG12	13:M:454:ILE:CD1	2.20	0.70
14:N:237:THR:HG23	14:N:237:THR:O	1.88	0.70
15:O:241:TYR:HA	15:O:245:PHE:HB3	1.73	0.70
49:AE:187:GLU:HB3	49:AE:201:ASP:HB3	1.71	0.70
2:B:123:ALA:HB1	4:D:89:PRO:HG3	1.73	0.70
7:G:117:MET:HE3	7:G:143:SER:HA	1.73	0.70
8:H:104:PHE:CE2	58:H:402:3PE:H362	2.26	0.70
21:V:12:VAL:HG13	21:V:13:GLY:H	1.56	0.70
49:AE:223:VAL:HB	47:Ac:264:THR:HB	1.72	0.70
4:D:254:ARG:NH1	43:r:25:GLN:HB2	2.06	0.70
15:O:135:LEU:HB3	15:O:139:ARG:HH12	1.56	0.70
16:P:172:ALA:O	16:P:185:ALA:HB2	1.91	0.70
21:V:56:LEU:HD12	21:V:56:LEU:C	2.16	0.70
30:e:83:ARG:HH11	30:e:92:TYR:HE2	1.38	0.70
37:l:184:TYR:HA	40:o:36:GLU:HA	1.72	0.70
38:m:45:ARG:NH2	39:n:150:MET:HE3	2.06	0.70
45:Aa:68:THR:HG22	45:Aa:136:LEU:HD23	1.73	0.70
49:Ae:178:HIS:HB2	49:Ae:210:TRP:CZ3	2.26	0.70
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.55	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.71	0.70
10:J:13:LEU:HD21	11:K:14:LEU:HD12	1.74	0.70
10:J:123:TRP:CH2	30:e:73:MET:CA	2.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:559:GLU:O	12:L:564:LYS:HB2	1.92	0.70
15:O:275:TYR:OH	21:V:23:ARG:NH1	2.24	0.70
46:AB:92:LYS:HE2	46:AB:143:ALA:HB1	1.72	0.70
49:AE:159:ILE:HG23	49:AE:163:LYS:HE3	1.74	0.70
49:Ae:220:LEU:HD12	49:Ae:239:HIS:CE1	2.27	0.70
7:G:463:CYS:O	7:G:467:LYS:HG2	1.92	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
10:J:127:GLU:OE2	25:Z:120:LEU:HA	1.91	0.70
12:L:604:ILE:O	24:Y:5:LYS:HD2	1.91	0.70
25:Z:12:PRO:HD3	25:Z:16:TYR:CZ	2.25	0.70
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE1	2.27	0.70
47:Ac:151:SER:HB3	47:Ac:161:VAL:HG21	1.72	0.70
49:Ae:207:LYS:HB2	49:Ae:210:TRP:HB2	1.73	0.70
14:N:156:MET:HE2	24:Y:138:PHE:CE2	2.27	0.70
14:N:254:LEU:HD12	14:N:255:PRO:HD3	1.72	0.70
21:V:35:LEU:HA	21:V:38:PHE:CD1	2.27	0.70
23:X:124:GLN:O	27:b:70:PRO:HB2	1.91	0.70
28:c:55:TRP:CZ2	29:d:66:THR:HG22	2.25	0.70
37:l:38:PRO:HG2	38:m:71:ALA:HB2	1.73	0.70
45:AA:113:VAL:HG13	46:AB:299:ILE:HD11	1.72	0.70
45:AA:407:THR:HB	45:AA:408:PRO:HD3	1.73	0.70
49:Ae:199:GLN:O	49:Ae:248:ARG:HD3	1.90	0.70
58:D:501:3PE:H361	12:L:566:THR:HG21	1.73	0.70
8:H:274:ARG:HH22	61:H:401:UQ9:H1MB	1.57	0.70
12:L:445:GLU:OE2	35:j:54:GLN:HG3	1.91	0.70
12:L:446:ASN:HD21	35:j:51:THR:HG21	1.55	0.70
12:L:593:ILE:HG21	24:Y:41:TYR:CE2	2.25	0.70
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.74	0.70
18:R:70:ASN:HB2	18:R:111:PHE:HD1	1.55	0.70
23:X:18:VAL:HG21	25:Z:74:LEU:HD11	1.74	0.70
12:L:428:TYR:HA	12:L:432:MET:CG	2.21	0.70
13:M:447:LEU:HD21	13:M:454:ILE:HD13	1.73	0.70
25:Z:110:VAL:HG21	30:e:72:THR:HG23	1.73	0.70
45:AA:399:LEU:HD12	45:AA:426:LEU:CD2	2.21	0.70
48:AD:295:MET:HG2	53:AJ:36:PHE:CZ	2.26	0.70
7:G:362:ASP:HB2	19:S:71:PHE:CD1	2.27	0.70
9:I:62:MET:HE2	9:I:62:MET:HA	1.72	0.70
13:M:134:THR:O	13:M:142:ARG:HD2	1.91	0.70
49:AE:207:LYS:HB2	49:AE:210:TRP:HB2	1.73	0.70
49:AE:220:LEU:HD12	49:AE:239:HIS:CE1	2.26	0.70
6:F:41:ILE:HD11	6:F:262:PHE:HE1	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:480:LEU:HD23	12:L:480:LEU:O	1.92	0.70
40:o:22:ILE:HA	40:o:105:GLU:OE2	1.91	0.70
40:o:25:PHE:HE2	40:o:109:LEU:HD22	1.57	0.70
49:AE:267:SER:HB3	49:AE:270:VAL:HB	1.72	0.70
46:Ab:46:GLY:HA3	46:Ab:216:ALA:HA	1.73	0.70
67:Ac:403:HEM:CGA	68:Ac:406:UQ6:H4M2	2.21	0.70
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HE3	1.74	0.70
12:L:285:THR:HG22	12:L:415:ALA:CB	2.22	0.69
16:P:55:VAL:HG12	16:P:123:SER:HA	1.74	0.69
46:AB:183:LYS:HG3	46:AB:254:ARG:HB3	1.74	0.69
45:Aa:74:TRP:CZ3	45:Aa:232:ALA:HB3	2.27	0.69
49:Ae:202:LEU:HA	49:Ae:205:VAL:HG22	1.74	0.69
8:H:93:HIS:HB3	26:a:27:HIS:ND1	2.07	0.69
25:Z:107:GLY:HA2	30:e:75:ARG:NH2	2.06	0.69
49:Ae:192:VAL:HA	49:Ae:195:LEU:HD12	1.73	0.69
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.41	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
8:H:30:TYR:CZ	26:a:1:MET:O	2.45	0.69
13:M:17:LEU:HD21	62:M:503:CDL:H522	1.74	0.69
16:P:148:ILE:HB	16:P:149:PRO:HD3	1.74	0.69
23:X:50:GLU:CG	23:X:138:PRO:HG3	2.23	0.69
25:Z:110:VAL:HG11	30:e:72:THR:HG22	1.74	0.69
34:i:104:ILE:HG13	40:o:48:ASP:HB3	1.74	0.69
45:AA:342:GLN:NE2	45:AA:357:HIS:HB3	2.02	0.69
46:Ab:183:LYS:HG3	46:Ab:254:ARG:HB3	1.74	0.69
2:B:131:MET:HE3	2:B:152:MET:CE	2.23	0.69
6:F:63:TYR:HB3	6:F:256:ARG:NE	2.04	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
10:J:123:TRP:CZ3	30:e:73:MET:CA	2.75	0.69
14:N:248:LEU:HD13	14:N:296:LEU:HD23	1.75	0.69
52:Ah:72:PHE:CE2	52:Ah:76:ARG:HD2	2.28	0.69
5:E:222:PHE:H	5:E:225:GLU:HG2	1.55	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69
8:H:92:PRO:HD3	8:H:255:TYR:CD2	2.27	0.69
8:H:274:ARG:NH2	61:H:401:UQ9:H1MB	2.06	0.69
13:M:216:LEU:HD11	13:M:236:LEU:HD11	1.72	0.69
18:R:67:GLN:HG2	18:R:109:LEU:CD2	2.21	0.69
24:Y:143:VAL:HG22	33:h:161:ARG:HD2	1.73	0.69
49:AI:5:ALA:HA	49:AI:12:ALA:HB2	1.74	0.69
10:J:22:LYS:HZ2	11:K:22:PHE:HA	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:50:LYS:HE2	13:M:52:PHE:CE1	2.25	0.69
13:M:142:ARG:NH2	14:N:303:THR:HG22	2.07	0.69
13:M:369:LEU:HD23	13:M:371:PRO:CD	2.12	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
16:P:69:VAL:HG21	16:P:129:LEU:HD11	1.74	0.69
37:l:122:THR:HG21	37:l:129:MET:HE1	1.73	0.69
38:m:25:VAL:HA	38:m:30:ARG:HD3	1.73	0.69
48:Ad:249:TYR:CZ	48:Ad:252:VAL:HA	2.28	0.69
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.27	0.69
12:L:305:SER:HB2	12:L:422:TYR:HE1	1.58	0.69
16:P:320:GLU:O	16:P:324:ILE:HG12	1.93	0.69
16:P:344:PRO:HD2	16:P:347:LEU:HD22	1.74	0.69
20:T:138:LEU:HD13	20:T:144:ILE:CG1	2.22	0.69
25:Z:98:MET:SD	30:e:79:ILE:HA	2.31	0.69
33:h:96:ALA:HB3	41:p:63:TYR:HD1	1.57	0.69
38:m:127:ILE:CG2	41:p:136:THR:HG23	2.23	0.69
45:AA:279:ASP:OD1	51:AG:12:ARG:NE	2.25	0.69
2:B:92:PRO:HG3	2:B:119:VAL:HG13	1.73	0.69
2:B:99:CYS:HB2	4:D:141:TYR:CG	2.28	0.69
4:D:279:THR:HG23	21:V:13:GLY:CA	2.19	0.69
5:E:151:LEU:HD23	5:E:170:LEU:HD13	1.73	0.69
6:F:81:LYS:HE2	6:F:97:LEU:HD23	1.75	0.69
7:G:43:VAL:HG12	7:G:55:LYS:HD3	1.75	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
8:H:23:VAL:HG11	26:a:9:LEU:HD21	1.72	0.69
12:L:542:LEU:HD21	37:l:116:ARG:HD2	1.73	0.69
13:M:173:THR:CG2	33:h:147:ALA:CB	2.71	0.69
14:N:215:MET:HE2	14:N:248:LEU:CD2	2.23	0.69
46:AB:45:ASN:HD22	46:AB:239:ASN:HA	1.57	0.69
49:AE:192:VAL:HA	49:AE:195:LEU:HD12	1.73	0.69
54:AK:33:VAL:HG12	54:AK:42:LEU:HG	1.75	0.69
50:Af:35:ASP:HB2	50:Af:90:TYR:CE1	2.28	0.69
2:B:92:PRO:HG2	2:B:121:PHE:HA	1.75	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
4:D:254:ARG:HH11	43:r:25:GLN:CB	2.06	0.69
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.69
7:G:335:GLY:HA2	7:G:362:ASP:O	1.93	0.69
8:H:42:PRO:HB3	42:q:27:PHE:CE2	2.28	0.69
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:51:LEU:HD13	19:S:95:LEU:HD12	1.75	0.69
40:o:19:PRO:HA	40:o:22:ILE:HD11	1.74	0.69
3:C:85:ILE:CD1	3:C:140:ILE:CD1	2.70	0.68
8:H:90:PRO:HD3	8:H:162:LEU:HD23	1.75	0.68
8:H:224:PHE:HB3	61:H:401:UQ9:C20	2.22	0.68
12:L:18:PRO:O	12:L:21:ILE:HG22	1.92	0.68
12:L:312:LEU:HD21	12:L:395:ILE:HG21	1.75	0.68
12:L:332:HIS:NE2	12:L:336:LYS:HG3	2.07	0.68
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.75	0.68
13:M:263:LEU:CD1	38:m:102:TYR:HD1	2.05	0.68
25:Z:110:VAL:HG11	30:e:72:THR:CA	2.24	0.68
36:k:34:PRO:CD	36:k:59:TYR:CD1	2.75	0.68
6:F:41:ILE:HD11	6:F:262:PHE:CE1	2.28	0.68
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.74	0.68
9:I:78:PHE:HB3	43:r:8:ILE:HG22	1.76	0.68
15:O:140:LEU:HG	15:O:304:VAL:HG12	1.74	0.68
30:e:95:PRO:HG2	30:e:97:HIS:HB2	1.75	0.68
37:l:78:LEU:HD11	37:l:104:PRO:HB2	1.74	0.68
46:AB:164:VAL:HG23	49:AI:34:VAL:HG23	1.73	0.68
48:AD:214:LEU:HD11	48:AD:237:PHE:HB2	1.75	0.68
49:AE:180:THR:H	49:AE:183:GLU:HB2	1.58	0.68
53:AJ:17:ARG:HD2	53:AJ:20:THR:HG23	1.75	0.68
46:Ab:412:VAL:HG13	46:Ab:415:GLN:HE21	1.58	0.68
48:Ad:214:LEU:HD11	48:Ad:237:PHE:HB2	1.75	0.68
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.90	0.68
8:H:34:ARG:HH22	61:H:401:UQ9:H4M	1.58	0.68
15:O:60:ILE:HD12	15:O:203:ALA:HB3	1.73	0.68
24:Y:77:CYS:SG	24:Y:78:VAL:N	2.66	0.68
46:AB:233:VAL:HA	46:AB:236:GLN:HG2	1.76	0.68
49:AE:219:HIS:CD2	47:Ac:287:LYS:HG3	2.28	0.68
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.74	0.68
12:L:516:ALA:HB1	12:L:520:SER:HB2	1.74	0.68
15:O:256:LEU:HB3	15:O:258:TYR:CE1	2.29	0.68
20:T:87:LEU:HD22	20:T:104:PHE:HE1	1.58	0.68
20:T:100:VAL:HB	20:T:142:GLN:HB2	1.74	0.68
23:X:142:TYR:O	23:X:143:HIS:C	2.36	0.68
48:AD:215:LEU:HD11	69:AD:401:HEC:HMB3	1.73	0.68
49:AI:69:GLY:HA3	49:AI:72:VAL:HB	1.76	0.68
4:D:259:GLU:O	4:D:263:THR:HG22	1.93	0.68
12:L:578:THR:CG2	14:N:168:GLY:HA2	2.23	0.68
13:M:143:LEU:HD21	14:N:303:THR:HG23	1.72	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:379:LEU:O	13:M:383:MET:HG3	1.93	0.68
20:T:116:VAL:HG12	20:T:120:MET:HE2	1.75	0.68
48:AD:249:TYR:CZ	48:AD:252:VAL:HA	2.28	0.68
51:AG:19:LEU:HD11	51:AG:23:GLU:CG	2.24	0.68
51:AG:73:LYS:HZ3	52:AH:63:GLU:HA	1.58	0.68
50:Af:99:ILE:HG23	50:Af:102:ARG:HH21	1.58	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
5:E:39:VAL:HG22	7:G:205:GLN:NE2	2.09	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
7:G:651:PRO:HG3	19:S:57:GLU:H	1.58	0.68
12:L:9:LEU:HD11	58:i:201:3PE:H2A2	1.74	0.68
12:L:211:ILE:N	12:L:212:PRO:HD2	2.08	0.68
12:L:383:MET:SD	12:L:384:PRO:HD2	2.33	0.68
14:N:215:MET:HE1	14:N:248:LEU:HD21	1.71	0.68
37:l:156:VAL:HG11	40:o:95:TYR:CZ	2.29	0.68
40:o:7:ARG:HA	40:o:11:TRP:HD1	1.58	0.68
49:AE:197:ASP:HB3	49:AE:257:ASN:CG	2.19	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
4:D:279:THR:HA	21:V:12:VAL:CG1	2.24	0.68
4:D:279:THR:HA	21:V:12:VAL:HG13	1.75	0.68
13:M:39:LEU:HD23	13:M:67:ILE:HD13	1.74	0.68
20:U:100:VAL:O	20:U:141:PRO:HG2	1.94	0.68
23:X:142:TYR:CB	25:Z:115:ARG:HD3	2.23	0.68
26:a:31:ASN:ND2	26:a:36:LYS:HB2	2.08	0.68
32:g:140:PHE:CE2	41:p:74:ILE:CG2	2.77	0.68
43:r:20:LEU:C	43:r:20:LEU:HD12	2.18	0.68
47:AC:287:LYS:CG	49:Ae:219:HIS:HD2	2.07	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
10:J:100:VAL:O	10:J:103:ILE:HG12	1.94	0.68
13:M:173:THR:HG23	33:h:147:ALA:CB	2.24	0.68
15:O:323:GLN:HE22	32:g:54:GLN:CB	2.03	0.68
15:O:352:ILE:HG21	29:d:52:PRO:HG2	1.75	0.68
24:Y:96:GLY:HA3	24:Y:121:GLY:HA2	1.75	0.68
37:l:101:TRP:NE1	38:m:62:ASP:HA	2.09	0.68
47:Ac:71:ARG:NE	48:Ad:199:TYR:OH	2.24	0.68
2:B:110:PRO:HB3	8:H:33:LEU:O	1.93	0.68
6:F:39:ASP:HB3	6:F:265:PHE:CZ	2.29	0.68
8:H:224:PHE:CG	61:H:401:UQ9:H20	2.29	0.68
10:J:59:TYR:HA	10:J:63:MET:CB	2.24	0.68
16:P:317:ASP:HB3	16:P:321:ARG:HH22	1.58	0.68
45:Aa:267:PRO:HD2	45:Aa:350:ASP:OD1	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:25:PRO:HB3	11:K:27:MET:HG3	1.75	0.68
37:l:122:THR:HG23	37:l:123:PRO:HD2	1.75	0.68
49:AE:202:LEU:HA	49:AE:205:VAL:HG22	1.74	0.68
45:Aa:101:THR:HG22	45:Aa:154:SER:HA	1.76	0.68
45:Aa:117:GLY:HA2	46:Ab:377:LYS:HG2	1.75	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
12:L:228:GLY:C	12:L:229:LEU:HG	2.19	0.67
12:L:358:LYS:HG2	39:n:80:TYR:CZ	2.29	0.67
13:M:311:GLY:HA2	13:M:314:MET:HE3	1.76	0.67
13:M:423:MET:SD	38:m:59:HIS:NE2	2.67	0.67
14:N:313:MET:CG	15:O:305:LEU:HD22	2.23	0.67
15:O:347:VAL:O	15:O:347:VAL:CG1	2.42	0.67
29:d:5:ARG:HD2	29:d:89:ASP:OD2	1.93	0.67
47:AC:16:HIS:CE1	47:AC:201:HIS:NE2	2.62	0.67
47:Ac:141:TRP:CD1	47:Ac:265:PRO:HD3	2.30	0.67
5:E:206:GLU:HB2	5:E:213:PRO:HG3	1.76	0.67
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.75	0.67
8:H:51:ASP:OD2	61:H:401:UQ9:H16A	1.94	0.67
8:H:54:LYS:HG3	8:H:55:LEU:N	2.08	0.67
16:P:185:ALA:O	16:P:188:GLU:HG2	1.94	0.67
19:S:19:ILE:HD12	19:S:94:VAL:HG11	1.76	0.67
23:X:44:MET:O	23:X:48:TRP:HE3	1.77	0.67
37:l:152:SER:HA	40:o:5:LEU:HD21	1.75	0.67
45:AA:101:THR:HG22	45:AA:154:SER:HA	1.76	0.67
48:Ad:215:LEU:HD11	69:Ad:401:HEC:HMB3	1.73	0.67
8:H:224:PHE:CD2	61:H:401:UQ9:H17A	2.28	0.67
19:S:16:LEU:HB3	19:S:69:TYR:HD1	1.58	0.67
22:W:121:PHE:HA	22:W:124:LYS:HE2	1.75	0.67
23:X:41:LYS:HD2	27:b:56:PRO:HB3	1.75	0.67
48:AD:156:ASP:HB2	48:AD:167:ARG:CG	2.24	0.67
46:Ab:40:PHE:CZ	46:Ab:406:TYR:HB2	2.29	0.67
54:Ak:43:ASP:HA	54:Ak:49:ASN:CG	2.19	0.67
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.76	0.67
4:D:375:MET:HE1	7:G:126:LEU:HA	1.75	0.67
6:F:225:LEU:H	17:Q:160:TYR:HE2	1.43	0.67
8:H:5:ASN:HD21	26:a:23:THR:HG23	1.58	0.67
8:H:33:LEU:HD21	43:r:25:GLN:HG2	1.74	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	2.30	0.67
18:R:48:PHE:CD2	42:q:125:VAL:HG21	2.29	0.67
23:X:158:LEU:HB3	29:d:21:LEU:HD21	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AA:367:ASP:O	45:AA:371:PHE:N	2.24	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
13:M:11:LEU:HB3	13:M:100:ILE:HD13	1.76	0.67
14:N:26:LEU:HD23	14:N:29:MET:SD	2.35	0.67
14:N:149:LEU:HD13	14:N:154:ILE:HG21	1.75	0.67
20:T:87:LEU:CD2	20:T:104:PHE:CZ	2.78	0.67
38:m:125:PHE:CE1	41:p:133:THR:HG22	2.29	0.67
45:AA:314:TYR:HB2	45:AA:371:PHE:HZ	1.60	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
13:M:30:TYR:O	13:M:34:ILE:HG12	1.95	0.67
32:g:109:ASP:CB	32:g:114:GLU:HB3	2.24	0.67
47:AC:34:GLY:C	67:AC:402:HEM:HMA1	2.19	0.67
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.58	0.67
7:G:304:GLU:OE2	16:P:41:ILE:HG12	1.94	0.67
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.25	0.67
13:M:98:MET:HE2	13:M:131:ILE:HB	1.77	0.67
21:V:116:ILE:HG23	21:V:116:ILE:O	1.92	0.67
23:X:158:LEU:HD13	29:d:17:GLU:HG3	1.77	0.67
38:m:45:ARG:HD2	39:n:150:MET:HE1	1.76	0.67
38:m:49:LEU:HD23	39:n:140:LEU:HD23	1.76	0.67
45:Aa:400:VAL:HG11	46:Ab:58:LEU:HG	1.76	0.67
53:Aj:17:ARG:HD2	53:Aj:20:THR:HG23	1.75	0.67
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.60	0.67
13:M:424:ILE:HG13	38:m:57:VAL:O	1.95	0.67
24:Y:76:THR:HG22	24:Y:92:TYR:HA	1.77	0.67
29:d:14:LEU:O	29:d:14:LEU:CD1	2.37	0.67
45:AA:120:LEU:HB3	46:AB:299:ILE:HG13	1.75	0.67
46:AB:412:VAL:HG13	46:AB:415:GLN:HE21	1.58	0.67
53:AJ:30:LEU:HD12	54:AK:34:TRP:HB2	1.77	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
7:G:382:ARG:HD2	19:S:56:ARG:CD	2.25	0.67
9:I:92:PRO:HA	42:q:91:HIS:O	1.95	0.67
12:L:81:LYS:N	12:L:135:ASN:ND2	2.43	0.67
15:O:249:MET:HB3	15:O:253:CYS:SG	2.34	0.67
35:j:99:ILE:HA	40:o:108:LEU:CD2	2.25	0.67
37:l:106:HIS:HD2	37:l:107:TRP:H	1.43	0.67
45:Aa:402:HIS:CD2	45:Aa:403:LEU:CD1	2.70	0.67
50:Af:83:LYS:HB2	50:Af:86:GLU:HG3	1.76	0.67
3:C:149:LEU:CD1	22:W:80:ARG:NH2	2.56	0.67
6:F:42:PHE:HA	6:F:137:LYS:HZ2	1.58	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:552:LEU:CD2	12:L:553:LEU:HD12	2.25	0.67
13:M:285:LEU:HD13	13:M:342:MET:HE1	1.76	0.67
30:e:14:LEU:CD1	30:e:15:ASP:HB2	2.25	0.67
42:q:13:GLN:HE22	62:q:201:CDL:HA31	1.60	0.67
51:Ag:19:LEU:HD11	51:Ag:23:GLU:CG	2.24	0.67
7:G:126:LEU:CD1	18:R:89:PRO:CB	2.73	0.66
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.66
12:L:389:PHE:CZ	35:j:79:ALA:HB1	2.30	0.66
13:M:270:ILE:HG22	13:M:271:MET:HE2	1.76	0.66
15:O:209:VAL:HG12	15:O:260:SER:HB2	1.76	0.66
15:O:326:ARG:NH2	32:g:56:ASP:OD1	2.27	0.66
49:Ae:180:THR:H	49:Ae:183:GLU:HB2	1.58	0.66
52:Ah:32:ARG:O	52:Ah:36:GLU:HG2	1.94	0.66
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.26	0.66
7:G:617:ARG:HH12	22:W:129:HIS:N	1.93	0.66
12:L:201:ILE:HG22	12:L:266:LEU:HD11	1.76	0.66
18:R:97:LYS:HE3	18:R:100:LYS:HD3	1.78	0.66
20:U:128:PHE:CZ	20:U:148:ILE:HD12	2.30	0.66
37:l:38:PRO:CB	38:m:75:ASN:HD22	2.02	0.66
40:o:89:TYR:CE2	40:o:93:LEU:HD11	2.30	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
9:I:68:ARG:HH22	25:Z:26:PRO:HD2	1.60	0.66
12:L:446:ASN:HD21	35:j:51:THR:CG2	2.08	0.66
13:M:361:MET:CB	13:M:441:MET:HE3	2.25	0.66
24:Y:71:MET:HG3	24:Y:102:THR:CG2	2.26	0.66
25:Z:128:ARG:HA	30:e:98:HIS:CD2	2.31	0.66
35:j:38:VAL:HG12	35:j:39:HIS:N	2.10	0.66
40:o:42:THR:HG22	40:o:44:GLN:H	1.59	0.66
46:AB:229:VAL:O	46:AB:232:GLN:HG2	1.95	0.66
49:Ae:197:ASP:HB3	49:Ae:257:ASN:CG	2.19	0.66
54:Ak:36:THR:HG1	54:Ak:38:TRP:CD1	2.12	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
8:H:92:PRO:HD3	8:H:255:TYR:HD2	1.58	0.66
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.78	0.66
15:O:343:TYR:HD1	15:O:352:ILE:HG23	1.59	0.66
23:X:44:MET:CE	25:Z:73:PRO:HA	2.25	0.66
46:AB:298:HIS:H	46:AB:304:ASN:HD21	1.43	0.66
48:Ad:131:ALA:H	48:Ad:134:HIS:CE1	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Ah:51:CYS:HB2	52:Ah:54:ARG:CZ	2.25	0.66
2:B:98:ALA:HB2	2:B:136:THR:H	1.61	0.66
12:L:364:LYS:CE	36:k:67:ILE:HD11	2.25	0.66
12:L:407:TRP:CE3	12:L:410:LEU:HD11	2.30	0.66
13:M:151:PHE:CZ	14:N:291:PHE:HB2	2.31	0.66
15:O:205:ILE:HD11	15:O:273:ILE:HG12	1.77	0.66
18:R:76:ILE:HD11	18:R:92:TYR:HB3	1.77	0.66
33:h:102:PRO:HD2	33:h:105:TYR:HB2	1.78	0.66
39:n:149:ILE:H	39:n:149:ILE:HD12	1.59	0.66
46:AB:50:ALA:HB3	46:AB:221:VAL:HG22	1.77	0.66
52:AH:51:CYS:HA	52:AH:54:ARG:HB3	1.77	0.66
7:G:246:ARG:NH2	17:Q:123:ASN:OD1	2.28	0.66
7:G:655:ARG:NH1	19:S:59:SER:CB	2.58	0.66
13:M:318:ALA:HB2	13:M:373:ILE:HG23	1.75	0.66
16:P:268:PRO:HG2	16:P:344:PRO:HA	1.76	0.66
20:T:83:VAL:HG22	20:T:126:PHE:CZ	2.31	0.66
21:V:72:LEU:HD12	21:V:72:LEU:C	2.19	0.66
31:f:38:ARG:HD3	31:f:56:TRP:NE1	2.10	0.66
47:AC:153:ILE:HB	47:AC:157:GLY:CA	2.25	0.66
48:AD:147:ALA:O	48:AD:151:GLU:HG3	1.94	0.66
47:Ac:137:GLN:NE2	47:Ac:141:TRP:HE1	1.94	0.66
47:Ac:147:THR:O	47:Ac:161:VAL:HG22	1.95	0.66
1:A:3:LEU:HD23	58:H:402:3PE:H251	1.77	0.66
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.66
10:J:59:TYR:CD2	10:J:63:MET:HG2	2.31	0.66
12:L:116:ARG:HG2	12:L:120:TYR:CE2	2.31	0.66
12:L:174:TYR:CD2	12:L:232:TRP:CD1	2.68	0.66
15:O:132:GLN:NE2	64:O:401:ADP:HN62	1.93	0.66
19:S:24:CYS:SG	19:S:61:VAL:O	2.53	0.66
21:V:72:LEU:O	21:V:72:LEU:CD1	2.42	0.66
47:Ac:45:ILE:HA	67:Ac:402:HEM:HAB	1.77	0.66
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.31	0.66
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.66
15:O:200:PRO:HG3	15:O:282:PRO:HD2	1.78	0.66
38:m:129:TYR:CZ	41:p:144:LEU:O	2.49	0.66
47:Ac:146:ILE:HG13	70:Ac:405:U10:H4M2	1.78	0.66
50:Af:106:GLU:O	50:Af:110:LYS:HG3	1.95	0.66
52:Ah:49:GLU:HA	52:Ah:52:ASP:OD2	1.96	0.66
5:E:43:THR:OG1	5:E:44:PRO:HD2	1.96	0.66
7:G:388:ASN:H	7:G:514:ASN:HB3	1.61	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:ASN:OD1	12:L:25:ASN:O	2.14	0.66
15:O:48:LYS:HD2	15:O:288:ASP:HB2	1.78	0.66
15:O:62:VAL:HA	15:O:205:ILE:O	1.96	0.66
25:Z:110:VAL:CG1	30:e:72:THR:HG22	2.26	0.66
36:k:34:PRO:CG	36:k:59:TYR:CE1	2.72	0.66
52:AH:48:LEU:O	52:AH:51:CYS:SG	2.54	0.66
54:AK:14:ALA:O	54:AK:18:ILE:HG12	1.96	0.66
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.78	0.66
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.31	0.66
5:E:138:PRO:HD2	59:E:301:FES:S2	2.36	0.66
12:L:66:TRP:HZ3	12:L:68:TRP:CD1	2.14	0.66
12:L:552:LEU:HD23	12:L:553:LEU:HD12	1.77	0.66
16:P:288:PHE:CZ	16:P:290:PRO:HB3	2.30	0.66
52:Ah:81:ALA:HA	52:Ah:84:LEU:HB3	1.77	0.66
9:I:200:GLU:OE2	42:q:93:MET:SD	2.53	0.65
10:J:44:LEU:CD2	10:J:52:GLY:HA3	2.26	0.65
18:R:70:ASN:HB2	18:R:111:PHE:CD1	2.31	0.65
21:V:38:PHE:CD1	21:V:95:LEU:HD21	2.31	0.65
34:i:15:LEU:HD21	39:n:164:PRO:HB2	1.78	0.65
41:p:70:ARG:CZ	41:p:91:GLN:HE21	2.09	0.65
52:Ah:39:GLU:O	52:Ah:42:VAL:HG12	1.96	0.65
54:Ak:37:ASP:HB3	54:Ak:42:LEU:HD11	1.77	0.65
13:M:373:ILE:CD1	13:M:454:ILE:HD11	2.25	0.65
15:O:38:TYR:HB3	15:O:299:GLN:NE2	2.11	0.65
23:X:160:PRO:HG3	29:d:22:PRO:HD3	1.78	0.65
30:e:95:PRO:HD2	30:e:98:HIS:ND1	2.08	0.65
45:AA:276:ARG:NH1	45:AA:278:ARG:HD2	2.11	0.65
47:AC:138:MET:HA	47:AC:138:MET:HE3	1.77	0.65
49:AE:206:LYS:HB2	49:AE:265:PHE:CE2	2.30	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.77	0.65
14:N:307:THR:CB	15:O:319:ILE:HD11	2.22	0.65
20:T:118:ILE:HG23	20:T:122:MET:HE3	1.78	0.65
22:W:65:LYS:HE2	22:W:110:PHE:HA	1.78	0.65
38:m:15:PRO:CG	38:m:18:LEU:HD12	2.27	0.65
48:AD:133:ARG:HG2	48:AD:171:LEU:O	1.96	0.65
49:AE:122:THR:HG21	53:AJ:25:ILE:HD13	1.79	0.65
49:AE:220:LEU:O	47:Ac:145:VAL:HA	1.97	0.65
3:C:102:HIS:CE1	21:V:48:THR:HG22	2.27	0.65
14:N:220:MET:C	14:N:223:ASN:H	2.04	0.65
16:P:263:PHE:HD1	16:P:333:PRO:HB2	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:h:201:CDL:H112	58:i:201:3PE:H331	1.77	0.65
45:AA:314:TYR:HB2	45:AA:371:PHE:CZ	2.30	0.65
52:AH:58:ARG:O	52:AH:61:THR:HG22	1.97	0.65
46:Ab:229:VAL:O	46:Ab:232:GLN:HG2	1.95	0.65
13:M:367:LEU:CD2	13:M:408:MET:HE2	2.25	0.65
18:R:42:ASP:HB3	18:R:44:ARG:HH11	1.61	0.65
19:S:16:LEU:HB3	19:S:69:TYR:CD1	2.32	0.65
21:V:44:TYR:CE1	21:V:48:THR:HG23	2.30	0.65
37:l:82:SER:HA	37:l:112:TYR:HB3	1.79	0.65
45:Aa:192:PHE:HB3	45:Aa:195:THR:OG1	1.96	0.65
46:Ab:138:LEU:HB3	46:Ab:237:PHE:CG	2.31	0.65
49:Ae:122:THR:HG21	53:Aj:25:ILE:HD13	1.79	0.65
50:Af:32:LEU:HD21	50:Af:66:ALA:HB2	1.77	0.65
52:Ah:29:THR:O	52:Ah:33:GLU:HG3	1.97	0.65
12:L:190:SER:HB2	12:L:196:TRP:HE1	1.60	0.65
12:L:386:LEU:HD11	35:j:69:ILE:HD11	1.79	0.65
14:N:258:THR:HB	14:N:333:SER:O	1.96	0.65
16:P:135:GLU:HB2	16:P:140:ASP:HA	1.78	0.65
18:R:32:THR:HG22	18:R:36:GLN:N	2.09	0.65
19:S:58:CYS:HB2	19:S:61:VAL:HG12	1.78	0.65
45:Aa:273:SER:HB3	51:Ag:19:LEU:HD12	1.78	0.65
46:Ab:278:ILE:HG22	46:Ab:331:SER:N	2.12	0.65
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.32	0.65
3:C:73:GLN:NE2	21:V:112:TRP:HE1	1.95	0.65
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
8:H:221:ALA:HA	61:H:401:UQ9:H20A	1.79	0.65
12:L:88:LEU:HD23	12:L:326:PHE:CE2	2.32	0.65
32:g:108:PRO:O	32:g:109:ASP:OD1	2.13	0.65
37:l:185:ASP:O	40:o:34:ARG:HD3	1.96	0.65
39:n:30:TRP:CD2	39:n:76:HIS:HD2	2.15	0.65
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.77	0.65
5:E:147:ILE:HD11	5:E:183:PRO:HB3	1.77	0.65
7:G:126:LEU:CD1	18:R:89:PRO:HB3	2.25	0.65
8:H:138:GLN:HG3	8:H:139:THR:N	2.11	0.65
58:L:705:3PE:H2A1	58:L:705:3PE:H261	1.79	0.65
13:M:263:LEU:HD11	38:m:102:TYR:CD1	2.31	0.65
15:O:343:TYR:CE1	15:O:355:LYS:HB2	2.31	0.65
19:S:48:HIS:CE1	19:S:95:LEU:CD2	2.80	0.65
35:j:47:PHE:HA	36:k:63:PHE:CZ	2.32	0.65
45:AA:68:THR:O	45:AA:406:THR:HG21	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
12:L:141:PHE:CD2	13:M:370:PRO:HG3	2.31	0.65
12:L:591:PHE:HE1	14:N:113:PHE:HD2	1.42	0.65
13:M:122:PHE:HD1	13:M:238:LEU:HG	1.62	0.65
58:M:501:3PE:H12	14:N:276:LEU:HD22	1.79	0.65
16:P:141:PHE:CD2	16:P:179:LYS:HD2	2.28	0.65
20:T:130:ILE:HG23	20:T:131:PRO:HD2	1.77	0.65
33:h:127:ASP:OD1	33:h:127:ASP:O	2.15	0.65
41:p:24:THR:HG22	41:p:26:LEU:H	1.62	0.65
47:AC:45:ILE:HA	67:AC:401:HEM:HAB	1.77	0.65
47:Ac:223:TYR:O	48:Ad:311:TRP:NE1	2.27	0.65
48:Ad:248:ILE:HG22	48:Ad:263:MET:HG3	1.79	0.65
2:B:98:ALA:CB	2:B:136:THR:H	2.10	0.65
6:F:110:PRO:HB3	6:F:152:ARG:HH12	1.62	0.65
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.65
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.65
11:K:66:PHE:CZ	14:N:35:PHE:CE1	2.84	0.65
12:L:387:THR:HG22	12:L:465:GLY:H	1.61	0.65
12:L:594:ASN:CG	14:N:110:PRO:CB	2.69	0.65
23:X:162:LYS:HB3	23:X:166:ARG:HH21	1.62	0.65
46:AB:43:LEU:HD12	46:AB:47:LEU:HD23	1.77	0.65
52:AH:48:LEU:CD1	52:AH:65:CYS:HB3	2.26	0.65
48:Ad:186:ARG:HE	48:Ad:193:LEU:HB2	1.62	0.65
48:Ad:201:VAL:HG21	48:Ad:275:ARG:HA	1.79	0.65
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
5:E:136:THR:HG22	5:E:137:THR:H	1.62	0.64
6:F:152:ARG:NH2	44:s:60:PRO:HG3	2.13	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.13	0.64
8:H:90:PRO:HD3	8:H:162:LEU:CD2	2.27	0.64
12:L:368:PHE:HB3	12:L:445:GLU:OE2	1.97	0.64
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.77	0.64
15:O:194:THR:HG23	15:O:307:TYR:HB2	1.79	0.64
16:P:166:HIS:HB3	16:P:200:ILE:CD1	2.27	0.64
17:Q:163:ASN:OD1	17:Q:164:PHE:N	2.31	0.64
40:o:71:ARG:HB3	40:o:71:ARG:HH11	1.61	0.64
41:p:74:ILE:HD13	41:p:85:ILE:HG13	1.80	0.64
47:AC:248:ASP:OD2	48:AD:202:ARG:NH1	2.30	0.64
68:AC:403:UQ6:H3M3	68:AC:403:UQ6:H4M2	1.78	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
13:M:119:TYR:CD1	13:M:160:LEU:HD22	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:166:LEU:HD11	58:M:501:3PE:H11	1.77	0.64
13:M:167:ILE:O	13:M:171:VAL:HG12	1.98	0.64
18:R:52:GLN:HE21	42:q:122:GLU:C	2.04	0.64
20:T:120:MET:HG2	22:W:44:ARG:HH11	1.61	0.64
23:X:167:PHE:HD2	23:X:170:TRP:NE1	1.94	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
4:D:137:ASP:OD1	4:D:148:GLU:OE2	2.14	0.64
7:G:386:LEU:HD21	7:G:523:VAL:CG1	2.28	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
10:J:22:LYS:NZ	11:K:22:PHE:CA	2.56	0.64
13:M:307:TRP:CD1	13:M:459:MET:SD	2.91	0.64
31:f:8:ARG:HE	31:f:8:ARG:HA	1.63	0.64
37:l:38:PRO:C	38:m:75:ASN:ND2	2.55	0.64
37:l:122:THR:CG2	37:l:123:PRO:HD2	2.27	0.64
47:AC:153:ILE:HG21	47:AC:156:ILE:HG12	1.79	0.64
49:Ae:156:LEU:HB2	49:Ae:269:ASP:C	2.23	0.64
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.64
12:L:556:ILE:CG2	38:m:80:PHE:CZ	2.81	0.64
14:N:307:THR:HG22	14:N:308:ASN:N	2.12	0.64
24:Y:137:LEU:HD23	24:Y:138:PHE:CG	2.31	0.64
45:AA:74:TRP:CZ3	45:AA:232:ALA:HB3	2.32	0.64
45:Aa:407:THR:HB	45:Aa:408:PRO:HD3	1.79	0.64
46:Ab:297:PRO:HB3	46:Ab:302:GLY:HA3	1.79	0.64
54:Ak:45:VAL:HB	54:Ak:48:ILE:HG22	1.78	0.64
1:A:67:LEU:CD1	11:K:68:ALA:CB	2.75	0.64
7:G:617:ARG:NH1	22:W:129:HIS:CA	2.59	0.64
10:J:25:PRO:HB3	11:K:27:MET:CG	2.28	0.64
12:L:81:LYS:N	12:L:135:ASN:HD21	1.96	0.64
29:d:60:ARG:O	29:d:61:GLN:C	2.40	0.64
32:g:140:PHE:CE2	41:p:74:ILE:HG22	2.33	0.64
62:h:201:CDL:HA62	62:h:201:CDL:H551	1.78	0.64
46:AB:164:VAL:HG23	49:AI:34:VAL:CG2	2.28	0.64
48:AD:248:ILE:HG22	48:AD:263:MET:HG3	1.79	0.64
49:Ae:234:TYR:HB2	49:Ae:243:TYR:HB2	1.79	0.64
12:L:385:PHE:HE2	35:j:73:PHE:HD1	1.45	0.64
13:M:300:SER:HB3	13:M:381:ILE:HG23	1.78	0.64
14:N:37:LEU:HD12	14:N:63:GLN:HB3	1.79	0.64
15:O:117:PHE:CE1	15:O:173:MET:CE	2.77	0.64
15:O:132:GLN:HE22	64:O:401:ADP:HN62	1.45	0.64
35:j:84:PHE:HE2	40:o:88:ASP:HB3	1.63	0.64
40:o:105:GLU:O	40:o:106:ARG:C	2.39	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.27	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
12:L:40:ILE:HD13	12:L:97:THR:HG22	1.79	0.64
12:L:56:HIS:HA	40:o:74:PHE:CD1	2.33	0.64
12:L:366:MET:CG	12:L:443:ILE:HG21	2.28	0.64
13:M:160:LEU:HD11	13:M:203:PHE:CZ	2.33	0.64
13:M:344:MET:HE1	38:m:59:HIS:NE2	2.13	0.64
41:p:5:TRP:HH2	41:p:12:GLU:OE1	1.81	0.64
45:Aa:249:HIS:O	45:Aa:250:LEU:HB2	1.97	0.64
46:Ab:300:LYS:HG2	46:Ab:301:ARG:HG3	1.79	0.64
1:A:62:PHE:HE2	10:J:62:GLY:HA3	1.63	0.64
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.64
2:B:99:CYS:CB	4:D:141:TYR:CG	2.80	0.64
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.64
12:L:41:LYS:HG3	12:L:98:TRP:CE2	2.33	0.64
16:P:88:VAL:HG12	16:P:92:MET:HE2	1.80	0.64
16:P:169:HIS:H	16:P:184:LYS:HE3	1.63	0.64
19:S:15:GLY:HA3	19:S:17:ARG:HH22	1.63	0.64
19:S:16:LEU:HD12	19:S:16:LEU:C	2.22	0.64
45:AA:337:LEU:HD21	45:AA:367:ASP:CG	2.22	0.64
47:AC:37:LEU:CB	67:AC:402:HEM:CMB	2.76	0.64
49:Ae:127:TYR:HA	54:Ak:34:TRP:HH2	1.62	0.64
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.80	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
8:H:316:PRO:HG3	25:Z:57:ARG:HB3	1.80	0.64
12:L:385:PHE:CD1	35:j:72:ARG:HG3	2.32	0.64
12:L:441:ILE:HD12	35:j:46:GLU:O	1.98	0.64
12:L:480:LEU:HD22	35:j:84:PHE:CD2	2.33	0.64
14:N:179:MET:HG3	14:N:216:PHE:HE1	1.63	0.64
19:S:69:TYR:CD2	19:S:75:LYS:HG3	2.33	0.64
20:T:83:VAL:HG23	20:T:126:PHE:HZ	1.63	0.64
20:T:87:LEU:HD21	20:T:104:PHE:CZ	2.32	0.64
25:Z:65:LEU:O	25:Z:68:ARG:HG2	1.98	0.64
27:b:48:ALA:O	27:b:49:THR:C	2.40	0.64
29:d:100:ASP:HB3	33:h:159:LEU:HD21	1.80	0.64
46:AB:91:THR:HB	46:AB:143:ALA:O	1.98	0.64
48:AD:111:ARG:HG3	48:AD:140:TYR:CZ	2.33	0.64
45:Aa:478:LEU:HD11	58:Ac:401:3PE:H11	1.80	0.64
1:A:52:SER:HB3	1:A:55:PHE:HB2	1.80	0.64
6:F:278:ILE:HG22	6:F:282:VAL:HG21	1.80	0.64
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:246:LEU:HD12	12:L:246:LEU:C	2.23	0.64
13:M:196:TRP:HZ3	13:M:261:PHE:HE2	1.44	0.64
17:Q:112:MET:SD	42:q:126:PRO:HB2	2.38	0.64
46:AB:326:PHE:HD1	49:AI:11:PHE:CG	2.16	0.64
48:AD:323:PRO:HG2	48:AD:325:LYS:HD2	1.80	0.64
49:AE:188:ALA:HA	49:AE:200:HIS:NE2	2.13	0.64
3:C:206:TYR:C	3:C:223:VAL:HG23	2.23	0.63
4:D:97:LEU:O	4:D:99:LEU:HG	1.98	0.63
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.79	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
12:L:586:LEU:HD21	24:Y:47:PRO:HD3	1.80	0.63
58:L:701:3PE:H262	58:L:701:3PE:H342	1.78	0.63
13:M:267:TRP:CZ2	13:M:271:MET:HE3	2.32	0.63
62:M:503:CDL:H132	14:N:242:THR:HG21	1.80	0.63
14:N:220:MET:HA	14:N:223:ASN:HA	1.79	0.63
21:V:38:PHE:CE1	21:V:95:LEU:HD21	2.33	0.63
62:d:201:CDL:H531	62:d:201:CDL:H711	1.79	0.63
31:f:56:TRP:CD1	33:h:134:GLU:OE1	2.51	0.63
34:i:29:SER:HB2	34:i:32:GLU:OE1	1.97	0.63
62:q:201:CDL:H1	43:r:3:SER:HB2	1.80	0.63
48:Ad:323:PRO:HG2	48:Ad:325:LYS:HD2	1.80	0.63
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.79	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
10:J:51:LEU:H	10:J:51:LEU:HD12	1.63	0.63
14:N:143:ILE:HA	14:N:194:LEU:HD11	1.79	0.63
19:S:16:LEU:CD2	19:S:19:ILE:HD11	2.28	0.63
35:j:84:PHE:CE2	40:o:88:ASP:HB3	2.34	0.63
37:l:106:HIS:CD2	37:l:107:TRP:N	2.67	0.63
39:n:95:GLU:HA	39:n:98:LYS:HG3	1.80	0.63
40:o:6:THR:HA	40:o:10:LEU:HD13	1.80	0.63
49:AI:43:LEU:HD13	46:Ab:160:ILE:HG23	1.80	0.63
49:AI:70:LEU:HD11	46:Ab:100:THR:HG23	1.79	0.63
45:Aa:190:THR:HA	45:Aa:193:GLN:HE21	1.62	0.63
46:Ab:117:GLU:OE2	46:Ab:331:SER:N	2.22	0.63
49:Ae:93:ARG:HA	51:Ag:25:ARG:HG3	1.79	0.63
49:Ae:188:ALA:HA	49:Ae:200:HIS:NE2	2.13	0.63
12:L:381:THR:HG21	12:L:498:PHE:CE2	2.33	0.63
15:O:167:PHE:HZ	15:O:244:THR:HB	1.61	0.63
15:O:176:GLN:HB2	15:O:178:TYR:CD2	2.32	0.63
20:T:93:ILE:CG2	20:T:110:LEU:HD13	2.28	0.63
40:o:15:VAL:HG23	40:o:16:GLU:N	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:426:LYS:O	46:AB:429:LYS:HG2	1.97	0.63
48:AD:255:TYR:OH	48:AD:266:VAL:HA	1.98	0.63
46:Ab:426:LYS:O	46:Ab:429:LYS:HG2	1.97	0.63
1:A:90:MET:SD	10:J:152:MET:HE3	2.39	0.63
1:A:104:TYR:HE2	10:J:167:ILE:CD1	2.11	0.63
10:J:151:MET:CE	14:N:28:LEU:HD13	2.24	0.63
13:M:250:LEU:O	13:M:250:LEU:CD1	2.44	0.63
13:M:368:ALA:HB1	13:M:375:LEU:CD1	2.25	0.63
16:P:284:THR:HG23	16:P:356:HIS:HB2	1.79	0.63
16:P:297:VAL:O	16:P:300:TRP:HB3	1.98	0.63
30:e:87:MET:HG2	30:e:92:TYR:O	1.99	0.63
32:g:75:ASP:OD1	32:g:76:SER:N	2.32	0.63
45:AA:388:VAL:HG22	45:AA:441:LEU:HD13	1.81	0.63
46:AB:90:THR:HG23	46:AB:95:SER:HA	1.79	0.63
45:Aa:182:VAL:HG22	49:Ae:80:HIS:CE1	2.34	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.63
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.63
10:J:46:PHE:CZ	11:K:46:VAL:HG13	2.34	0.63
12:L:100:ILE:HD13	12:L:341:MET:SD	2.39	0.63
12:L:305:SER:HB2	12:L:422:TYR:CE1	2.34	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
13:M:118:PHE:O	13:M:122:PHE:N	2.25	0.63
13:M:231:LEU:HA	13:M:235:LEU:HD12	1.80	0.63
15:O:63:ASP:OD2	15:O:165:SER:HB3	1.99	0.63
16:P:163:ARG:CD	16:P:253:THR:HA	2.27	0.63
25:Z:70:ALA:O	25:Z:73:PRO:HD2	1.99	0.63
36:k:34:PRO:HG2	36:k:59:TYR:CD1	2.34	0.63
45:AA:204:PRO:HB2	45:AA:206:GLU:OE1	1.99	0.63
48:Ad:158:PRO:HA	48:Ad:163:GLU:C	2.23	0.63
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.63
12:L:80:PHE:C	12:L:135:ASN:HD21	2.06	0.63
12:L:202:MET:HE3	12:L:265:PRO:CG	2.25	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:220:HIS:NE2	13:M:231:LEU:HB3	2.13	0.63
16:P:166:HIS:HE1	16:P:168:SER:HB2	1.63	0.63
18:R:112:LYS:O	18:R:113:GLN:C	2.40	0.63
39:n:133:TRP:HA	39:n:136:GLU:OE2	1.98	0.63
45:AA:63:GLN:HA	45:AA:235:GLY:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AI:20:ARG:HG2	49:AI:20:ARG:O	1.97	0.63
2:B:99:CYS:CB	4:D:141:TYR:CD2	2.82	0.63
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.64	0.63
5:E:176:LEU:HB2	5:E:184:MET:CE	2.29	0.63
7:G:117:MET:HE3	7:G:143:SER:CA	2.28	0.63
12:L:358:LYS:HG3	39:n:80:TYR:CE2	2.32	0.63
14:N:149:LEU:HD13	14:N:154:ILE:CG2	2.28	0.63
20:U:140:CYS:SG	20:U:143:GLU:OE2	2.53	0.63
23:X:83:THR:HA	23:X:86:TRP:CD1	2.34	0.63
23:X:160:PRO:HG3	29:d:22:PRO:CD	2.28	0.63
34:i:28:LEU:HD22	34:i:32:GLU:HG2	1.79	0.63
47:AC:197:LEU:HD11	68:AC:403:UQ6:H72	1.80	0.63
48:AD:186:ARG:HE	48:AD:193:LEU:HB2	1.62	0.63
50:AF:110:LYS:HA	54:Ak:10:TYR:HE1	1.62	0.63
1:A:67:LEU:CD1	11:K:68:ALA:HB3	2.29	0.63
2:B:92:PRO:HD2	2:B:121:PHE:N	2.13	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
4:D:348:LEU:O	25:Z:11:PRO:HB3	1.98	0.63
5:E:245:GLN:HB2	6:F:257:ARG:C	2.23	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.63
12:L:361:ASN:OD1	12:L:361:ASN:O	2.17	0.63
14:N:131:LEU:O	14:N:135:LYS:HG2	1.98	0.63
15:O:305:LEU:HD12	15:O:305:LEU:C	2.24	0.63
16:P:165:ILE:HA	16:P:199:ILE:O	1.98	0.63
30:e:69:ARG:HD2	30:e:72:THR:HG21	1.80	0.63
33:h:155:GLU:O	33:h:159:LEU:HD13	1.99	0.63
35:j:89:PRO:O	40:o:103:GLU:HG2	1.98	0.63
48:AD:321:TYR:HB2	50:AF:61:PHE:CZ	2.33	0.63
49:AE:234:TYR:HB2	49:AE:243:TYR:HB2	1.79	0.63
51:AG:79:GLU:HA	52:AH:58:ARG:CD	2.29	0.63
52:AH:26:ASP:HB3	52:AH:29:THR:HG23	1.79	0.63
45:Aa:341:PHE:CD2	45:Aa:368:MET:HE3	2.32	0.63
4:D:253:LEU:HD22	43:r:23:LYS:HB2	1.81	0.63
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.63
13:M:129:THR:HG21	13:M:235:LEU:HD13	1.80	0.63
19:S:16:LEU:HA	19:S:69:TYR:HA	1.79	0.63
27:b:66:VAL:HG22	27:b:75:GLY:HA3	1.81	0.63
36:k:42:LEU:HG	39:n:39:TYR:HD1	1.64	0.63
48:AD:217:GLY:O	48:AD:235:PRO:HD2	1.99	0.63
52:AH:54:ARG:CZ	52:AH:63:GLU:HB3	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.34	0.62
12:L:598:ILE:HG21	14:N:100:MET:HE2	1.81	0.62
16:P:239:PRO:HG2	16:P:345:LEU:HD12	1.80	0.62
20:T:138:LEU:HD12	20:T:138:LEU:C	2.24	0.62
20:T:138:LEU:O	20:T:138:LEU:CD1	2.40	0.62
23:X:25:LEU:HD11	26:a:50:ARG:NH2	2.13	0.62
43:r:109:ASP:O	43:r:110:GLN:HG2	1.99	0.62
49:AE:213:LEU:HD23	49:AE:260:VAL:HG22	1.81	0.62
47:Ac:150:LEU:CD1	47:Ac:164:ILE:HD12	2.29	0.62
48:Ad:217:GLY:O	48:Ad:235:PRO:HD2	1.99	0.62
5:E:48:PRO:HA	5:E:95:SER:HB2	1.81	0.62
7:G:127:ASP:HA	18:R:106:TYR:OH	1.99	0.62
12:L:445:GLU:HB2	12:L:450:LEU:CD2	2.29	0.62
14:N:100:MET:HE3	14:N:111:PHE:CZ	2.34	0.62
14:N:158:ALA:O	14:N:162:ILE:HG12	1.99	0.62
16:P:164:PHE:HE2	16:P:166:HIS:HB2	1.63	0.62
16:P:172:ALA:H	16:P:202:ARG:HH21	1.45	0.62
16:P:217:PHE:HA	16:P:220:TYR:HD2	1.63	0.62
22:W:55:LEU:CB	22:W:107:MET:HE2	2.30	0.62
23:X:130:LYS:HZ2	27:b:63:MET:HB2	1.64	0.62
39:n:31:CYS:SG	39:n:36:LYS:NZ	2.71	0.62
45:AA:117:GLY:HA2	46:AB:377:LYS:HG2	1.81	0.62
47:AC:147:THR:HG22	47:AC:161:VAL:HG13	1.80	0.62
49:AE:161:GLU:HA	49:AE:178:HIS:CG	2.34	0.62
46:Ab:233:VAL:HA	46:Ab:236:GLN:HG2	1.81	0.62
48:Ad:158:PRO:HB2	48:Ad:162:GLY:HA2	1.81	0.62
5:E:140:MET:HE1	6:F:366:ALA:HA	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
8:H:51:ASP:HA	8:H:54:LYS:HG2	1.80	0.62
8:H:248:TYR:HB3	8:H:250:ASN:OD1	2.00	0.62
12:L:437:PHE:CE1	12:L:441:ILE:CG1	2.69	0.62
15:O:61:THR:HB	15:O:160:GLU:O	2.00	0.62
32:g:106:TYR:CE2	33:h:86:ILE:HD12	2.35	0.62
45:AA:249:HIS:O	45:AA:250:LEU:HB2	1.97	0.62
45:Aa:204:PRO:HB2	45:Aa:206:GLU:OE1	1.99	0.62
47:Ac:9:PRO:HA	47:Ac:12:LYS:HE2	1.80	0.62
6:F:35:LEU:HD11	6:F:39:ASP:O	1.99	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
12:L:539:MET:SD	38:m:11:LEU:HD21	2.38	0.62
13:M:73:LEU:CD2	13:M:103:GLN:NE2	2.61	0.62
13:M:318:ALA:CB	13:M:373:ILE:HG23	2.29	0.62
15:O:121:PRO:O	15:O:122:LYS:CG	2.46	0.62
18:R:51:ARG:NH2	42:q:125:VAL:HG12	2.14	0.62
22:W:55:LEU:CB	22:W:107:MET:CE	2.75	0.62
31:f:13:HIS:O	31:f:17:PRO:HD2	2.00	0.62
49:AE:222:CYS:SG	47:Ac:145:VAL:HG22	2.40	0.62
48:Ad:255:TYR:OH	48:Ad:266:VAL:HA	1.98	0.62
50:Af:56:TYR:O	50:Af:60:MET:HG2	1.99	0.62
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
57:I:301:PC1:H361	57:I:301:PC1:H322	1.79	0.62
13:M:307:TRP:CE3	13:M:383:MET:HE3	2.34	0.62
15:O:132:GLN:HE22	15:O:169:PHE:HB2	1.64	0.62
23:X:115:LEU:HD13	23:X:117:TRP:CH2	2.34	0.62
24:Y:64:THR:OG1	24:Y:106:ARG:HG2	2.00	0.62
31:f:41:SER:OG	33:h:134:GLU:HG2	2.00	0.62
46:AB:94:ALA:HB1	46:AB:98:LYS:HD3	1.82	0.62
45:Aa:280:ASP:N	51:Ag:12:ARG:HG2	2.13	0.62
48:Ad:235:PRO:HA	48:Ad:240:GLN:HG3	1.82	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:289:LEU:HD23	8:H:289:LEU:C	2.25	0.62
12:L:365:ILE:HD11	12:L:366:MET:HE2	1.82	0.62
13:M:129:THR:HG21	13:M:235:LEU:CD1	2.30	0.62
13:M:307:TRP:HD1	13:M:459:MET:SD	2.23	0.62
15:O:113:SER:HB3	15:O:116:LYS:HB2	1.80	0.62
20:T:103:HIS:CD2	20:T:106:LYS:HD2	2.34	0.62
38:m:17:THR:O	38:m:18:LEU:HB2	1.99	0.62
48:AD:201:VAL:HG21	48:AD:275:ARG:HA	1.79	0.62
50:AF:108:TRP:CZ2	46:Ab:101:ARG:HB3	2.34	0.62
49:Ae:161:GLU:HA	49:Ae:178:HIS:CG	2.34	0.62
49:Ae:218:THR:CG2	49:Ae:256:LEU:O	2.45	0.62
2:B:99:CYS:HB2	4:D:141:TYR:CD1	2.35	0.62
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.81	0.62
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.77	0.62
7:G:339:ALA:C	7:G:545:LEU:HD12	2.25	0.62
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.81	0.62
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:LEU:HD11	10:J:56:PHE:CZ	2.35	0.62
12:L:153:LEU:HD11	13:M:360:LEU:HD11	1.81	0.62
14:N:207:ILE:O	14:N:211:LEU:HG	2.00	0.62
46:Ab:215:SER:CB	46:Ab:242:GLY:HA2	2.29	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.62
8:H:289:LEU:HD23	8:H:289:LEU:O	1.99	0.62
12:L:9:LEU:HD22	34:i:82:VAL:HG13	1.82	0.62
13:M:56:PHE:HE1	13:M:108:MET:HG2	1.64	0.62
16:P:43:HIS:H	16:P:51:VAL:HG13	1.64	0.62
20:U:112:SER:HB2	39:n:17:LEU:HD11	1.82	0.62
23:X:69:ASN:O	23:X:73:GLN:HG3	2.00	0.62
23:X:130:LYS:NZ	27:b:63:MET:HB2	2.14	0.62
37:l:57:MET:HG2	37:l:104:PRO:HG2	1.82	0.62
40:o:25:PHE:HB3	40:o:29:LEU:HD22	1.82	0.62
43:r:20:LEU:HD12	43:r:21:GLN:N	2.14	0.62
48:AD:235:PRO:HA	48:AD:240:GLN:HG3	1.82	0.62
46:Ab:40:PHE:HZ	46:Ab:396:ILE:HG23	1.65	0.62
46:Ab:412:VAL:O	46:Ab:415:GLN:HG2	2.00	0.62
1:A:71:LEU:HD21	11:K:65:VAL:HG21	1.81	0.62
1:A:90:MET:HG2	10:J:145:TYR:CD1	2.35	0.62
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.62
6:F:71:LYS:HE2	6:F:71:LYS:HA	1.82	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.62
10:J:129:ASP:OD2	10:J:135:LEU:HD13	2.00	0.62
13:M:395:LEU:HD21	38:m:101:TRP:CZ2	2.34	0.62
14:N:109:ALA:CB	14:N:110:PRO:HD3	2.30	0.62
27:b:67:PRO:HD2	27:b:72:ASP:HB2	1.82	0.62
40:o:39:MET:HE1	40:o:58:TYR:HA	1.81	0.62
48:Ad:159:ASN:HB2	48:Ad:165:PHE:HE2	1.64	0.62
49:Ae:179:ARG:HH12	49:Ae:201:ASP:HB2	1.64	0.62
1:A:73:LEU:N	1:A:74:PRO:HD2	2.15	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
5:E:131:ILE:HD11	5:E:168:PHE:HD2	1.65	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.62
7:G:311:LYS:HE3	7:G:313:LEU:HD13	1.82	0.62
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.34	0.62
13:M:98:MET:HE3	13:M:128:PRO:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:335:MET:O	14:N:335:MET:CG	2.41	0.62
15:O:117:PHE:HD1	15:O:128:SER:HA	1.64	0.62
23:X:164:GLY:O	23:X:165:THR:C	2.41	0.62
25:Z:28:ARG:HG3	25:Z:28:ARG:O	1.99	0.62
29:d:109:TYR:HB3	41:p:156:LEU:HD21	1.80	0.62
45:AA:313:HIS:CE1	45:AA:342:GLN:HA	2.35	0.62
46:AB:412:VAL:O	46:AB:415:GLN:HG2	2.00	0.62
52:AH:65:CYS:HA	52:AH:68:GLU:OE1	2.00	0.62
3:C:149:LEU:HD11	22:W:80:ARG:HH21	1.58	0.61
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
12:L:559:GLU:HA	12:L:563:PRO:HG2	1.82	0.61
14:N:338:PRO:HB3	62:d:201:CDL:H712	1.80	0.61
20:U:128:PHE:CZ	20:U:148:ILE:HG23	2.35	0.61
49:Ae:244:ASP:HB3	49:Ae:250:ARG:HH11	1.65	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
12:L:173:LEU:HD23	58:L:702:3PE:C32	2.30	0.61
18:R:98:GLU:CD	18:R:98:GLU:H	2.07	0.61
40:o:69:CYS:C	40:o:80:CYS:SG	2.82	0.61
41:p:5:TRP:CH2	41:p:12:GLU:OE1	2.53	0.61
46:AB:167:GLN:HE22	49:AI:33:ALA:C	2.08	0.61
47:AC:137:GLN:NE2	47:AC:141:TRP:HE1	1.98	0.61
47:AC:197:LEU:HD12	68:AC:403:UQ6:C1	2.30	0.61
67:AC:402:HEM:HBA1	68:AC:403:UQ6:C4M	2.30	0.61
49:AE:179:ARG:HH12	49:AE:201:ASP:HB2	1.64	0.61
45:Aa:388:VAL:HG22	45:Aa:441:LEU:HD13	1.81	0.61
49:Ae:213:LEU:HD23	49:Ae:260:VAL:HG22	1.82	0.61
4:D:109:CYS:O	4:D:111:PRO:HD3	1.99	0.61
5:E:222:PHE:N	5:E:225:GLU:HG2	2.15	0.61
12:L:10:LEU:HD23	12:L:46:ILE:HG21	1.82	0.61
13:M:73:LEU:CB	13:M:103:GLN:OE1	2.48	0.61
13:M:422:HIS:NE2	13:M:425:ASN:OD1	2.33	0.61
14:N:218:ALA:HB1	14:N:240:MET:SD	2.40	0.61
15:O:117:PHE:HE1	15:O:128:SER:HB2	1.63	0.61
15:O:326:ARG:HH21	32:g:56:ASP:CG	2.06	0.61
23:X:129:THR:HG23	27:b:68:SER:HA	1.81	0.61
23:X:158:LEU:HD13	29:d:17:GLU:CG	2.30	0.61
45:AA:366:ASP:O	45:AA:369:VAL:HB	2.01	0.61
52:AH:31:VAL:HG13	52:AH:83:LYS:HG3	1.81	0.61
7:G:334:GLU:OE1	19:S:71:PHE:CE1	2.51	0.61
8:H:81:LEU:HD22	8:H:108:THR:HG23	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.61
13:M:81:GLN:O	13:M:85:LYS:HB2	2.01	0.61
13:M:458:THR:HG21	41:p:148:ALA:HB1	1.81	0.61
14:N:17:PRO:HG2	14:N:133:TRP:CE2	2.35	0.61
16:P:41:ILE:HB	16:P:43:HIS:CE1	2.35	0.61
20:T:103:HIS:ND1	20:T:140:CYS:SG	2.73	0.61
34:i:95:TYR:OH	41:p:11:PRO:O	2.18	0.61
38:m:100:PHE:O	38:m:104:VAL:HG23	2.00	0.61
45:AA:367:ASP:O	45:AA:368:MET:C	2.41	0.61
50:AF:92:GLU:HB3	50:AF:93:PRO:HD3	1.81	0.61
1:A:90:MET:CG	10:J:145:TYR:CD1	2.82	0.61
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.61
4:D:94:VAL:O	4:D:94:VAL:HG23	1.99	0.61
6:F:266:GLY:HA3	6:F:271:SER:HA	1.82	0.61
13:M:98:MET:HE1	13:M:128:PRO:HA	1.83	0.61
13:M:139:GLN:HB3	13:M:222:GLU:HG3	1.83	0.61
13:M:318:ALA:HB2	13:M:373:ILE:CG2	2.30	0.61
13:M:373:ILE:H	13:M:448:THR:HG22	1.65	0.61
13:M:433:GLU:O	13:M:437:MET:HG2	2.01	0.61
14:N:175:MET:HE1	14:N:227:ILE:HA	1.80	0.61
15:O:140:LEU:HD21	15:O:304:VAL:O	2.00	0.61
16:P:156:SER:HB2	16:P:161:VAL:HG21	1.81	0.61
20:U:138:LEU:HB3	20:U:144:ILE:HG12	1.82	0.61
40:o:25:PHE:CE2	40:o:109:LEU:HD22	2.34	0.61
50:Af:29:LYS:HA	50:Af:81:TRP:CE2	2.35	0.61
1:A:90:MET:HG3	10:J:145:TYR:CE1	2.34	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:114:TYR:OH	10:J:33:ILE:HD12	1.99	0.61
12:L:468:ILE:O	12:L:472:ILE:HG23	2.00	0.61
13:M:162:ILE:HG23	14:N:271:MET:CE	2.29	0.61
14:N:273:ASN:HD21	24:Y:143:VAL:HA	1.63	0.61
15:O:213:GLU:O	15:O:217:ARG:HG3	2.00	0.61
32:g:123:LEU:HD12	41:p:98:VAL:CG1	2.31	0.61
37:l:62:TYR:CZ	37:l:64:PRO:HG3	2.36	0.61
42:q:10:GLY:HA2	62:q:201:CDL:OA6	2.00	0.61
42:q:34:ARG:NE	42:q:58:ARG:NH2	2.48	0.61
49:AE:218:THR:CG2	49:AE:256:LEU:O	2.45	0.61
68:Ac:406:UQ6:C13	68:Ac:406:UQ6:H101	2.30	0.61
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CE2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HE21	21:V:112:TRP:HE1	1.47	0.61
3:C:98:PHE:HA	21:V:90:LEU:CD1	2.28	0.61
5:E:222:PHE:CE1	6:F:48:ARG:HG3	2.36	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
8:H:87:VAL:HG13	8:H:95:LEU:HD23	1.83	0.61
8:H:224:PHE:HB3	61:H:401:UQ9:H20B	1.81	0.61
15:O:114:LEU:HA	15:O:131:LEU:CD2	2.30	0.61
15:O:140:LEU:HD11	15:O:198:TYR:CZ	2.35	0.61
19:S:48:HIS:HE1	19:S:95:LEU:HD22	1.63	0.61
33:h:106:ILE:O	33:h:106:ILE:HG22	1.99	0.61
42:q:71:LYS:O	42:q:72:ASN:CG	2.43	0.61
47:AC:287:LYS:HZ1	49:Ae:219:HIS:HA	1.65	0.61
50:Af:92:GLU:O	50:Af:96:LYS:HG3	2.01	0.61
2:B:98:ALA:O	55:B:301:SF4:S3	2.59	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:116:ILE:HD12	8:H:135:ALA:CB	2.30	0.61
8:H:301:CYS:O	8:H:305:ILE:HG13	2.01	0.61
16:P:268:PRO:CG	16:P:344:PRO:HA	2.30	0.61
49:AE:156:LEU:HB2	49:AE:269:ASP:CA	2.30	0.61
47:Ac:21:LEU:HD11	47:Ac:201:HIS:ND1	2.15	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
5:E:193:GLU:HB2	5:E:217:PRO:HG3	1.81	0.61
5:E:204:ILE:HG22	5:E:208:LYS:HG3	1.82	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.61
12:L:100:ILE:HG21	12:L:246:LEU:HD23	1.82	0.61
13:M:109:THR:HG22	13:M:121:LEU:HB3	1.82	0.61
17:Q:167:ASN:O	17:Q:168:LYS:CG	2.48	0.61
28:c:55:TRP:HE1	29:d:66:THR:HG21	1.66	0.61
36:k:47:LEU:HD12	39:n:43:LEU:HD23	1.83	0.61
45:AA:341:PHE:HE2	45:AA:372:LEU:HD13	1.64	0.61
48:AD:248:ILE:HD11	69:AD:401:HEC:HBB1	1.83	0.61
50:AF:83:LYS:HB2	50:AF:86:GLU:HB2	1.83	0.61
48:Ad:154:VAL:N	48:Ad:167:ARG:O	2.30	0.61
50:Af:75:ILE:HD12	50:Af:81:TRP:HZ2	1.65	0.61
51:Ag:64:ASN:O	51:Ag:68:GLU:HG2	2.01	0.61
8:H:127:TYR:CD2	8:H:207:LEU:HG	2.36	0.61
10:J:56:PHE:HA	10:J:60:LEU:HD13	1.82	0.61
12:L:182:PHE:CE2	12:L:186:MET:SD	2.94	0.61
13:M:1:MET:CE	13:M:111:SER:HB2	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AB:40:PHE:O	46:AB:40:PHE:HD1	1.84	0.61
46:Ab:307:SER:HB2	46:Ab:310:SER:HB2	1.83	0.61
46:Ab:313:VAL:HG21	46:Ab:323:VAL:HG21	1.83	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.60
10:J:166:ILE:HA	10:J:169:ILE:HG22	1.83	0.60
13:M:423:MET:O	13:M:424:ILE:C	2.44	0.60
18:R:32:THR:HA	18:R:55:VAL:HG23	1.83	0.60
24:Y:18:THR:HG22	24:Y:19:GLN:HG3	1.83	0.60
27:b:11:ASN:O	27:b:15:LYS:N	2.31	0.60
32:g:109:ASP:HB3	32:g:114:GLU:HB3	1.83	0.60
42:q:74:PHE:CD2	42:q:75:TRP:CD1	2.88	0.60
45:AA:92:PHE:HD1	45:AA:168:ILE:HD12	1.66	0.60
48:AD:95:PRO:HG2	52:AH:85:PHE:HB2	1.83	0.60
48:AD:133:ARG:HH22	49:AE:144:ALA:HB1	1.66	0.60
48:Ad:218:TYR:CD1	48:Ad:246:PRO:HG3	2.36	0.60
50:Af:108:TRP:HA	50:Af:111:LYS:NZ	2.15	0.60
1:A:64:LEU:CD1	10:J:163:ILE:HD13	2.31	0.60
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.83	0.60
7:G:35:PHE:O	7:G:101:ASN:HA	2.01	0.60
7:G:64:CYS:HG	7:G:75:CYS:HG	1.47	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
13:M:209:LEU:HD23	13:M:210:TYR:N	2.16	0.60
19:S:23:LEU:O	19:S:23:LEU:CD1	2.41	0.60
20:T:79:ILE:CB	20:T:145:VAL:HG13	2.28	0.60
21:V:35:LEU:HA	21:V:38:PHE:HD1	1.65	0.60
23:X:159:LYS:O	23:X:160:PRO:C	2.43	0.60
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.37	0.60
12:L:466:PHE:HB3	35:j:68:TRP:HZ2	1.65	0.60
14:N:59:TYR:CZ	14:N:63:GLN:HG3	2.36	0.60
21:V:82:LEU:O	21:V:86:LYS:HG3	2.00	0.60
25:Z:143:TYR:O	25:Z:144:THR:C	2.45	0.60
33:h:89:VAL:HG21	33:h:117:ILE:HD11	1.83	0.60
46:AB:171:THR:HA	49:AI:14:VAL:HG13	1.83	0.60
47:AC:150:LEU:HD11	47:AC:164:ILE:HD12	1.82	0.60
48:AD:321:TYR:HB2	50:AF:61:PHE:CE1	2.36	0.60
48:Ad:215:LEU:CD1	69:Ad:401:HEC:CMB	2.73	0.60
50:Af:42:GLU:HA	50:Af:45:LYS:HD3	1.82	0.60
4:D:80:MET:O	4:D:100:GLU:HA	2.02	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
4:D:304:LYS:HE2	9:I:35:THR:N	2.16	0.60
5:E:175:CYS:SG	6:F:122:PRO:HA	2.42	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:ILE:HD12	12:L:101:MET:HG3	1.83	0.60
16:P:55:VAL:CG1	16:P:123:SER:HA	2.30	0.60
31:f:49:ARG:NH2	33:h:106:ILE:HG22	2.15	0.60
51:AG:78:TYR:HB3	52:AH:63:GLU:HG3	1.81	0.60
48:Ad:155:GLN:HA	48:Ad:166:MET:HA	1.82	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
7:G:306:MET:HG2	7:G:316:TYR:HA	1.84	0.60
8:H:195:ARG:O	8:H:199:ASP:HB2	2.02	0.60
9:I:64:THR:HG21	57:I:301:PC1:H121	1.83	0.60
12:L:9:LEU:HD21	58:i:201:3PE:H2B1	1.83	0.60
14:N:100:MET:HE3	14:N:111:PHE:HZ	1.66	0.60
23:X:127:LYS:HD3	27:b:66:VAL:HG21	1.83	0.60
43:r:12:ARG:HB3	43:r:20:LEU:HD21	1.84	0.60
48:Ad:248:ILE:HD11	69:Ad:401:HEC:HBB1	1.84	0.60
53:Aj:31:PHE:HD1	54:Ak:47:TYR:HD2	1.48	0.60
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.31	0.60
7:G:126:LEU:HD11	18:R:89:PRO:HB3	1.82	0.60
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.66	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.84	0.60
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.60
12:L:42:PHE:O	12:L:46:ILE:HG12	2.01	0.60
12:L:222:GLY:CA	12:L:229:LEU:HD11	2.26	0.60
29:d:16:ASP:O	29:d:19:ARG:HG3	2.01	0.60
33:h:87:THR:HA	62:h:201:CDL:H512	1.83	0.60
45:Aa:192:PHE:HB2	45:Aa:198:ALA:HB2	1.84	0.60
6:F:158:ILE:CD1	6:F:166:ALA:HB2	2.32	0.60
7:G:343:GLY:HA3	7:G:550:ALA:HA	1.82	0.60
10:J:150:TRP:CD1	14:N:28:LEU:HD21	2.36	0.60
13:M:207:MET:HG3	13:M:239:GLY:HA3	1.83	0.60
13:M:269:MET:HE3	13:M:399:ASN:CB	2.32	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
62:Y:201:CDL:H361	62:Y:201:CDL:H151	1.83	0.60
32:g:106:TYR:OH	33:h:86:ILE:HG23	2.02	0.60
48:AD:218:TYR:CD1	48:AD:246:PRO:HG3	2.36	0.60
6:F:191:TYR:HE2	6:F:193:PHE:HD2	1.50	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
10:J:37:PHE:O	10:J:41:LEU:HG	2.02	0.60
16:P:136:THR:CG2	16:P:139:PHE:HB2	2.31	0.60
19:S:16:LEU:CB	19:S:69:TYR:HD1	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:73:PHE:HD2	33:h:74:TYR:CD1	2.20	0.60
49:AE:207:LYS:HD2	49:AE:210:TRP:HD1	1.66	0.60
46:Ab:38:LEU:HD22	46:Ab:406:TYR:CD2	2.37	0.60
2:B:141:MET:HE2	4:D:115:LEU:HD23	1.84	0.60
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.60
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.83	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
12:L:141:PHE:CD2	13:M:370:PRO:CG	2.85	0.60
12:L:204:SER:HA	12:L:207:ASN:HD22	1.67	0.60
13:M:144:ASN:HA	13:M:147:ILE:HD12	1.82	0.60
13:M:370:PRO:HA	13:M:375:LEU:HD22	1.83	0.60
14:N:276:LEU:C	14:N:276:LEU:HD12	2.26	0.60
16:P:146:VAL:HG23	16:P:187:GLY:HA2	1.83	0.60
16:P:350:ILE:HB	16:P:366:ILE:CG2	2.32	0.60
23:X:20:VAL:HG12	23:X:25:LEU:HD21	1.84	0.60
25:Z:120:LEU:HG	30:e:69:ARG:NH2	2.16	0.60
34:i:74:HIS:C	34:i:78:PRO:HG2	2.24	0.60
39:n:143:GLU:OE1	39:n:155:PRO:HB3	2.02	0.60
47:AC:94:LEU:HD13	67:AC:402:HEM:HAB	1.84	0.60
51:AG:64:ASN:O	51:AG:68:GLU:HG2	2.01	0.60
52:AH:46:GLU:O	52:AH:50:LEU:HG	2.01	0.60
49:Ae:207:LYS:HD2	49:Ae:210:TRP:HD1	1.66	0.60
6:F:44:ASN:OD1	6:F:49:HIS:HB2	2.02	0.60
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
12:L:56:HIS:O	40:o:71:ARG:HG3	2.01	0.60
62:L:703:CDL:H341	33:h:71:MET:SD	2.42	0.60
13:M:77:LEU:HD23	13:M:99:LEU:HD12	1.83	0.60
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.84	0.60
15:O:76:GLU:HG3	15:O:266:PRO:HG2	1.83	0.60
45:AA:61:SER:HB3	45:AA:242:LEU:HD22	1.84	0.60
47:AC:16:HIS:NE2	47:AC:201:HIS:NE2	2.49	0.60
45:Aa:402:HIS:HD2	45:Aa:403:LEU:HD11	1.66	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.59
4:D:253:LEU:HB2	43:r:23:LYS:CD	2.31	0.59
5:E:225:GLU:HG3	5:E:226:PRO:O	2.01	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.17	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.59
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.32	0.59
8:H:104:PHE:HE2	58:H:402:3PE:H362	1.66	0.59
12:L:556:ILE:HG23	38:m:80:PHE:CE2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:126:LEU:HD21	13:M:153:THR:HB	1.83	0.59
14:N:258:THR:CG2	14:N:336:THR:HG22	2.32	0.59
15:O:54:HIS:HB2	15:O:56:TYR:CE1	2.37	0.59
16:P:229:VAL:HB	16:P:323:HIS:CD2	2.37	0.59
24:Y:137:LEU:CD2	24:Y:138:PHE:CD2	2.84	0.59
33:h:102:PRO:HD2	33:h:105:TYR:CB	2.32	0.59
47:AC:116:GLY:C	67:AC:402:HEM:HMC2	2.27	0.59
47:AC:149:LEU:CA	49:Ae:220:LEU:HD22	2.21	0.59
47:AC:302:ALA:O	47:AC:305:PRO:HD2	2.02	0.59
51:AG:78:TYR:CZ	52:AH:62:GLU:HB2	2.36	0.59
50:Af:85:GLU:CD	50:Af:85:GLU:H	2.09	0.59
1:A:7:ILE:HD12	58:H:402:3PE:H392	1.84	0.59
2:B:115:ASP:HA	2:B:119:VAL:O	2.02	0.59
6:F:90:GLY:O	6:F:350:GLY:HA2	2.01	0.59
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
10:J:123:TRP:HH2	30:e:72:THR:C	2.09	0.59
10:J:168:GLU:CD	14:N:5:THR:HG21	2.27	0.59
20:U:90:TYR:CZ	20:U:92:LYS:HD2	2.35	0.59
22:W:64:ASP:O	22:W:68:GLU:HG3	2.02	0.59
26:a:3:PHE:CE2	62:q:201:CDL:HA4	2.35	0.59
33:h:73:PHE:CD2	33:h:74:TYR:CD1	2.90	0.59
50:AF:33:MET:HE3	50:AF:88:LYS:HG2	1.82	0.59
48:Ad:233:PHE:HA	48:Ad:240:GLN:O	2.02	0.59
50:Af:15:ASP:HA	50:Af:18:ARG:HB2	1.84	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
7:G:388:ASN:H	7:G:514:ASN:CB	2.15	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
12:L:123:LEU:HD22	12:L:150:MET:CG	2.33	0.59
12:L:247:LEU:HD12	12:L:248:HIS:CG	2.36	0.59
13:M:115:LEU:O	13:M:118:PHE:HB3	2.02	0.59
16:P:164:PHE:HB3	16:P:198:ALA:HB1	1.83	0.59
46:AB:46:GLY:HA3	46:AB:216:ALA:HA	1.82	0.59
46:AB:138:LEU:CD2	46:AB:238:LEU:HG	2.32	0.59
51:AG:14:VAL:O	51:AG:14:VAL:HG13	2.01	0.59
45:Aa:80:ARG:HH12	45:Aa:197:LEU:HD22	1.66	0.59
47:Ac:302:ALA:O	47:Ac:305:PRO:HD2	2.02	0.59
49:Ae:132:VAL:HA	49:Ae:135:GLN:NE2	2.17	0.59
49:Ae:163:LYS:O	49:Ae:177:ARG:HG3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.59
8:H:116:ILE:HD12	8:H:135:ALA:HB1	1.85	0.59
12:L:313:MET:HE2	12:L:328:HIS:CE1	2.38	0.59
12:L:598:ILE:HD11	14:N:153:ILE:CG1	2.32	0.59
13:M:127:ILE:HG12	14:N:254:LEU:HD21	1.84	0.59
13:M:294:MET:HE3	13:M:319:HIS:CD2	2.37	0.59
15:O:126:GLY:CA	32:g:51:MET:HE1	2.32	0.59
16:P:180:SER:O	16:P:184:LYS:HG3	2.03	0.59
17:Q:167:ASN:HB3	44:s:64:ARG:HE	1.67	0.59
18:R:40:GLU:HA	18:R:45:ARG:CZ	2.33	0.59
23:X:124:GLN:HA	23:X:127:LYS:HE3	1.83	0.59
25:Z:54:ASN:O	25:Z:58:ARG:HG2	2.02	0.59
35:j:94:ASP:HB3	35:j:99:ILE:HB	1.83	0.59
46:AB:255:GLY:HA3	46:AB:435:LYS:HD2	1.85	0.59
49:AE:132:VAL:HA	49:AE:135:GLN:NE2	2.17	0.59
45:Aa:193:GLN:OE1	45:Aa:271:THR:HG21	2.02	0.59
10:J:2:ASN:HB3	10:J:121:GLY:CA	2.31	0.59
12:L:81:LYS:HB2	12:L:135:ASN:OD1	2.03	0.59
33:h:69:ARG:O	33:h:73:PHE:HB2	2.02	0.59
45:AA:399:LEU:HD12	45:AA:426:LEU:HD23	1.84	0.59
46:AB:101:ARG:HB3	50:Af:108:TRP:CZ2	2.37	0.59
46:AB:313:VAL:HG21	46:AB:323:VAL:HG21	1.83	0.59
49:AE:220:LEU:HA	47:Ac:148:ASN:HB2	1.83	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
8:H:183:MET:HE2	57:I:301:PC1:H291	1.85	0.59
12:L:312:LEU:CD2	12:L:395:ILE:HG21	2.33	0.59
19:S:63:PRO:HB2	19:S:79:LEU:HB2	1.85	0.59
20:T:83:VAL:CG2	20:T:126:PHE:CZ	2.83	0.59
20:U:120:MET:HE1	39:n:24:LEU:HD12	1.83	0.59
22:W:104:THR:O	22:W:108:ARG:HG3	2.02	0.59
25:Z:120:LEU:HD11	30:e:69:ARG:HG2	1.84	0.59
31:f:38:ARG:HD3	31:f:56:TRP:CD1	2.38	0.59
35:j:52:ARG:NE	35:j:52:ARG:HA	2.17	0.59
38:m:37:LEU:HA	38:m:40:ARG:HG2	1.83	0.59
42:q:51:ASP:O	42:q:59:HIS:HB2	2.02	0.59
42:q:96:ASP:OD1	42:q:97:PRO:CD	2.50	0.59
42:q:98:PRO:O	42:q:99:THR:C	2.45	0.59
42:q:137:TRP:CZ2	42:q:140:PRO:HD3	2.38	0.59
48:AD:160:ASP:O	48:Ad:183:GLU:HB3	2.02	0.59
50:Af:75:ILE:HD12	50:Af:81:TRP:CZ2	2.37	0.59
51:Ag:19:LEU:CD2	51:Ag:24:GLN:HB3	2.29	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:PRO:CG	2:B:119:VAL:HG13	2.31	0.59
8:H:172:MET:HE1	25:Z:46:GLY:CA	2.33	0.59
8:H:224:PHE:CD2	61:H:401:UQ9:H20B	2.37	0.59
10:J:134:MET:HE1	27:b:51:TYR:CE1	2.37	0.59
12:L:227:PHE:CD2	12:L:283:LEU:CD2	2.86	0.59
12:L:424:MET:HE2	12:L:502:LEU:HB2	1.85	0.59
12:L:460:GLY:HA2	58:L:701:3PE:O12	2.02	0.59
13:M:209:LEU:HD23	13:M:211:GLY:H	1.67	0.59
13:M:350:MET:HG2	39:n:99:VAL:HG12	1.83	0.59
15:O:343:TYR:HE1	15:O:355:LYS:HB2	1.66	0.59
16:P:328:MET:HG3	16:P:330:THR:H	1.67	0.59
16:P:357:ARG:HD3	16:P:361:TRP:O	2.03	0.59
21:V:90:LEU:HD21	21:V:94:MET:CE	2.33	0.59
24:Y:141:PRO:HB2	33:h:161:ARG:NH1	2.17	0.59
32:g:139:TYR:HD2	32:g:140:PHE:CD1	2.20	0.59
62:h:201:CDL:H531	62:h:201:CDL:HA31	1.85	0.59
45:AA:172:MET:HE1	45:AA:205:SER:HA	1.85	0.59
46:AB:286:PHE:CE1	46:AB:427:ALA:HB1	2.38	0.59
47:AC:215:ALA:HA	51:AG:11:ILE:HD11	1.84	0.59
47:AC:345:HIS:CE1	47:AC:346:PRO:HB3	2.37	0.59
49:AE:244:ASP:HB3	49:AE:250:ARG:HH11	1.65	0.59
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.85	0.59
3:C:102:HIS:HE1	21:V:48:THR:CG2	2.12	0.59
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.59
12:L:605:ASN:O	12:L:606:LEU:C	2.46	0.59
13:M:275:ILE:HD11	13:M:288:TYR:CB	2.33	0.59
14:N:300:THR:HG23	14:N:301:SER:N	2.17	0.59
18:R:42:ASP:HB3	18:R:44:ARG:NH1	2.17	0.59
24:Y:110:TYR:CD2	58:m:201:3PE:H112	2.37	0.59
25:Z:98:MET:HB2	25:Z:104:TRP:NE1	2.18	0.59
26:a:36:LYS:HA	26:a:59:ARG:HH22	1.68	0.59
30:e:41:ILE:CD1	33:h:174:PRO:HB2	2.33	0.59
33:h:96:ALA:O	41:p:63:TYR:HE1	1.85	0.59
49:AE:220:LEU:CD2	47:Ac:149:LEU:HA	2.33	0.59
46:Ab:236:GLN:HG3	46:Ab:237:PHE:CD2	2.38	0.59
51:Ag:35:ILE:HD11	62:Ag:102:CDL:H322	1.84	0.59
1:A:104:TYR:CE2	10:J:167:ILE:CD1	2.86	0.59
4:D:67:ASN:HB2	15:O:193:LEU:HD22	1.84	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
7:G:337:ALA:O	7:G:543:LYS:N	2.36	0.59
12:L:173:LEU:HD23	58:L:702:3PE:H322	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:542:LEU:CD2	37:l:116:ARG:HD2	2.32	0.59
13:M:14:LEU:HD21	13:M:26:ASN:HB2	1.84	0.59
14:N:200:LEU:HD22	14:N:269:GLU:HG3	1.84	0.59
15:O:167:PHE:CZ	15:O:244:THR:HB	2.38	0.59
20:U:105:MET:SD	20:U:139:MET:HE1	2.42	0.59
23:X:120:PRO:HB2	23:X:125:LEU:HD11	1.85	0.59
25:Z:105:LYS:O	25:Z:106:VAL:C	2.46	0.59
27:b:8:PHE:HA	27:b:11:ASN:ND2	2.18	0.59
36:k:58:ARG:HD2	39:n:34:ARG:HG3	1.83	0.59
39:n:111:GLU:O	39:n:114:MET:HG2	2.03	0.59
48:AD:233:PHE:HA	48:AD:240:GLN:O	2.02	0.59
49:AE:159:ILE:O	49:AE:210:TRP:HH2	1.86	0.59
45:Aa:55:ASN:HB3	45:Aa:226:ALA:HB1	1.84	0.59
49:Ae:159:ILE:O	49:Ae:210:TRP:HH2	1.86	0.59
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.59
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.59
14:N:243:MET:HG2	29:d:44:MET:HE2	1.85	0.59
23:X:44:MET:HE1	25:Z:73:PRO:HA	1.84	0.59
27:b:6:SER:O	27:b:9:LEU:HB3	2.03	0.59
45:AA:363:MET:N	45:AA:363:MET:SD	2.76	0.59
46:AB:117:GLU:OE2	46:AB:331:SER:N	2.22	0.59
49:AI:62:ARG:HB3	49:AI:63:PRO:HD2	1.84	0.59
54:AK:37:ASP:O	54:AK:39:ARG:HG3	2.03	0.59
46:Ab:43:LEU:HD12	46:Ab:47:LEU:HD23	1.84	0.59
48:Ad:223:THR:HG21	52:Ah:52:ASP:CA	2.19	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.58
10:J:19:LEU:HD21	11:K:31:LEU:O	2.03	0.58
10:J:56:PHE:CE1	10:J:60:LEU:HD22	2.38	0.58
10:J:164:PHE:CD2	14:N:8:ILE:HG13	2.36	0.58
12:L:230:HIS:N	12:L:231:PRO:CD	2.66	0.58
12:L:417:SER:HB3	12:L:493:ILE:CG1	2.31	0.58
12:L:532:ILE:HG21	37:l:133:LEU:HD22	1.85	0.58
13:M:210:TYR:O	13:M:213:HIS:CD2	2.56	0.58
13:M:396:MET:HG3	13:M:396:MET:O	2.03	0.58
14:N:319:LYS:HA	15:O:302:THR:HG21	1.84	0.58
15:O:323:GLN:NE2	32:g:54:GLN:C	2.61	0.58
20:T:90:TYR:CE2	20:T:92:LYS:HB3	2.38	0.58
21:V:31:THR:HG22	21:V:88:LEU:HD13	1.85	0.58
30:e:45:HIS:CD2	33:h:176:LYS:HZ2	2.21	0.58
33:h:95:GLU:HB3	33:h:114:LYS:HG2	1.85	0.58
37:l:155:PRO:HG3	40:o:4:HIS:CG	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:26:PRO:HB2	40:o:28:ASP:OD1	2.02	0.58
62:q:201:CDL:H722	62:q:201:CDL:H512	1.84	0.58
49:AE:152:ILE:HG21	49:AE:273:VAL:C	2.28	0.58
51:AG:19:LEU:CD2	51:AG:24:GLN:HB3	2.29	0.58
49:AI:78:PHE:HZ	46:Ab:168:ASN:ND2	1.99	0.58
47:Ac:119:LEU:HD22	67:Ac:403:HEM:HBB2	1.84	0.58
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.58
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
12:L:466:PHE:CE1	12:L:470:TYR:HE2	2.21	0.58
14:N:77:ASN:OD1	14:N:81:LEU:HD12	2.04	0.58
14:N:109:ALA:CB	14:N:110:PRO:CD	2.81	0.58
20:T:103:HIS:HB2	20:T:106:LYS:HB2	1.83	0.58
20:U:119:ILE:HD11	20:U:138:LEU:HB2	1.85	0.58
23:X:53:PRO:HD3	25:Z:116:TRP:CG	2.38	0.58
25:Z:144:THR:HA	26:a:45:TRP:CZ3	2.35	0.58
28:c:30:TYR:HB2	28:c:34:PRO:HD3	1.85	0.58
34:i:111:LEU:HD11	41:p:20:PRO:HD3	1.84	0.58
40:o:12:ASP:HB3	40:o:15:VAL:HG22	1.84	0.58
47:AC:146:ILE:O	47:AC:149:LEU:HB3	2.02	0.58
47:Ac:345:HIS:CE1	47:Ac:346:PRO:HB3	2.38	0.58
4:D:51:VAL:HG21	4:D:58:THR:HG22	1.83	0.58
12:L:556:ILE:HD11	38:m:76:ILE:HG22	1.83	0.58
14:N:179:MET:CG	14:N:216:PHE:HE1	2.16	0.58
15:O:124:ASN:O	32:g:51:MET:HG2	2.03	0.58
23:X:78:CYS:SG	23:X:110:CYS:HB3	2.42	0.58
23:X:127:LYS:HD3	27:b:66:VAL:CG2	2.34	0.58
31:f:11:TRP:O	31:f:14:ILE:HG22	2.02	0.58
37:l:113:ILE:HG12	37:l:114:ARG:H	1.67	0.58
41:p:37:TYR:CZ	41:p:41:VAL:HG11	2.38	0.58
45:AA:68:THR:HG22	45:AA:136:LEU:HD23	1.83	0.58
51:AG:11:ILE:HG22	51:AG:12:ARG:N	2.18	0.58
46:Ab:276:ALA:HB2	46:Ab:282:GLU:HB3	1.85	0.58
48:Ad:111:ARG:HG3	48:Ad:140:TYR:CZ	2.39	0.58
4:D:37:TRP:CZ2	4:D:39:PRO:HA	2.38	0.58
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.19	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
12:L:407:TRP:CZ3	12:L:410:LEU:HD11	2.38	0.58
12:L:525:LEU:HD21	39:n:77:PRO:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:318:LYS:O	16:P:322:ILE:HG13	2.02	0.58
17:Q:166:TRP:CE3	44:s:67:PRO:HG3	2.38	0.58
19:S:47:ALA:O	19:S:49:PRO:HD3	2.03	0.58
20:U:105:MET:CG	20:U:139:MET:HE1	2.33	0.58
25:Z:122:GLY:O	25:Z:126:GLY:N	2.34	0.58
27:b:27:GLY:O	27:b:30:ILE:HG22	2.02	0.58
37:l:105:ILE:HG23	37:l:109:LEU:HD22	1.84	0.58
46:Ab:286:PHE:CE1	46:Ab:427:ALA:HB1	2.38	0.58
47:Ac:98:VAL:HG22	67:Ac:403:HEM:HBC2	1.85	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
12:L:404:THR:HG22	12:L:405:ASN:N	2.19	0.58
41:p:128:GLU:O	41:p:131:GLN:N	2.37	0.58
47:AC:214:ASP:HB3	51:AG:9:ALA:HB2	1.85	0.58
49:AE:168:LYS:HD2	47:Ac:262:LEU:CD1	2.33	0.58
45:Aa:92:PHE:HD1	45:Aa:168:ILE:HD12	1.66	0.58
50:Af:19:LYS:HG2	50:Af:84:TYR:CG	2.39	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
13:M:196:TRP:HZ3	13:M:261:PHE:CE2	2.21	0.58
15:O:49:THR:O	15:O:53:LEU:HG	2.04	0.58
19:S:16:LEU:HD11	19:S:51:LEU:CD1	2.29	0.58
32:g:147:LEU:HD11	41:p:163:MET:HB3	1.86	0.58
38:m:75:ASN:O	38:m:75:ASN:OD1	2.20	0.58
49:Ae:156:LEU:HD13	49:Ae:210:TRP:NE1	2.19	0.58
1:A:55:PHE:O	1:A:56:PHE:C	2.46	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.86	0.58
4:D:375:MET:HE1	7:G:126:LEU:CA	2.34	0.58
7:G:49:VAL:HB	7:G:91:ALA:HA	1.86	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:288:LEU:HA	8:H:292:ASN:HB2	1.86	0.58
14:N:147:PRO:HB2	14:N:148:LEU:HD12	1.86	0.58
21:V:28:TYR:HE2	21:V:59:VAL:HG21	1.69	0.58
25:Z:135:ASN:O	25:Z:139:GLY:HA3	2.04	0.58
33:h:96:ALA:HB3	41:p:63:TYR:CD1	2.38	0.58
48:AD:218:TYR:CG	48:AD:246:PRO:HG3	2.38	0.58
49:AE:163:LYS:O	49:AE:177:ARG:HG3	2.02	0.58
48:Ad:218:TYR:CG	48:Ad:246:PRO:HG3	2.38	0.58
49:Ae:160:PRO:O	49:Ae:178:HIS:HB3	2.03	0.58
3:C:120:THR:OG1	17:Q:128:PHE:HA	2.04	0.58
4:D:166:ARG:HH22	25:Z:10:MET:HG2	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
5:E:126:VAL:HG21	5:E:130:HIS:ND1	2.19	0.58
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.58
6:F:116:ASN:OD1	6:F:244:ASN:HA	2.03	0.58
12:L:15:LEU:O	12:L:18:PRO:HD2	2.03	0.58
13:M:73:LEU:HB2	13:M:103:GLN:OE1	2.02	0.58
58:M:501:3PE:O22	14:N:276:LEU:HD13	2.03	0.58
14:N:26:LEU:O	14:N:27:MET:C	2.46	0.58
16:P:275:HIS:HB3	16:P:372:ALA:HB1	1.86	0.58
23:X:167:PHE:HB3	23:X:170:TRP:CD1	2.39	0.58
25:Z:110:VAL:CG1	30:e:72:THR:HG23	2.33	0.58
29:d:14:LEU:HD12	29:d:14:LEU:C	2.27	0.58
38:m:127:ILE:HG22	41:p:136:THR:HG23	1.84	0.58
50:Af:41:THR:H	50:Af:44:VAL:HB	1.68	0.58
2:B:112:TYR:CZ	9:I:84:ILE:HD11	2.37	0.58
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.85	0.58
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.86	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.58
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.58
12:L:550:LEU:HB2	13:M:275:ILE:HG22	1.86	0.58
14:N:149:LEU:HD11	14:N:195:PRO:HG3	1.84	0.58
20:U:100:VAL:C	20:U:141:PRO:HG2	2.28	0.58
23:X:154:ILE:HG22	29:d:88:HIS:CE1	2.38	0.58
31:f:39:ASN:O	31:f:45:GLN:HG3	2.04	0.58
45:AA:51:SER:HB2	45:AA:243:LEU:HD13	1.85	0.58
47:AC:245:PHE:HE1	48:AD:102:LEU:HD23	1.69	0.58
51:AG:11:ILE:HG21	51:AG:14:VAL:HG11	1.84	0.58
7:G:387:LEU:HD21	7:G:516:LEU:HB3	1.85	0.58
12:L:232:TRP:CZ3	12:L:233:LEU:HD21	2.37	0.58
13:M:109:THR:HG22	13:M:121:LEU:CB	2.34	0.58
14:N:33:LEU:HD11	14:N:141:ILE:HD12	1.86	0.58
17:Q:166:TRP:HE3	44:s:67:PRO:HG3	1.67	0.58
20:T:90:TYR:CE2	20:T:92:LYS:CB	2.87	0.58
23:X:20:VAL:C	26:a:54:ILE:HD13	2.29	0.58
30:e:14:LEU:HD12	30:e:15:ASP:CB	2.33	0.58
32:g:121:GLU:HA	32:g:124:VAL:HG22	1.86	0.58
45:AA:276:ARG:HH12	45:AA:278:ARG:CD	2.16	0.58
45:AA:295:GLY:O	45:AA:301:ASN:ND2	2.35	0.58
47:AC:141:TRP:O	47:AC:145:VAL:HG23	2.04	0.58
48:AD:155:GLN:CB	48:AD:166:MET:HG2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:152:ILE:HD13	49:AE:169:TRP:CD1	2.38	0.58
45:Aa:220:LEU:O	45:Aa:224:TYR:HB2	2.04	0.58
48:Ad:120:VAL:O	69:Ad:401:HEC:HMC3	2.04	0.58
5:E:135:THR:OG1	5:E:172:GLU:CG	2.52	0.57
6:F:109:ARG:NH2	6:F:232:ASP:O	2.36	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.57
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.57
12:L:425:ARG:HG3	12:L:429:PHE:CE2	2.39	0.57
15:O:63:ASP:OD2	15:O:165:SER:CB	2.52	0.57
15:O:76:GLU:HG3	15:O:266:PRO:CG	2.34	0.57
15:O:117:PHE:CD1	15:O:128:SER:CB	2.87	0.57
32:g:140:PHE:CZ	41:p:74:ILE:HG22	2.39	0.57
49:AE:114:SER:HB2	51:AG:22:PHE:HE2	1.68	0.57
50:AF:106:GLU:O	50:AF:110:LYS:HG3	2.03	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
10:J:133:VAL:HG22	25:Z:68:ARG:CZ	2.33	0.57
12:L:593:ILE:CG2	24:Y:41:TYR:CE2	2.87	0.57
20:U:125:GLU:OE2	35:j:44:TYR:OH	2.21	0.57
24:Y:63:PHE:HE2	24:Y:106:ARG:HE	1.53	0.57
25:Z:129:THR:HB	25:Z:132:GLU:HG3	1.86	0.57
48:AD:94:TYR:HE2	52:AH:84:LEU:HD23	1.68	0.57
50:Af:89:PHE:HB3	50:Af:92:GLU:HB2	1.85	0.57
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.85	0.57
4:D:279:THR:CG2	21:V:13:GLY:HA3	2.22	0.57
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.57
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
11:K:96:LEU:O	11:K:97:GLN:C	2.47	0.57
12:L:592:LEU:O	12:L:596:ILE:HG12	2.04	0.57
19:S:65:LEU:HB2	19:S:79:LEU:HD11	1.84	0.57
25:Z:86:ILE:HG23	25:Z:128:ARG:NE	2.15	0.57
40:o:15:VAL:HG23	40:o:16:GLU:H	1.69	0.57
45:AA:87:ASN:HD21	45:AA:199:GLN:HB2	1.69	0.57
45:AA:220:LEU:O	45:AA:224:TYR:HB2	2.04	0.57
47:AC:145:VAL:HG22	49:Ae:222:CYS:SG	2.44	0.57
45:Aa:118:ALA:O	46:Ab:298:HIS:HB3	2.04	0.57
45:Aa:172:MET:HE1	45:Aa:205:SER:HA	1.85	0.57
1:A:104:TYR:HE2	10:J:167:ILE:HD13	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:151:MET:HE2	10:J:151:MET:HA	1.86	0.57
13:M:230:ILE:HG13	13:M:235:LEU:HG	1.87	0.57
13:M:296:LEU:HD22	13:M:396:MET:HE1	1.85	0.57
13:M:297:VAL:O	13:M:301:ILE:HG12	2.03	0.57
14:N:154:ILE:HG12	14:N:195:PRO:HG2	1.86	0.57
14:N:253:GLY:N	14:N:290:LEU:HD11	2.19	0.57
16:P:56:ALA:HA	16:P:125:VAL:O	2.03	0.57
21:V:31:THR:O	21:V:35:LEU:HG	2.04	0.57
48:AD:94:TYR:HB3	52:AH:85:PHE:CE2	2.40	0.57
45:Aa:171:GLU:O	45:Aa:175:ASN:N	2.37	0.57
45:Aa:286:HIS:CD2	45:Aa:359:VAL:HG13	2.38	0.57
52:Ah:51:CYS:CA	52:Ah:54:ARG:HB3	2.33	0.57
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.34	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
13:M:172:GLY:C	13:M:173:THR:HG23	2.28	0.57
13:M:447:LEU:HD21	13:M:454:ILE:CD1	2.33	0.57
15:O:80:GLN:CG	15:O:270:VAL:HG21	2.18	0.57
25:Z:120:LEU:HB2	25:Z:123:GLU:HG3	1.87	0.57
30:e:101:ARG:NE	30:e:101:ARG:HA	2.20	0.57
45:AA:51:SER:CB	45:AA:243:LEU:HD13	2.34	0.57
45:AA:171:GLU:O	45:AA:175:ASN:N	2.37	0.57
46:AB:162:LYS:NZ	46:AB:194:ASP:OD1	2.38	0.57
48:AD:120:VAL:O	69:AD:401:HEC:HMC3	2.04	0.57
48:AD:249:TYR:CE2	48:AD:252:VAL:HA	2.40	0.57
51:AG:35:ILE:HB	51:AG:36:PRO:HD3	1.87	0.57
48:Ad:249:TYR:CE2	48:Ad:252:VAL:HA	2.40	0.57
49:Ae:127:TYR:HA	54:Ak:34:TRP:CH2	2.39	0.57
51:Ag:27:PHE:HB3	51:Ag:30:TYR:HB2	1.87	0.57
52:Ah:58:ARG:HG2	52:Ah:61:THR:HB	1.86	0.57
3:C:104:ASN:O	43:r:97:PRO:HD3	2.04	0.57
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
7:G:73:GLY:HA2	59:G:803:FES:S1	2.45	0.57
8:H:64:LEU:HD12	16:P:362:LEU:HD11	1.86	0.57
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.86	0.57
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.86	0.57
10:J:122:ASP:O	10:J:123:TRP:CD1	2.50	0.57
13:M:444:LEU:O	13:M:448:THR:HG23	2.04	0.57
14:N:284:MET:O	14:N:287:LEU:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:354:LEU:HG	28:c:44:VAL:HG22	1.86	0.57
37:l:166:LEU:HB2	37:l:170:ARG:NH2	2.19	0.57
48:AD:284:HIS:NE2	48:AD:288:MET:HE3	2.19	0.57
50:AF:110:LYS:HA	54:Ak:10:TYR:CE1	2.39	0.57
45:Aa:338:CYS:HB2	45:Aa:368:MET:SD	2.45	0.57
48:Ad:290:LEU:CD2	53:Aj:44:TYR:HB2	2.32	0.57
54:Ak:14:ALA:O	54:Ak:18:ILE:HG12	2.05	0.57
1:A:83:LYS:CE	10:J:146:SER:CB	2.58	0.57
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.87	0.57
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.19	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:136:GLU:CD	17:Q:87:MET:HG3	2.29	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
10:J:85:ASN:O	10:J:89:LEU:HG	2.04	0.57
12:L:227:PHE:CD2	12:L:283:LEU:HD21	2.38	0.57
12:L:425:ARG:HG3	12:L:429:PHE:HE2	1.68	0.57
13:M:4:ILE:CG2	13:M:107:ILE:HD13	2.29	0.57
13:M:14:LEU:HD11	13:M:26:ASN:HB3	1.87	0.57
13:M:73:LEU:HD22	13:M:103:GLN:NE2	2.19	0.57
15:O:100:ASP:O	28:c:31:VAL:HG23	2.04	0.57
20:U:93:ILE:HD11	20:U:110:LEU:HD11	1.86	0.57
20:U:155:TYR:OH	33:h:52:LYS:HD2	2.04	0.57
49:AE:155:LYS:HG3	49:AE:269:ASP:O	2.04	0.57
49:AE:156:LEU:HD13	49:AE:210:TRP:NE1	2.19	0.57
50:AF:24:ALA:O	51:AG:48:ARG:NH2	2.36	0.57
52:AH:35:CYS:HB3	52:AH:79:CYS:SG	2.45	0.57
47:Ac:8:HIS:CE1	47:Ac:10:LEU:HB3	2.39	0.57
48:Ad:213:SER:HB3	48:Ad:236:TYR:CD2	2.40	0.57
52:Ah:39:GLU:O	52:Ah:43:LYS:HG3	2.04	0.57
1:A:62:PHE:CE2	10:J:62:GLY:HA3	2.40	0.57
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.04	0.57
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.45	0.57
8:H:90:PRO:HA	8:H:94:PRO:HB3	1.86	0.57
8:H:210:GLY:HA2	8:H:213:VAL:HG23	1.87	0.57
13:M:388:TRP:NE1	38:m:109:ARG:HD2	2.20	0.57
15:O:354:LEU:HD21	28:c:44:VAL:HG11	1.87	0.57
16:P:214:LEU:HD23	16:P:352:VAL:CG1	2.34	0.57
17:Q:77:VAL:HG12	17:Q:101:PHE:HA	1.86	0.57
17:Q:167:ASN:O	17:Q:168:LYS:HG2	2.04	0.57
23:X:58:LYS:HA	23:X:61:LYS:HE2	1.87	0.57
34:i:103:ARG:O	41:p:18:PRO:HG3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:160:PRO:O	49:AE:178:HIS:HB3	2.04	0.57
52:AH:87:ASN:O	52:AH:87:ASN:OD1	2.23	0.57
50:Af:107:GLU:HA	50:Af:110:LYS:HD2	1.86	0.57
1:A:104:TYR:CE2	10:J:167:ILE:HD13	2.40	0.57
4:D:84:PHE:CE2	4:D:91:ALA:HB2	2.40	0.57
7:G:267:THR:HB	17:Q:115:ALA:HB2	1.85	0.57
8:H:86:TRP:NE1	8:H:233:LEU:HB2	2.20	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
12:L:306:THR:HA	12:L:336:LYS:HZ2	1.67	0.57
13:M:42:LEU:HD11	13:M:67:ILE:CD1	2.34	0.57
14:N:179:MET:HG3	14:N:216:PHE:CE1	2.39	0.57
14:N:273:ASN:O	14:N:274:ASN:HB2	2.05	0.57
20:T:130:ILE:HD11	20:T:148:ILE:HD11	1.86	0.57
67:AC:402:HEM:HBA1	68:AC:403:UQ6:O4	2.05	0.57
49:AE:219:HIS:HD2	47:Ac:287:LYS:HG3	1.67	0.57
46:Ab:41:THR:OG1	46:Ab:49:ILE:HB	2.04	0.57
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
7:G:171:THR:HB	7:G:173:MET:HG3	1.87	0.57
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.57
12:L:246:LEU:HD12	12:L:247:LEU:CA	2.34	0.57
12:L:253:VAL:CG2	12:L:310:LEU:HD11	2.35	0.57
13:M:269:MET:HE3	13:M:399:ASN:HB2	1.86	0.57
14:N:109:ALA:HB1	14:N:110:PRO:HD3	1.86	0.57
14:N:314:MET:HB2	15:O:305:LEU:HD11	1.86	0.57
17:Q:125:VAL:HG23	17:Q:125:VAL:O	2.05	0.57
33:h:175:GLU:HB3	33:h:177:GLU:HG2	1.86	0.57
34:i:87:LYS:HG2	34:i:87:LYS:O	2.05	0.57
40:o:6:THR:O	40:o:10:LEU:HB2	2.05	0.57
42:q:65:THR:HG22	42:q:66:THR:N	2.20	0.57
48:AD:213:SER:HB3	48:AD:236:TYR:CD2	2.40	0.57
49:AE:207:LYS:HB3	49:AE:209:GLU:OE1	2.05	0.57
7:G:41:VAL:HG21	7:G:56:VAL:HB	1.86	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
10:J:138:GLY:HA2	10:J:141:VAL:HG12	1.86	0.56
12:L:60:GLU:CG	12:L:83:ASP:HA	2.35	0.56
12:L:247:LEU:CD1	12:L:248:HIS:NE2	2.53	0.56
12:L:553:LEU:HD11	38:m:93:ALA:HB1	1.86	0.56
13:M:12:LEU:HB2	13:M:13:PRO:HD3	1.86	0.56
13:M:282:LEU:HD13	13:M:342:MET:HE2	1.87	0.56
13:M:310:MET:O	13:M:314:MET:HG3	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:38:TYR:HB3	15:O:299:GLN:HE22	1.70	0.56
15:O:125:ASP:OD1	15:O:126:GLY:N	2.38	0.56
16:P:211:ASP:OD1	16:P:214:LEU:HB3	2.04	0.56
31:f:49:ARG:HB2	31:f:50:PRO:HD2	1.87	0.56
42:q:14:VAL:HG13	42:q:23:LEU:CD2	2.35	0.56
45:AA:392:LYS:O	45:AA:396:ARG:HG3	2.05	0.56
46:Ab:51:SER:HB2	46:Ab:230:LEU:CD1	2.33	0.56
47:Ac:277:ALA:HB1	70:Ac:405:U10:H1M2	1.87	0.56
49:Ae:152:ILE:HG21	49:Ae:174:LEU:HD22	1.86	0.56
50:Af:78:LYS:O	50:Af:81:TRP:HB2	2.05	0.56
7:G:102:ILE:H	7:G:102:ILE:HD12	1.70	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
8:H:113:VAL:O	8:H:116:ILE:HG12	2.05	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
12:L:594:ASN:OD1	14:N:110:PRO:CB	2.53	0.56
13:M:264:LEU:HD23	38:m:98:LEU:HD11	1.87	0.56
24:Y:57:ARG:HG2	24:Y:60:ARG:HH21	1.69	0.56
24:Y:92:TYR:CE1	24:Y:128:LYS:HD3	2.40	0.56
25:Z:7:LYS:HB2	25:Z:7:LYS:NZ	2.20	0.56
39:n:81:ILE:CD1	39:n:87:GLY:O	2.53	0.56
67:AC:402:HEM:CAA	68:AC:403:UQ6:O4	2.54	0.56
48:AD:131:ALA:CA	48:AD:174:TYR:HA	2.32	0.56
49:AE:218:THR:HG21	49:AE:256:LEU:C	2.30	0.56
45:Aa:403:LEU:HD22	45:Aa:426:LEU:CG	2.34	0.56
47:Ac:35:SER:HA	68:Ac:406:UQ6:H122	1.87	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.87	0.56
57:B:303:PC1:H143	42:q:29:ARG:O	2.05	0.56
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.15	0.56
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.56
5:E:151:LEU:CD2	5:E:170:LEU:HD13	2.35	0.56
6:F:171:VAL:HA	6:F:174:ARG:HH12	1.70	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.56
8:H:19:PHE:CE1	26:a:11:ILE:HD12	2.40	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
10:J:19:LEU:HD22	10:J:32:LEU:HD13	1.87	0.56
10:J:126:TYR:O	25:Z:120:LEU:HD22	2.06	0.56
13:M:196:TRP:HE1	13:M:250:LEU:HD13	1.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:M:501:3PE:H12	14:N:276:LEU:CD2	2.35	0.56
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
14:N:313:MET:HG2	15:O:305:LEU:HD22	1.85	0.56
15:O:173:MET:HE2	15:O:179:ILE:HG23	1.87	0.56
15:O:209:VAL:HG23	15:O:209:VAL:O	2.05	0.56
15:O:242:LYS:HA	15:O:246:LEU:HD12	1.88	0.56
16:P:168:SER:HA	16:P:184:LYS:HE3	1.87	0.56
18:R:38:TYR:HE2	42:q:127:TYR:CB	1.97	0.56
18:R:62:ASP:O	18:R:66:GLN:HG3	2.05	0.56
20:T:134:ASP:OD1	20:T:134:ASP:O	2.23	0.56
23:X:137:LEU:HD13	27:b:58:ARG:HE	1.70	0.56
23:X:168:PHE:O	23:X:169:PHE:CD1	2.58	0.56
32:g:140:PHE:HB3	41:p:75:THR:HG21	1.86	0.56
42:q:129:THR:O	42:q:129:THR:HG22	2.03	0.56
45:AA:369:VAL:O	45:AA:370:PHE:C	2.47	0.56
47:AC:197:LEU:CD1	68:AC:403:UQ6:C1	2.84	0.56
49:AE:152:ILE:HG13	49:AE:154:ILE:CD1	2.35	0.56
49:AE:263:TYR:HB3	49:AE:273:VAL:HG13	1.86	0.56
50:AF:83:LYS:HB2	50:AF:86:GLU:CB	2.35	0.56
51:AG:33:LYS:C	51:AG:36:PRO:HD2	2.30	0.56
2:B:98:ALA:H	2:B:135:GLY:HA3	1.69	0.56
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.40	0.56
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.86	0.56
11:K:16:LEU:HA	11:K:36:MET:HE2	1.85	0.56
13:M:57:SER:HB3	13:M:113:THR:HG22	1.87	0.56
13:M:118:PHE:O	13:M:122:PHE:CB	2.54	0.56
15:O:149:HIS:CE1	15:O:153:THR:HG21	2.40	0.56
18:R:37:VAL:O	18:R:38:TYR:C	2.44	0.56
18:R:59:PHE:O	18:R:63:LEU:HG	2.06	0.56
18:R:77:ILE:HD11	18:R:111:PHE:CG	2.41	0.56
25:Z:115:ARG:NE	30:e:35:ALA:HB1	2.20	0.56
39:n:50:GLU:HG2	39:n:51:HIS:N	2.20	0.56
40:o:7:ARG:NH1	40:o:106:ARG:HH12	2.03	0.56
41:p:39:LEU:O	41:p:44:PRO:HD3	2.06	0.56
45:AA:190:THR:OG1	45:AA:273:SER:HB2	2.05	0.56
47:AC:18:PHE:HE1	68:AC:403:UQ6:C8	2.19	0.56
49:Ae:219:HIS:HB2	49:Ae:254:ALA:HA	1.88	0.56
52:Ah:79:CYS:HA	52:Ah:82:HIS:CD2	2.40	0.56
4:D:359:ASP:O	7:G:150:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.31	0.56
10:J:123:TRP:CZ3	30:e:73:MET:N	2.74	0.56
13:M:78:MET:O	13:M:432:ARG:HD2	2.06	0.56
14:N:120:GLN:O	14:N:176:ARG:CZ	2.54	0.56
15:O:275:TYR:CZ	21:V:23:ARG:NH1	2.64	0.56
17:Q:110:PRO:HB3	18:R:43:TYR:OH	2.06	0.56
34:i:101:LYS:HG2	41:p:116:ARG:O	2.05	0.56
45:Aa:68:THR:HG22	45:Aa:136:LEU:CD2	2.35	0.56
48:Ad:142:GLU:HG2	48:Ad:171:LEU:CD1	2.35	0.56
48:Ad:308:ARG:HD3	51:Ag:27:PHE:CZ	2.41	0.56
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD1	2.40	0.56
50:Af:93:PRO:HA	50:Af:96:LYS:HD2	1.87	0.56
51:Ag:35:ILE:HB	51:Ag:36:PRO:HD3	1.86	0.56
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.56
4:D:72:LEU:CD1	14:N:50:PRO:HG3	2.34	0.56
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.56
5:E:84:LEU:HD12	44:s:46:LEU:HD13	1.88	0.56
5:E:200:ILE:O	5:E:204:ILE:HG13	2.06	0.56
8:H:19:PHE:HB3	26:a:12:MET:HG3	1.87	0.56
8:H:142:TYR:HE1	8:H:285:LEU:HD23	1.71	0.56
14:N:149:LEU:CD1	14:N:154:ILE:HG21	2.35	0.56
14:N:196:TYR:HB3	14:N:273:ASN:OD1	2.05	0.56
14:N:253:GLY:H	14:N:290:LEU:HD11	1.71	0.56
33:h:55:PHE:HB2	34:i:28:LEU:HD21	1.87	0.56
34:i:110:ILE:HD13	41:p:16:ARG:HD2	1.88	0.56
47:AC:171:ASP:CG	47:AC:172:LYS:H	2.13	0.56
48:AD:223:THR:HG21	52:AH:52:ASP:HA	1.86	0.56
47:Ac:171:ASP:CG	47:Ac:172:LYS:H	2.13	0.56
51:Ag:33:LYS:C	51:Ag:36:PRO:HD2	2.30	0.56
13:M:25:THR:HG22	32:g:84:ASN:CG	2.31	0.56
15:O:316:GLU:HG3	32:g:51:MET:HE2	1.87	0.56
16:P:145:PHE:O	16:P:149:PRO:HG2	2.05	0.56
23:X:44:MET:SD	23:X:48:TRP:HZ3	2.29	0.56
23:X:142:TYR:HB2	25:Z:115:ARG:NH1	2.17	0.56
30:e:14:LEU:HD12	30:e:14:LEU:C	2.31	0.56
38:m:15:PRO:HG3	38:m:18:LEU:HD12	1.86	0.56
39:n:133:TRP:HA	39:n:136:GLU:HG2	1.87	0.56
49:AE:154:ILE:HD13	49:AE:273:VAL:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:197:ASP:HB3	49:AE:257:ASN:OD1	2.06	0.56
48:Ad:116:VAL:HA	48:Ad:253:LEU:HD21	1.88	0.56
49:Ae:197:ASP:HB3	49:Ae:257:ASN:OD1	2.06	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
6:F:39:ASP:HB3	6:F:265:PHE:HZ	1.69	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
8:H:4:ILE:H	8:H:4:ILE:HD12	1.71	0.56
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.19	0.56
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.88	0.56
9:I:35:THR:CG2	43:r:107:SER:HA	2.36	0.56
13:M:370:PRO:CA	13:M:375:LEU:CD2	2.83	0.56
14:N:258:THR:OG1	14:N:336:THR:HG22	2.05	0.56
35:j:99:ILE:HD12	40:o:107:ARG:HB2	1.86	0.56
38:m:6:TYR:CE2	38:m:15:PRO:HD3	2.40	0.56
41:p:74:ILE:CD1	41:p:85:ILE:HG13	2.36	0.56
48:AD:131:ALA:HB2	48:AD:174:TYR:CD2	2.41	0.56
48:AD:222:PRO:HG3	52:AH:66:THR:HA	1.86	0.56
49:AE:177:ARG:HB3	49:AE:211:VAL:HG13	1.88	0.56
50:AF:15:ASP:OD2	50:AF:19:LYS:NZ	2.39	0.56
47:Ac:97:HIS:CE1	47:Ac:100:ARG:HH21	2.24	0.56
49:Ae:191:GLU:H	49:Ae:191:GLU:CD	2.14	0.56
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.56
9:I:80:GLU:HB3	43:r:26:LEU:HD11	1.88	0.56
10:J:71:THR:O	10:J:72:ALA:C	2.49	0.56
12:L:397:GLU:HB2	12:L:482:MET:SD	2.46	0.56
20:U:90:TYR:CD1	36:k:51:TRP:CE2	2.94	0.56
20:U:90:TYR:HD1	36:k:51:TRP:CE2	2.23	0.56
26:a:14:VAL:O	26:a:18:ILE:HG13	2.06	0.56
30:e:85:LYS:O	30:e:88:LYS:HB3	2.06	0.56
46:AB:236:GLN:HG3	46:AB:237:PHE:CD2	2.41	0.56
49:Ae:207:LYS:HB3	49:Ae:209:GLU:OE1	2.05	0.56
49:Ae:218:THR:HG21	49:Ae:256:LEU:C	2.30	0.56
50:Af:91:LEU:HD12	50:Af:94:TYR:HB2	1.88	0.56
5:E:180:VAL:HG21	6:F:286:CYS:HA	1.88	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
8:H:318:MET:HE3	25:Z:57:ARG:HH21	1.71	0.56
12:L:597:LEU:HD21	24:Y:37:ILE:HD12	1.87	0.56
13:M:309:PHE:O	13:M:313:THR:HG23	2.06	0.56
14:N:25:ASN:HB3	30:e:15:ASP:OD2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:313:MET:HG3	15:O:305:LEU:HD22	1.87	0.56
16:P:273:LEU:O	16:P:277:VAL:HG23	2.06	0.56
17:Q:58:LYS:O	17:Q:59:LEU:C	2.49	0.56
20:T:90:TYR:HE2	20:T:92:LYS:CB	2.19	0.56
23:X:124:GLN:C	23:X:125:LEU:HD12	2.31	0.56
23:X:169:PHE:CD2	23:X:169:PHE:O	2.59	0.56
24:Y:76:THR:CG2	24:Y:95:GLY:HA3	2.34	0.56
25:Z:85:GLN:O	25:Z:89:GLU:HG3	2.06	0.56
25:Z:92:GLU:O	25:Z:96:ILE:HG13	2.05	0.56
37:l:111:MET:HE3	37:l:112:TYR:CZ	2.41	0.56
51:AG:11:ILE:HG21	51:AG:14:VAL:CG1	2.36	0.56
51:AG:27:PHE:HB3	51:AG:30:TYR:HB2	1.87	0.56
52:AH:48:LEU:HD12	52:AH:65:CYS:HB3	1.88	0.56
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.41	0.55
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.21	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
10:J:22:LYS:HZ2	11:K:22:PHE:CA	2.16	0.55
10:J:161:ALA:O	10:J:165:ILE:HD12	2.06	0.55
12:L:94:LEU:HD23	12:L:125:LEU:HD21	1.88	0.55
12:L:375:ILE:HG12	35:j:65:MET:SD	2.46	0.55
13:M:4:ILE:H	13:M:4:ILE:HD12	1.70	0.55
13:M:73:LEU:CD2	13:M:103:GLN:CD	2.79	0.55
14:N:193:ILE:HD11	14:N:269:GLU:HB2	1.89	0.55
15:O:114:LEU:HA	15:O:131:LEU:HD22	1.88	0.55
16:P:251:ASN:OD1	16:P:254:LYS:HE3	2.06	0.55
17:Q:166:TRP:CE3	44:s:67:PRO:CG	2.88	0.55
20:T:87:LEU:HD22	20:T:104:PHE:CZ	2.41	0.55
30:e:101:ARG:CZ	30:e:102:GLU:H	2.19	0.55
40:o:8:ARG:HD2	40:o:16:GLU:HB3	1.88	0.55
49:AE:132:VAL:O	49:AE:135:GLN:HG2	2.06	0.55
49:AE:219:HIS:HB2	49:AE:254:ALA:HA	1.88	0.55
46:Ab:305:THR:O	46:Ab:311:GLN:NE2	2.39	0.55
46:Ab:366:LEU:HD21	46:Ab:425:VAL:HG22	1.87	0.55
48:Ad:155:GLN:HA	48:Ad:165:PHE:O	2.06	0.55
48:Ad:222:PRO:O	48:Ad:225:VAL:HG12	2.06	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
1:A:96:THR:O	1:A:100:LEU:HG	2.06	0.55
4:D:57:GLU:HA	4:D:60:HIS:CD2	2.41	0.55
4:D:199:PRO:HD3	4:D:261:MET:HE1	1.87	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:538:PRO:O	12:L:542:LEU:HD13	2.06	0.55
15:O:256:LEU:HD23	15:O:258:TYR:OH	2.05	0.55
16:P:188:GLU:HA	16:P:191:VAL:HG12	1.89	0.55
17:Q:163:ASN:OD1	17:Q:163:ASN:C	2.49	0.55
20:U:130:ILE:HD11	20:U:148:ILE:CD1	2.36	0.55
24:Y:137:LEU:HD23	24:Y:138:PHE:CD2	2.41	0.55
27:b:8:PHE:CG	27:b:9:LEU:N	2.74	0.55
34:i:19:ARG:HA	39:n:171:VAL:HG13	1.89	0.55
36:k:47:LEU:CD1	39:n:43:LEU:HD23	2.36	0.55
39:n:57:MET:HE2	39:n:57:MET:HA	1.87	0.55
46:AB:164:VAL:HG22	49:AI:34:VAL:HG23	1.87	0.55
47:AC:197:LEU:CD1	68:AC:403:UQ6:C6	2.82	0.55
48:AD:183:GLU:HB3	48:Ad:160:ASP:O	2.06	0.55
49:AE:114:SER:HB2	51:AG:22:PHE:CE2	2.41	0.55
49:AE:152:ILE:HG13	49:AE:154:ILE:HD11	1.89	0.55
46:Ab:162:LYS:NZ	46:Ab:194:ASP:OD1	2.38	0.55
6:F:213:ILE:CG2	6:F:235:VAL:HA	2.36	0.55
7:G:264:SER:HB2	7:G:272:ARG:HG2	1.88	0.55
7:G:666:GLN:NE2	19:S:38:VAL:HG13	2.21	0.55
12:L:94:LEU:CD2	12:L:125:LEU:HD21	2.35	0.55
14:N:325:MET:HE3	14:N:329:LEU:HD11	1.88	0.55
16:P:217:PHE:HA	16:P:220:TYR:CD2	2.42	0.55
16:P:265:PHE:CZ	16:P:338:LEU:HD12	2.41	0.55
18:R:36:GLN:HG2	42:q:127:TYR:CD2	2.40	0.55
30:e:45:HIS:CD2	33:h:176:LYS:CD	2.89	0.55
33:h:116:PRO:O	33:h:119:ARG:HG2	2.06	0.55
40:o:73:SER:HA	41:p:24:THR:OG1	2.05	0.55
45:AA:183:VAL:HG21	45:AA:286:HIS:HB2	1.88	0.55
45:AA:313:HIS:ND1	45:AA:341:PHE:HD1	2.02	0.55
48:AD:124:CYS:HG	69:AD:401:HEC:CAC	2.19	0.55
48:AD:253:LEU:HD12	48:AD:253:LEU:C	2.32	0.55
52:AH:43:LYS:HA	52:AH:46:GLU:CD	2.32	0.55
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.55
1:A:54:LYS:HE3	1:A:111:LEU:O	2.06	0.55
3:C:217:ARG:HH12	22:W:112:GLU:CB	2.13	0.55
4:D:145:MET:O	4:D:148:GLU:N	2.39	0.55
4:D:254:ARG:HH11	43:r:25:GLN:CA	2.19	0.55
7:G:94:MET:CE	7:G:100:TRP:HH2	2.20	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
12:L:54:PHE:O	12:L:58:ASN:CA	2.55	0.55
12:L:150:MET:HE3	62:L:703:CDL:H552	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:466:PHE:HB2	35:j:68:TRP:CH2	2.40	0.55
15:O:170:LEU:HG	15:O:179:ILE:HD13	1.87	0.55
23:X:20:VAL:HG13	23:X:24:VAL:HB	1.86	0.55
24:Y:71:MET:CG	24:Y:102:THR:HG21	2.37	0.55
33:h:90:ASN:HD21	62:h:201:CDL:PA1	2.29	0.55
47:AC:37:LEU:HD13	67:AC:402:HEM:C3B	2.42	0.55
67:AC:402:HEM:HMA2	68:AC:403:UQ6:O5	2.06	0.55
48:AD:157:GLY:O	48:AD:164:MET:HA	2.05	0.55
48:AD:222:PRO:O	48:AD:225:VAL:HG12	2.06	0.55
52:AH:79:CYS:HB2	52:AH:83:LYS:NZ	2.21	0.55
1:A:56:PHE:HA	10:J:69:TYR:CE2	2.41	0.55
3:C:85:ILE:HD11	3:C:140:ILE:CD1	2.34	0.55
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
7:G:126:LEU:CD1	18:R:89:PRO:HB2	2.37	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
8:H:25:ARG:HH11	61:H:401:UQ9:H15	1.72	0.55
8:H:111:LEU:HD11	10:J:56:PHE:CE2	2.41	0.55
10:J:46:PHE:CE2	11:K:46:VAL:HG13	2.41	0.55
12:L:69:VAL:HG11	12:L:71:MET:HE2	1.88	0.55
12:L:149:ILE:HG13	13:M:369:LEU:HD12	1.89	0.55
12:L:513:MET:HE1	39:n:30:TRP:HB3	1.89	0.55
16:P:206:ILE:HG13	65:P:401:NDP:H42N	1.88	0.55
16:P:235:THR:OG1	16:P:273:LEU:CB	2.54	0.55
42:q:68:MET:HE1	42:q:81:MET:O	2.06	0.55
47:AC:152:ALA:HB1	47:AC:288:LEU:HD23	1.88	0.55
52:AH:49:GLU:HA	52:AH:52:ASP:OD2	2.07	0.55
45:Aa:168:ILE:O	45:Aa:171:GLU:HG2	2.05	0.55
47:Ac:141:TRP:O	47:Ac:145:VAL:HG23	2.05	0.55
48:Ad:141:THR:H	48:Ad:144:GLU:HB2	1.72	0.55
50:Af:47:ALA:HB1	50:Af:91:LEU:HD11	1.88	0.55
2:B:95:PHE:HE2	2:B:97:LEU:HD11	1.71	0.55
2:B:210:ARG:HD3	42:q:76:ASP:HB2	1.88	0.55
5:E:170:LEU:HD12	5:E:171:ILE:N	2.20	0.55
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.55
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55
11:K:66:PHE:CE1	14:N:35:PHE:CE1	2.95	0.55
12:L:230:HIS:N	12:L:231:PRO:HD3	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:561:THR:O	12:L:565:SER:HB2	2.07	0.55
13:M:244:ILE:O	41:p:149:TYR:OH	2.19	0.55
14:N:224:SER:HB2	14:N:229:SER:HB3	1.89	0.55
14:N:237:THR:O	14:N:237:THR:CG2	2.55	0.55
16:P:64:PHE:HE1	16:P:209:ARG:O	1.90	0.55
16:P:208:GLY:O	16:P:209:ARG:C	2.48	0.55
16:P:258:ALA:HA	16:P:263:PHE:HZ	1.71	0.55
38:m:18:LEU:HD21	39:n:69:GLU:HA	1.89	0.55
40:o:69:CYS:O	40:o:69:CYS:SG	2.65	0.55
54:AK:2:LEU:HB3	54:AK:5:PHE:CZ	2.42	0.55
45:Aa:285:ALA:O	45:Aa:360:CYS:N	2.36	0.55
46:Ab:40:PHE:CZ	46:Ab:396:ILE:HG23	2.41	0.55
46:Ab:60:ARG:HG3	46:Ab:124:GLU:HB3	1.89	0.55
68:Ac:406:UQ6:H101	68:Ac:406:UQ6:H13	1.88	0.55
48:Ad:110:ILE:HB	48:Ad:139:CYS:SG	2.47	0.55
48:Ad:253:LEU:C	48:Ad:253:LEU:HD12	2.32	0.55
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.89	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
7:G:356:ASP:O	7:G:360:LYS:HG3	2.06	0.55
12:L:162:THR:O	12:L:166:THR:HG23	2.06	0.55
14:N:230:ILE:O	14:N:233:LEU:HB2	2.07	0.55
15:O:319:ILE:HG13	15:O:320:GLY:H	1.72	0.55
16:P:219:ASN:ND2	16:P:313:TRP:HE1	2.04	0.55
17:Q:165:SER:HB3	17:Q:168:LYS:O	2.06	0.55
20:T:128:PHE:CE2	20:T:130:ILE:HG13	2.42	0.55
30:e:14:LEU:HD12	30:e:15:ASP:N	2.21	0.55
31:f:8:ARG:HA	31:f:8:ARG:NE	2.21	0.55
41:p:66:ARG:HD3	41:p:68:TYR:CZ	2.40	0.55
42:q:64:TYR:CE2	42:q:82:VAL:HG13	2.42	0.55
46:AB:366:LEU:HD21	46:AB:425:VAL:HG22	1.87	0.55
47:AC:97:HIS:CE1	47:AC:100:ARG:HH21	2.23	0.55
54:AK:8:PRO:HA	54:AK:11:ARG:CZ	2.37	0.55
49:Ae:156:LEU:HD22	49:Ae:210:TRP:CE2	2.42	0.55
50:Af:76:LEU:O	50:Af:81:TRP:NE1	2.39	0.55
4:D:262:LEU:O	4:D:263:THR:C	2.49	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
13:M:231:LEU:CA	13:M:235:LEU:HD12	2.36	0.55
13:M:453:LEU:HD12	13:M:454:ILE:CG2	2.34	0.55
15:O:66:ILE:HD12	15:O:67:CYS:SG	2.47	0.55
15:O:258:TYR:CZ	15:O:269:VAL:HG13	2.42	0.55
16:P:196:PRO:O	16:P:197:GLU:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:56:GLU:HA	25:Z:59:ARG:HH11	1.72	0.55
27:b:38:TYR:HA	27:b:41:TYR:CD2	2.42	0.55
34:i:83:HIS:HE1	34:i:87:LYS:HD2	1.71	0.55
36:k:30:ILE:CD1	36:k:39:GLN:HB2	2.33	0.55
45:AA:168:ILE:O	45:AA:171:GLU:HG2	2.05	0.55
49:AE:168:LYS:HD2	47:Ac:262:LEU:HD11	1.88	0.55
49:AE:191:GLU:CD	49:AE:191:GLU:H	2.15	0.55
50:AF:102:ARG:HH21	50:AF:103:LYS:HE3	1.72	0.55
47:Ac:147:THR:HG21	47:Ac:165:TRP:CD1	2.41	0.55
49:Ae:207:LYS:CD	49:Ae:210:TRP:HD1	2.20	0.55
1:A:103:ALA:O	1:A:107:THR:HG23	2.06	0.55
4:D:97:LEU:HG	4:D:99:LEU:HD21	1.89	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
8:H:51:ASP:CA	8:H:54:LYS:HG2	2.37	0.55
9:I:53:ALA:CA	27:b:14:ALA:HB2	2.36	0.55
11:K:45:SER:O	11:K:49:LEU:HG	2.07	0.55
13:M:62:SER:C	13:M:64:PRO:HD2	2.32	0.55
20:U:83:VAL:O	20:U:87:LEU:HG	2.07	0.55
26:a:1:MET:HG3	62:q:201:CDL:HB21	1.87	0.55
32:g:78:PRO:O	32:g:81:ASP:HB3	2.07	0.55
49:AE:156:LEU:HD22	49:AE:210:TRP:CE2	2.42	0.55
49:AE:248:ARG:HA	49:AE:257:ASN:CG	2.31	0.55
49:Ae:92:ARG:HA	51:Ag:24:GLN:HA	1.89	0.55
1:A:105:GLU:CG	1:A:111:LEU:HB3	2.37	0.55
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.55
10:J:19:LEU:HD11	11:K:31:LEU:HG	1.88	0.55
12:L:73:SER:HB3	41:p:100:GLN:NE2	2.22	0.55
12:L:261:VAL:O	12:L:264:HIS:HD2	1.89	0.55
12:L:357:ARG:HG2	39:n:32:ILE:HG12	1.89	0.55
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.42	0.55
16:P:195:PHE:HD1	16:P:198:ALA:HB2	1.72	0.55
16:P:208:GLY:H	16:P:211:ASP:CB	2.18	0.55
19:S:30:SER:O	19:S:31:GLN:C	2.49	0.55
33:h:73:PHE:CD2	33:h:74:TYR:CE1	2.94	0.55
34:i:83:HIS:CD2	41:p:37:TYR:CE2	2.95	0.55
45:AA:58:ARG:HD2	45:AA:417:LEU:HD12	1.89	0.55
46:AB:42:LYS:HG3	46:AB:48:VAL:HG22	1.88	0.55
48:AD:318:LYS:HD2	49:AE:86:PRO:HB2	1.89	0.55
49:AE:153:GLU:C	49:AE:154:ILE:HD12	2.32	0.55
49:AI:69:GLY:HA2	46:Ab:111:SER:HA	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:248:ARG:HA	49:Ae:257:ASN:CG	2.32	0.55
52:Ah:74:HIS:CD2	52:Ah:78:HIS:CE1	2.95	0.55
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
7:G:608:VAL:HG23	17:Q:103:THR:HG1	1.72	0.54
10:J:8:LEU:HD12	10:J:38:VAL:HG13	1.89	0.54
13:M:6:LEU:HB3	13:M:7:PRO:HD3	1.88	0.54
13:M:55:MET:HE1	62:d:201:CDL:H511	1.89	0.54
15:O:209:VAL:HG23	15:O:214:VAL:HG13	1.88	0.54
20:U:79:ILE:HD11	20:U:148:ILE:CG2	2.36	0.54
45:AA:412:ASP:HA	45:AA:415:ARG:NH2	2.22	0.54
47:AC:287:LYS:HB2	49:Ae:219:HIS:HD2	1.71	0.54
48:AD:308:ARG:HD3	51:AG:27:PHE:CE2	2.42	0.54
52:AH:35:CYS:O	52:AH:38:LEU:HB2	2.06	0.54
52:AH:79:CYS:O	52:AH:83:LYS:HG2	2.07	0.54
45:Aa:279:ASP:HA	51:Ag:12:ARG:HA	1.89	0.54
45:Aa:396:ARG:O	45:Aa:400:VAL:HG23	2.07	0.54
49:Ae:132:VAL:O	49:Ae:135:GLN:HG2	2.06	0.54
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.89	0.54
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.37	0.54
6:F:270:ASN:OD1	6:F:270:ASN:C	2.48	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:617:ARG:HH12	22:W:128:GLY:C	2.14	0.54
7:G:671:LEU:HD21	19:S:45:LYS:HG2	1.88	0.54
8:H:212:ASN:HB3	8:H:215:TYR:HB2	1.89	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
12:L:54:PHE:O	12:L:58:ASN:HA	2.08	0.54
12:L:258:PHE:HE1	12:L:262:ARG:HH21	1.56	0.54
12:L:371:SER:HB2	35:j:62:SER:OG	2.06	0.54
16:P:199:ILE:HD13	16:P:258:ALA:HB1	1.89	0.54
21:V:50:GLN:HE22	43:r:94:ALA:H	1.54	0.54
32:g:106:TYR:OH	33:h:86:ILE:HD12	2.07	0.54
38:m:18:LEU:HD11	39:n:72:TRP:CG	2.42	0.54
46:AB:93:GLY:HA3	46:AB:139:ASN:CG	2.33	0.54
48:AD:215:LEU:CD1	69:AD:401:HEC:CMB	2.73	0.54
49:AE:255:PRO:CG	47:Ac:287:LYS:NZ	2.71	0.54
48:Ad:214:LEU:CD1	48:Ad:237:PHE:HB2	2.38	0.54
49:Ae:152:ILE:HG22	49:Ae:273:VAL:O	2.07	0.54
49:Ae:177:ARG:HB3	49:Ae:211:VAL:HG13	1.88	0.54
49:Ae:190:VAL:HG11	49:Ae:195:LEU:HD21	1.90	0.54
52:Ah:51:CYS:O	52:Ah:55:VAL:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:THR:HG22	4:D:100:GLU:HG2	1.88	0.54
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.42	0.54
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.54
7:G:456:ALA:O	7:G:499:LYS:HE2	2.06	0.54
12:L:353:GLU:OE1	39:n:80:TYR:OH	2.24	0.54
12:L:362:ILE:HA	12:L:365:ILE:HG13	1.90	0.54
13:M:415:GLN:O	13:M:416:ARG:HG3	2.08	0.54
15:O:49:THR:HG21	15:O:151:LEU:HG	1.89	0.54
15:O:305:LEU:O	15:O:305:LEU:CD1	2.55	0.54
16:P:61:ALA:HB3	16:P:82:ILE:HG23	1.89	0.54
16:P:213:PHE:CE2	16:P:239:PRO:HB3	2.42	0.54
16:P:300:TRP:O	16:P:304:LEU:HG	2.08	0.54
16:P:315:THR:O	16:P:316:LYS:C	2.49	0.54
19:S:79:LEU:HA	19:S:82:LEU:CD1	2.24	0.54
20:T:97:LYS:HG3	20:T:97:LYS:O	2.08	0.54
25:Z:24:ASN:OD1	25:Z:24:ASN:O	2.24	0.54
25:Z:53:TRP:O	25:Z:57:ARG:HG3	2.06	0.54
31:f:56:TRP:CE3	33:h:131:LYS:HG3	2.42	0.54
34:i:16:ARG:O	34:i:20:ARG:HG2	2.08	0.54
45:AA:87:ASN:H	45:AA:207:ASN:HD22	1.53	0.54
45:AA:396:ARG:HA	45:AA:399:LEU:CD2	2.27	0.54
47:AC:30:TRP:HB3	47:AC:100:ARG:HD3	1.90	0.54
49:AE:152:ILE:HD13	49:AE:169:TRP:CG	2.42	0.54
49:AE:161:GLU:HA	49:AE:178:HIS:CD2	2.43	0.54
49:AE:190:VAL:HG11	49:AE:195:LEU:HD21	1.90	0.54
50:AF:51:LEU:HD23	50:AF:94:TYR:CE2	2.42	0.54
45:Aa:204:PRO:CB	49:Ae:82:ASP:HA	2.38	0.54
47:Ac:277:ALA:CB	70:Ac:405:U10:H1M2	2.37	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
4:D:35:ARG:O	4:D:36:GLN:C	2.47	0.54
6:F:275:LEU:HA	6:F:289:GLU:HA	1.90	0.54
6:F:382:CYS:SG	55:F:502:SF4:FE2	1.89	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
10:J:122:ASP:C	10:J:123:TRP:CD1	2.86	0.54
12:L:190:SER:HB2	12:L:196:TRP:NE1	2.22	0.54
12:L:232:TRP:O	12:L:236:ALA:N	2.40	0.54
13:M:127:ILE:CG1	14:N:254:LEU:HD21	2.37	0.54
13:M:446:LEU:HD13	32:g:101:THR:CG2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:318:LYS:HA	16:P:321:ARG:NH1	2.22	0.54
26:a:58:ASN:HB2	26:a:61:TYR:CD2	2.43	0.54
27:b:8:PHE:O	27:b:9:LEU:C	2.50	0.54
40:o:103:GLU:OE2	40:o:106:ARG:HD2	2.07	0.54
46:AB:60:ARG:HG3	46:AB:124:GLU:HB3	1.89	0.54
46:AB:298:HIS:H	46:AB:304:ASN:ND2	2.05	0.54
51:AG:39:LEU:O	51:AG:42:THR:HG22	2.08	0.54
45:Aa:295:GLY:O	45:Aa:301:ASN:ND2	2.35	0.54
49:Ae:161:GLU:HA	49:Ae:178:HIS:CD2	2.43	0.54
52:Ah:83:LYS:HA	52:Ah:86:LYS:CD	2.36	0.54
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.43	0.54
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.54
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.54
5:E:40:HIS:HB2	7:G:209:TYR:CZ	2.41	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:J:29:GLY:CA	11:K:31:LEU:HD21	2.37	0.54
10:J:77:GLU:O	10:J:78:TYR:C	2.51	0.54
12:L:131:LEU:CD1	12:L:140:LEU:CD1	2.78	0.54
12:L:389:PHE:CZ	35:j:79:ALA:CB	2.90	0.54
13:M:373:ILE:HD11	13:M:454:ILE:HD11	1.88	0.54
16:P:376:ASN:OD1	16:P:376:ASN:C	2.50	0.54
23:X:8:PRO:HG2	23:X:57:LEU:HD11	1.90	0.54
33:h:90:ASN:OD1	33:h:115:HIS:NE2	2.40	0.54
47:AC:223:TYR:O	48:AD:311:TRP:NE1	2.34	0.54
47:AC:287:LYS:CB	49:Ae:219:HIS:HD2	2.21	0.54
45:Aa:183:VAL:HG21	45:Aa:286:HIS:HB2	1.88	0.54
46:Ab:60:ARG:CZ	46:Ab:390:GLU:HB3	2.37	0.54
47:Ac:238:ILE:HD12	62:Ag:102:CDL:H772	1.88	0.54
2:B:141:MET:CE	4:D:115:LEU:HD23	2.37	0.54
4:D:58:THR:HG23	4:D:61:TRP:CZ3	2.41	0.54
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.41	0.54
6:F:152:ARG:CZ	44:s:60:PRO:HG3	2.38	0.54
6:F:152:ARG:HD3	44:s:57:LEU:HD11	1.87	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.28	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
12:L:65:THR:HA	34:i:90:MET:HE2	1.90	0.54
12:L:141:PHE:CD2	13:M:370:PRO:CB	2.91	0.54
15:O:170:LEU:HG	15:O:179:ILE:CD1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:53:MET:HB2	22:W:55:LEU:HG	1.89	0.54
35:j:98:GLY:O	35:j:100:PRO:HD3	2.07	0.54
45:AA:276:ARG:NH1	45:AA:278:ARG:HB2	2.22	0.54
45:AA:402:HIS:CD2	45:AA:426:LEU:HD21	2.42	0.54
46:AB:60:ARG:CZ	46:AB:390:GLU:HB3	2.37	0.54
47:AC:222:PRO:HG2	47:AC:223:TYR:CD2	2.43	0.54
48:AD:131:ALA:H	48:AD:134:HIS:CE1	2.25	0.54
51:AG:78:TYR:HB3	52:AH:61:THR:OG1	2.08	0.54
52:AH:48:LEU:HD11	52:AH:65:CYS:HB3	1.88	0.54
45:Aa:55:ASN:HB3	45:Aa:226:ALA:CB	2.38	0.54
45:Aa:87:ASN:H	45:Aa:207:ASN:HD22	1.53	0.54
49:Ae:192:VAL:HA	49:Ae:195:LEU:CD1	2.37	0.54
50:Af:95:LEU:O	50:Af:99:ILE:HG12	2.08	0.54
51:Ag:39:LEU:O	51:Ag:42:THR:HG22	2.08	0.54
53:Aj:31:PHE:HD1	54:Ak:47:TYR:CD2	2.26	0.54
3:C:73:GLN:NE2	21:V:107:PRO:HB3	2.22	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
10:J:123:TRP:CZ3	30:e:73:MET:HG3	2.41	0.54
10:J:124:LEU:O	10:J:125:MET:C	2.49	0.54
10:J:164:PHE:HB3	14:N:5:THR:HG23	1.90	0.54
12:L:551:THR:HA	12:L:555:LEU:HD12	1.90	0.54
13:M:79:ALA:HB1	13:M:225:ILE:HD13	1.90	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
16:P:106:LEU:HD21	18:R:49:VAL:HG11	1.89	0.54
16:P:209:ARG:N	16:P:352:VAL:HG22	2.23	0.54
16:P:315:THR:HG22	16:P:316:LYS:N	2.21	0.54
17:Q:160:TYR:CZ	17:Q:164:PHE:HZ	2.26	0.54
24:Y:141:PRO:HB2	33:h:161:ARG:HH11	1.72	0.54
54:AK:37:ASP:O	54:AK:38:TRP:C	2.51	0.54
47:Ac:128:PHE:CE1	70:Ac:405:U10:H4M2	2.43	0.54
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.54
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.73	0.54
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.54
7:G:50:LEU:O	7:G:54:GLU:HG2	2.07	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
12:L:232:TRP:CH2	12:L:233:LEU:HD21	2.42	0.54
14:N:24:THR:HB	30:e:2:PRO:HG3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:60:ILE:O	15:O:158:VAL:HA	2.07	0.54
15:O:69:GLY:HA2	15:O:72:LYS:HZ3	1.72	0.54
20:T:140:CYS:HB2	20:T:143:GLU:HG2	1.90	0.54
22:W:43:TYR:CE1	22:W:63:ARG:HD3	2.43	0.54
22:W:67:ARG:HD2	22:W:71:MET:HE2	1.89	0.54
22:W:88:LYS:O	22:W:92:GLU:HG2	2.08	0.54
25:Z:53:TRP:NE1	25:Z:57:ARG:HD2	2.23	0.54
26:a:31:ASN:HD21	26:a:36:LYS:HB2	1.71	0.54
31:f:44:PHE:HE1	41:p:66:ARG:HH11	1.54	0.54
38:m:8:PRO:HB3	38:m:14:LEU:N	2.23	0.54
38:m:109:ARG:O	38:m:113:GLU:HG2	2.08	0.54
49:AE:122:THR:HG21	53:AJ:25:ILE:HG21	1.90	0.54
52:AH:45:ARG:O	52:AH:49:GLU:HG2	2.07	0.54
49:AI:64:LEU:HD12	49:AI:78:PHE:HA	1.89	0.54
49:Ae:122:THR:HG21	53:AJ:25:ILE:HG21	1.90	0.54
3:C:124:ARG:HD2	17:Q:140:LYS:NZ	2.23	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.07	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
6:F:171:VAL:HA	6:F:174:ARG:NH1	2.23	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.38	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:617:ARG:NH1	22:W:128:GLY:C	2.66	0.54
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.54
12:L:221:THR:HA	12:L:226:GLN:HG2	1.90	0.54
12:L:247:LEU:HD11	12:L:248:HIS:CE1	2.43	0.54
13:M:31:SER:HA	13:M:34:ILE:HG12	1.90	0.54
13:M:231:LEU:O	13:M:236:LEU:HG	2.06	0.54
13:M:283:LYS:HG3	13:M:327:PHE:CE1	2.43	0.54
16:P:258:ALA:HA	16:P:263:PHE:CZ	2.43	0.54
20:T:83:VAL:HG22	20:T:126:PHE:HZ	1.66	0.54
20:U:86:VAL:CB	20:U:122:MET:HE1	2.37	0.54
35:j:101:PRO:O	35:j:102:ASP:C	2.49	0.54
37:l:119:THR:HG23	38:m:11:LEU:HA	1.89	0.54
39:n:20:TYR:CE2	39:n:24:LEU:CD1	2.91	0.54
48:AD:116:VAL:HA	48:AD:253:LEU:HD21	1.88	0.54
49:AE:207:LYS:CD	49:AE:210:TRP:HD1	2.20	0.54
45:Aa:341:PHE:HE2	45:Aa:372:LEU:HD13	1.67	0.54
47:Ac:222:PRO:HG2	47:Ac:223:TYR:CD2	2.43	0.54
1:A:64:LEU:HD13	10:J:163:ILE:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:127:ASP:HB3	6:F:245:VAL:CG2	2.38	0.54
7:G:94:MET:HE2	7:G:100:TRP:HH2	1.73	0.54
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.54
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
12:L:66:TRP:CZ3	12:L:68:TRP:CD1	2.96	0.54
12:L:586:LEU:CD2	24:Y:47:PRO:HD3	2.38	0.54
14:N:307:THR:CG2	14:N:308:ASN:H	2.19	0.54
16:P:142:GLU:HA	16:P:146:VAL:HG12	1.90	0.54
17:Q:52:LEU:HG	22:W:21:LYS:HG2	1.90	0.54
23:X:121:ASP:O	23:X:122:LEU:C	2.50	0.54
35:j:97:LEU:O	40:o:104:ARG:CG	2.55	0.54
39:n:133:TRP:CA	39:n:136:GLU:HG2	2.38	0.54
40:o:93:LEU:O	40:o:97:LYS:HG2	2.07	0.54
41:p:31:THR:O	41:p:35:LYS:HG3	2.07	0.54
46:Ab:50:ALA:HB3	46:Ab:221:VAL:HG22	1.90	0.54
47:Ac:164:ILE:O	47:Ac:177:ARG:HD2	2.08	0.54
48:Ad:294:LEU:HD11	53:Aj:43:ILE:HD12	1.89	0.54
49:Ae:136:PHE:O	49:Ae:137:VAL:C	2.51	0.54
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.36	0.53
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.53
6:F:297:LYS:O	6:F:301:GLU:HG2	2.08	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53
8:H:303:TRP:CZ3	27:b:28:LEU:HG	2.43	0.53
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.53
10:J:123:TRP:CH2	30:e:73:MET:N	2.76	0.53
12:L:158:TRP:CD1	39:n:97:TYR:HH	2.26	0.53
13:M:1:MET:HE2	13:M:52:PHE:CE2	2.43	0.53
13:M:175:ASN:ND2	33:h:143:GLU:HG2	2.21	0.53
14:N:179:MET:HE2	14:N:216:PHE:CE1	2.43	0.53
15:O:319:ILE:HG13	15:O:320:GLY:N	2.22	0.53
15:O:355:LYS:HE2	28:c:38:LYS:HA	1.90	0.53
16:P:311:GLU:O	16:P:312:PRO:C	2.49	0.53
17:Q:117:THR:HG22	17:Q:119:ASP:H	1.73	0.53
18:R:94:ASN:OD1	18:R:96:ASP:HB2	2.08	0.53
29:d:39:TYR:CE2	29:d:43:LEU:HD11	2.43	0.53
40:o:57:ASP:CG	40:o:59:CYS:H	2.16	0.53
42:q:95:ASP:OD1	42:q:96:ASP:N	2.41	0.53
48:AD:116:VAL:HG22	48:AD:253:LEU:HD21	1.89	0.53
48:Ad:116:VAL:HG22	48:Ad:253:LEU:HD21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ad:255:TYR:HB3	48:Ad:257:ASP:OD1	2.08	0.53
54:Ak:12:GLU:HA	54:Ak:15:ARG:HD3	1.90	0.53
1:A:68:GLU:CD	1:A:98:LEU:HG	2.33	0.53
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.43	0.53
3:C:224:GLU:OE1	16:P:48:ARG:O	2.26	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
8:H:69:SER:O	8:H:72:ILE:HG13	2.08	0.53
12:L:491:LEU:CD1	35:j:80:VAL:HG22	2.38	0.53
15:O:40:LEU:HG	15:O:292:HIS:CE1	2.44	0.53
15:O:250:SER:HA	15:O:255:VAL:CG2	2.38	0.53
16:P:211:ASP:OD2	16:P:352:VAL:HG11	2.08	0.53
16:P:355:ARG:HH11	16:P:356:HIS:CE1	2.25	0.53
17:Q:82:PRO:O	17:Q:94:THR:HG23	2.08	0.53
28:c:72:ARG:NH1	29:d:19:ARG:HD3	2.24	0.53
39:n:30:TRP:CD2	39:n:76:HIS:CD2	2.95	0.53
42:q:125:VAL:HG23	42:q:125:VAL:O	2.08	0.53
47:AC:164:ILE:O	47:AC:177:ARG:HD2	2.08	0.53
47:AC:253:PRO:O	48:AD:203:ALA:HA	2.09	0.53
48:AD:255:TYR:HB3	48:AD:257:ASP:OD1	2.08	0.53
45:Aa:120:LEU:HB3	46:Ab:299:ILE:HA	1.90	0.53
48:Ad:156:ASP:HB2	48:Ad:167:ARG:CG	2.38	0.53
49:Ae:195:LEU:HD11	49:Ae:248:ARG:HH11	1.73	0.53
53:Aj:19:SER:HA	54:Ak:24:TRP:CH2	2.43	0.53
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.53
8:H:172:MET:HE1	25:Z:46:GLY:HA3	1.91	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
12:L:79:SER:CB	12:L:135:ASN:HB2	2.36	0.53
12:L:109:HIS:O	12:L:110:SER:HB2	2.08	0.53
12:L:362:ILE:CD1	12:L:430:VAL:CG1	2.82	0.53
12:L:400:ASN:HD21	12:L:413:LEU:HD11	1.73	0.53
12:L:559:GLU:HG2	12:L:564:LYS:HD3	1.90	0.53
13:M:61:LEU:HD22	13:M:244:ILE:HG21	1.90	0.53
13:M:154:LEU:HD13	14:N:287:LEU:CD2	2.39	0.53
20:T:118:ILE:HG23	20:T:122:MET:CE	2.37	0.53
21:V:48:THR:HA	21:V:51:ILE:HD12	1.90	0.53
27:b:28:LEU:HA	27:b:31:ILE:HG22	1.91	0.53
35:j:38:VAL:CG1	35:j:39:HIS:N	2.72	0.53
38:m:28:GLU:HG2	38:m:31:ARG:HH22	1.73	0.53
39:n:56:ASP:O	39:n:57:MET:C	2.50	0.53
39:n:133:TRP:HA	39:n:136:GLU:CG	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:142:ARG:O	41:p:143:TYR:CD1	2.61	0.53
46:AB:237:PHE:O	46:AB:238:LEU:HB2	2.07	0.53
48:AD:214:LEU:CD1	48:AD:237:PHE:HB2	2.38	0.53
47:Ac:9:PRO:O	47:Ac:13:ILE:HG13	2.08	0.53
53:Aj:43:ILE:O	53:Aj:47:ILE:HG13	2.09	0.53
2:B:114:MET:SD	2:B:119:VAL:HG12	2.48	0.53
2:B:135:GLY:O	2:B:165:ALA:HB2	2.08	0.53
6:F:276:PHE:HD1	6:F:352:ALA:HB1	1.72	0.53
7:G:382:ARG:HD2	19:S:56:ARG:HD3	1.90	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
12:L:362:ILE:HD12	12:L:430:VAL:HG13	1.88	0.53
13:M:105:LEU:HD11	62:M:503:CDL:H472	1.91	0.53
16:P:164:PHE:HB3	16:P:198:ALA:CB	2.38	0.53
37:l:101:TRP:HE1	38:m:62:ASP:HA	1.72	0.53
39:n:125:TRP:CE3	39:n:128:LEU:HD12	2.43	0.53
41:p:103:MET:CE	41:p:135:VAL:HG12	2.38	0.53
42:q:56:PHE:HD1	42:q:59:HIS:NE2	2.06	0.53
47:AC:147:THR:HG21	47:AC:165:TRP:CD1	2.44	0.53
47:AC:148:ASN:ND2	47:AC:161:VAL:HG11	2.22	0.53
46:Ab:42:LYS:HA	46:Ab:48:VAL:HA	1.91	0.53
47:Ac:253:PRO:HG2	48:Ad:205:HIS:CE1	2.42	0.53
1:A:58:VAL:HG11	8:H:286:MET:HE1	1.89	0.53
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.09	0.53
6:F:270:ASN:ND2	6:F:338:ASP:HB2	2.23	0.53
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.53
7:G:161:GLU:OE1	18:R:97:LYS:HE2	2.09	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.53
9:I:78:PHE:CG	43:r:8:ILE:HG23	2.44	0.53
10:J:59:TYR:CZ	11:K:64:LEU:HD22	2.43	0.53
12:L:141:PHE:CE2	13:M:375:LEU:HD22	2.23	0.53
12:L:387:THR:HG22	12:L:465:GLY:N	2.24	0.53
14:N:120:GLN:HE22	14:N:174:GLN:CB	2.21	0.53
15:O:140:LEU:HD11	15:O:198:TYR:OH	2.09	0.53
23:X:25:LEU:HD11	26:a:50:ARG:CZ	2.39	0.53
23:X:120:PRO:HG3	27:b:71:GLN:HE21	1.73	0.53
24:Y:50:SER:HB3	24:Y:53:GLU:HG2	1.91	0.53
33:h:57:VAL:HG12	39:n:99:VAL:HG21	1.89	0.53
37:l:38:PRO:CB	38:m:75:ASN:ND2	2.67	0.53
38:m:94:GLY:HA3	58:m:201:3PE:H2C1	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:132:LYS:HD3	42:q:135:HIS:ND1	2.23	0.53
45:AA:416:SER:HB3	45:AA:423:ARG:HA	1.90	0.53
47:AC:153:ILE:HB	47:AC:157:GLY:HA2	1.91	0.53
45:Aa:204:PRO:HB3	49:Ae:84:LYS:HZ3	1.73	0.53
1:A:56:PHE:CE1	11:K:79:VAL:HG21	2.43	0.53
4:D:51:VAL:HG21	4:D:58:THR:CG2	2.38	0.53
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.44	0.53
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.97	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:135:THR:OG1	5:E:135:THR:O	2.21	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:651:PRO:HD3	19:S:56:ARG:HB3	1.91	0.53
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.90	0.53
10:J:14:VAL:O	10:J:17:LEU:HB3	2.07	0.53
10:J:94:LEU:O	10:J:97:ILE:HG12	2.08	0.53
12:L:124:PHE:HZ	12:L:252:MET:HB2	1.74	0.53
13:M:55:MET:HG3	13:M:56:PHE:CD2	2.44	0.53
15:O:164:TYR:CE1	15:O:195:LEU:HD21	2.43	0.53
16:P:122:HIS:CB	18:R:46:VAL:CG1	2.85	0.53
16:P:370:LYS:HG3	16:P:370:LYS:O	2.08	0.53
21:V:114:TRP:O	21:V:115:PRO:C	2.52	0.53
34:i:98:VAL:HG13	41:p:115:GLN:HG2	1.91	0.53
45:AA:281:ALA:HB2	51:AG:10:ARG:HH22	1.74	0.53
48:AD:255:TYR:HH	48:AD:266:VAL:HA	1.73	0.53
49:AI:63:PRO:HD3	46:Ab:327:ASN:O	2.08	0.53
52:Ah:29:THR:HA	52:Ah:32:ARG:HD2	1.90	0.53
5:E:129:TYR:CZ	5:E:207:LEU:HB3	2.43	0.53
7:G:163:LYS:HE2	18:R:97:LYS:NZ	2.24	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.53
10:J:25:PRO:HG2	10:J:75:THR:OG1	2.08	0.53
10:J:104:CYS:O	10:J:107:ASN:HB3	2.08	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.90	0.53
12:L:450:LEU:HG	12:L:454:ILE:HD12	1.91	0.53
12:L:466:PHE:CE2	58:L:701:3PE:H331	2.44	0.53
12:L:542:LEU:HB3	13:M:278:ARG:HD2	1.91	0.53
13:M:57:SER:CB	13:M:113:THR:HG22	2.39	0.53
13:M:446:LEU:HD13	32:g:101:THR:HG21	1.89	0.53
25:Z:12:PRO:HD3	25:Z:16:TYR:CE1	2.43	0.53
25:Z:116:TRP:CZ2	25:Z:119:PRO:HD3	2.44	0.53
45:AA:204:PRO:HB3	49:AE:84:LYS:NZ	2.23	0.53
45:AA:274:GLU:OE2	45:AA:467:ASP:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:80:ARG:HH21	45:Aa:267:PRO:HG2	1.73	0.53
46:Ab:70:ARG:NH2	46:Ab:332:ASP:OD2	2.42	0.53
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.43	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.51	0.53
9:I:153:ILE:HD12	9:I:153:ILE:O	2.09	0.53
10:J:136:GLU:N	10:J:139:ILE:HD12	2.24	0.53
12:L:20:LEU:C	12:L:20:LEU:CD1	2.81	0.53
12:L:187:VAL:HG22	13:M:383:MET:HG2	1.90	0.53
12:L:361:ASN:HA	12:L:431:THR:O	2.09	0.53
12:L:511:LEU:HD11	36:k:38:VAL:HG22	1.91	0.53
13:M:269:MET:CE	13:M:396:MET:HA	2.36	0.53
13:M:310:MET:HG3	13:M:455:THR:CA	2.38	0.53
13:M:314:MET:HE1	13:M:380:PHE:CD2	2.44	0.53
14:N:307:THR:HB	15:O:319:ILE:CG1	2.39	0.53
19:S:82:LEU:HD13	19:S:86:GLU:OE1	2.08	0.53
20:T:103:HIS:HD1	20:T:140:CYS:HG	1.51	0.53
23:X:80:GLU:HB3	23:X:81:PRO:HD3	1.91	0.53
32:g:139:TYR:CD2	32:g:140:PHE:CD1	2.96	0.53
33:h:156:VAL:CG1	33:h:160:MET:HE3	2.39	0.53
35:j:52:ARG:HA	35:j:52:ARG:HE	1.74	0.53
38:m:49:LEU:HD23	39:n:140:LEU:CD2	2.39	0.53
42:q:68:MET:SD	42:q:81:MET:CB	2.95	0.53
42:q:88:ARG:HD2	42:q:94:THR:OG1	2.08	0.53
45:AA:52:ILE:CA	45:AA:58:ARG:HA	2.33	0.53
49:AE:195:LEU:HD11	49:AE:248:ARG:HH11	1.72	0.53
49:AE:220:LEU:HA	47:Ac:148:ASN:CB	2.38	0.53
52:AH:39:GLU:HA	52:AH:42:VAL:HG12	1.91	0.53
53:AJ:43:ILE:O	53:AJ:47:ILE:HG13	2.09	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.16	0.53
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:347:ASP:N	7:G:347:ASP:OD1	2.41	0.53
13:M:59:ASP:O	13:M:60:PRO:C	2.49	0.53
13:M:73:LEU:HD23	13:M:103:GLN:NE2	2.23	0.53
13:M:154:LEU:HD13	14:N:287:LEU:HD22	1.91	0.53
13:M:348:LEU:HD12	13:M:415:GLN:NE2	2.24	0.53
13:M:453:LEU:HD12	13:M:453:LEU:C	2.33	0.53
16:P:94:LEU:O	16:P:97:MET:HG2	2.09	0.53
23:X:171:THR:O	23:X:172:VAL:C	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:32:ARG:O	30:e:33:CYS:HB2	2.08	0.53
37:l:55:TYR:O	37:l:104:PRO:HG3	2.09	0.53
45:AA:255:ARG:O	45:AA:255:ARG:CG	2.51	0.53
46:AB:117:GLU:OE2	46:AB:330:TYR:HB3	2.09	0.53
49:AE:180:THR:N	49:AE:183:GLU:HB2	2.23	0.53
49:AE:207:LYS:HD2	49:AE:210:TRP:CD1	2.43	0.53
46:Ab:226:SER:O	46:Ab:229:VAL:HG22	2.09	0.53
47:Ac:42:MET:HE3	68:Ac:406:UQ6:H151	1.90	0.53
48:Ad:228:ARG:HG2	48:Ad:231:LEU:HD12	1.91	0.53
49:Ae:207:LYS:HD2	49:Ae:210:TRP:CD1	2.43	0.53
54:Ak:18:ILE:N	54:Ak:19:PRO:HD2	2.23	0.53
2:B:120:VAL:HG12	8:H:25:ARG:NH2	2.22	0.53
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.43	0.53
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.91	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.53
5:E:47:ASN:OD1	5:E:50:THR:HG23	2.09	0.53
5:E:131:ILE:HD13	5:E:151:LEU:HD11	1.90	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
12:L:247:LEU:O	12:L:252:MET:HB3	2.09	0.53
13:M:188:ALA:H	13:M:253:LEU:HD11	1.74	0.53
13:M:264:LEU:CD2	38:m:98:LEU:HD21	2.38	0.53
14:N:227:ILE:HA	14:N:230:ILE:CG2	2.38	0.53
18:R:69:VAL:HG12	18:R:112:LYS:N	2.24	0.53
19:S:16:LEU:O	19:S:16:LEU:CD1	2.51	0.53
19:S:16:LEU:HD13	19:S:19:ILE:CD1	2.38	0.53
21:V:12:VAL:CG1	21:V:13:GLY:N	2.72	0.53
25:Z:110:VAL:HG11	30:e:72:THR:HA	1.90	0.53
26:a:3:PHE:HE2	62:q:201:CDL:H112	1.74	0.53
28:c:55:TRP:HE1	29:d:66:THR:CG2	2.22	0.53
30:e:40:TRP:CG	30:e:40:TRP:O	2.61	0.53
38:m:85:LYS:O	38:m:85:LYS:HG2	2.09	0.53
39:n:132:SER:O	39:n:136:GLU:HG2	2.09	0.53
46:AB:362:ALA:HB2	46:AB:432:VAL:HG21	1.91	0.53
4:D:253:LEU:HB2	43:r:23:LYS:HD2	1.89	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:634:LEU:HD13	7:G:636:TYR:CZ	2.43	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.39	0.52
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.52
10:J:133:VAL:CG2	25:Z:68:ARG:NH1	2.71	0.52
12:L:128:MET:CG	12:L:251:THR:HB	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:400:ASN:HB3	12:L:486:LEU:HD22	1.91	0.52
13:M:15:THR:HG21	13:M:100:ILE:HD12	1.90	0.52
13:M:213:HIS:O	13:M:217:PRO:HD3	2.09	0.52
13:M:313:THR:HA	13:M:316:MET:HE3	1.89	0.52
13:M:447:LEU:HD11	13:M:454:ILE:HG23	1.90	0.52
15:O:170:LEU:HD13	15:O:187:TYR:CD2	2.44	0.52
15:O:347:VAL:HG11	28:c:29:PHE:CA	2.31	0.52
18:R:113:GLN:CD	18:R:113:GLN:N	2.66	0.52
24:Y:65:ALA:O	24:Y:68:ILE:HG12	2.09	0.52
39:n:39:TYR:CZ	39:n:43:LEU:HD11	2.44	0.52
45:AA:286:HIS:HA	45:AA:359:VAL:HG22	1.90	0.52
47:AC:152:ALA:HB1	47:AC:288:LEU:CD2	2.39	0.52
47:AC:170:VAL:HG23	47:AC:174:THR:CB	2.39	0.52
49:AE:241:SER:OG	49:AE:253:PRO:HD2	2.09	0.52
49:Ae:155:LYS:O	49:Ae:158:ASP:HB2	2.09	0.52
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.52
2:B:141:MET:HE1	4:D:86:PRO:HB2	1.90	0.52
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.09	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
11:K:89:TYR:HB3	11:K:91:GLN:OE1	2.09	0.52
12:L:108:MET:HB2	12:L:114:ILE:HD13	1.90	0.52
12:L:145:GLU:HG2	13:M:370:PRO:HD3	1.90	0.52
12:L:536:ILE:HG23	12:L:537:THR:N	2.25	0.52
13:M:73:LEU:HD21	13:M:100:ILE:HG12	1.91	0.52
13:M:160:LEU:CD2	13:M:164:LEU:HD13	2.39	0.52
13:M:354:LEU:O	13:M:357:THR:N	2.41	0.52
13:M:393:ILE:CG2	58:M:502:3PE:H381	2.39	0.52
15:O:121:PRO:C	15:O:122:LYS:HG2	2.33	0.52
17:Q:59:LEU:HD21	22:W:80:ARG:HH12	1.74	0.52
18:R:98:GLU:HA	18:R:113:GLN:CD	2.33	0.52
34:i:83:HIS:CD2	41:p:37:TYR:HE2	2.27	0.52
45:AA:165:ARG:HE	45:AA:209:ARG:HA	1.74	0.52
46:AB:348:GLY:HA2	46:AB:448:PRO:HD3	1.91	0.52
47:AC:107:TYR:HB2	47:AC:305:PRO:HG3	1.91	0.52
48:AD:227:LEU:HD12	48:AD:227:LEU:C	2.34	0.52
49:AE:89:SER:HA	49:AE:92:ARG:HB2	1.91	0.52
49:AE:127:TYR:HE1	53:AJ:33:GLU:HG3	1.74	0.52
49:AE:155:LYS:O	49:AE:158:ASP:HB2	2.09	0.52
46:Ab:42:LYS:HG3	46:Ab:48:VAL:HG22	1.90	0.52
46:Ab:362:ALA:HB2	46:Ab:432:VAL:HG21	1.91	0.52
52:Ah:45:ARG:O	52:Ah:49:GLU:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:MET:SD	8:H:126:LYS:HD3	2.49	0.52
7:G:30:ASN:O	7:G:45:PRO:HD3	2.09	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.91	0.52
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.91	0.52
10:J:141:VAL:HG23	11:K:58:PRO:HA	1.91	0.52
12:L:228:GLY:O	12:L:229:LEU:CG	2.47	0.52
13:M:403:THR:HA	13:M:406:TYR:CE2	2.44	0.52
15:O:310:ILE:HG13	15:O:311:PRO:HD2	1.91	0.52
16:P:239:PRO:HG2	16:P:345:LEU:CD1	2.40	0.52
16:P:283:MET:HE2	16:P:366:ILE:HG22	1.92	0.52
16:P:353:LEU:HA	16:P:356:HIS:HD2	1.74	0.52
18:R:95:LEU:HD21	18:R:111:PHE:CB	2.37	0.52
20:T:114:ASP:OD1	22:W:67:ARG:NH1	2.42	0.52
21:V:95:LEU:HA	21:V:100:TRP:CH2	2.35	0.52
25:Z:98:MET:SD	30:e:79:ILE:HG12	2.50	0.52
40:o:22:ILE:O	40:o:105:GLU:CD	2.52	0.52
42:q:3:LEU:HD13	62:q:201:CDL:OB6	2.09	0.52
45:AA:64:SER:OG	45:AA:235:GLY:HA2	2.10	0.52
49:AE:156:LEU:CB	49:AE:269:ASP:HA	2.38	0.52
47:Ac:30:TRP:HB3	47:Ac:100:ARG:HD3	1.90	0.52
47:Ac:107:TYR:HB2	47:Ac:305:PRO:HG3	1.92	0.52
49:Ae:180:THR:N	49:Ae:183:GLU:HB2	2.23	0.52
52:Ah:35:CYS:HA	52:Ah:38:LEU:HD13	1.92	0.52
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.90	0.52
5:E:178:ALA:HA	6:F:125:CYS:SG	2.49	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
8:H:317:TYR:O	8:H:318:MET:C	2.52	0.52
10:J:123:TRP:HZ2	30:e:76:MET:SD	2.32	0.52
11:K:38:LEU:HG	11:K:42:ILE:CD1	2.39	0.52
12:L:332:HIS:CD2	12:L:336:LYS:HG3	2.44	0.52
16:P:275:HIS:HA	16:P:278:LYS:HG2	1.91	0.52
24:Y:90:LEU:O	24:Y:91:ASN:C	2.51	0.52
26:a:64:LYS:HG3	26:a:66:LEU:H	1.75	0.52
30:e:69:ARG:HG3	30:e:72:THR:OG1	2.09	0.52
37:l:119:THR:HG22	38:m:13:THR:HG23	1.90	0.52
42:q:6:VAL:HG11	62:q:201:CDL:HB4	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:346:PRO:O	47:AC:349:ILE:HG22	2.10	0.52
48:AD:112:ARG:HD3	48:AD:257:ASP:OD2	2.09	0.52
45:Aa:49:GLN:HG2	45:Aa:239:HIS:CG	2.45	0.52
45:Aa:165:ARG:HE	45:Aa:209:ARG:HA	1.74	0.52
45:Aa:207:ASN:O	45:Aa:211:LEU:HG	2.09	0.52
47:Ac:170:VAL:HG23	47:Ac:174:THR:CB	2.39	0.52
48:Ad:321:TYR:HB2	50:Af:61:PHE:CG	2.45	0.52
48:Ad:321:TYR:CD2	48:Ad:323:PRO:HD3	2.45	0.52
2:B:103:GLU:O	2:B:106:HIS:HB2	2.10	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.52
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.52
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.52
7:G:36:VAL:CG1	7:G:56:VAL:HG11	2.34	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
11:K:57:MET:N	11:K:58:PRO:HD2	2.24	0.52
12:L:297:ASP:HB3	12:L:300:LYS:CG	2.39	0.52
13:M:68:LEU:HG	13:M:234:ILE:HD11	1.92	0.52
15:O:336:GLY:N	15:O:344:ASN:ND2	2.56	0.52
29:d:101:PHE:CZ	33:h:159:LEU:HD22	2.45	0.52
34:i:31:ARG:O	34:i:32:GLU:C	2.50	0.52
37:l:162:PRO:HG3	40:o:39:MET:HE3	1.92	0.52
48:AD:248:ILE:CG2	48:AD:263:MET:HG3	2.40	0.52
49:AE:248:ARG:HG2	49:AE:257:ASN:ND2	2.25	0.52
45:Aa:171:GLU:O	45:Aa:174:GLU:HG2	2.10	0.52
46:Ab:117:GLU:OE2	46:Ab:330:TYR:HB3	2.09	0.52
49:Ae:261:PRO:HB2	49:Ae:273:VAL:CG1	2.39	0.52
50:Af:44:VAL:O	50:Af:48:ILE:HG13	2.09	0.52
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.91	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.90	0.52
12:L:496:LEU:C	12:L:496:LEU:CD1	2.79	0.52
12:L:578:THR:HG21	14:N:168:GLY:HA2	1.92	0.52
13:M:17:LEU:HD13	31:f:11:TRP:CH2	2.45	0.52
13:M:196:TRP:HE1	13:M:254:THR:HB	1.75	0.52
14:N:10:TYR:O	14:N:13:ILE:HG22	2.09	0.52
20:T:87:LEU:HD23	20:T:122:MET:HE1	1.91	0.52
20:T:130:ILE:CG2	20:T:131:PRO:HD2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:37:ASP:OD1	23:X:38:LYS:N	2.43	0.52
23:X:49:GLU:HG2	23:X:138:PRO:HD2	1.91	0.52
32:g:70:ASP:OD1	39:n:108:HIS:NE2	2.42	0.52
42:q:13:GLN:HE22	62:q:201:CDL:CA3	2.21	0.52
42:q:29:ARG:HD3	42:q:74:PHE:CD1	2.44	0.52
46:AB:226:SER:O	46:AB:229:VAL:HG22	2.09	0.52
49:AE:242:HIS:CD2	49:AE:251:LYS:HB3	2.45	0.52
49:AI:62:ARG:HB2	49:AI:78:PHE:O	2.09	0.52
45:Aa:74:TRP:CZ2	45:Aa:411:GLU:HA	2.44	0.52
46:Ab:43:LEU:HB2	46:Ab:45:ASN:OD1	2.08	0.52
48:Ad:158:PRO:HA	48:Ad:164:MET:N	2.24	0.52
2:B:173:TYR:O	3:C:203:LEU:HD22	2.09	0.52
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.52
10:J:134:MET:HE2	27:b:51:TYR:CD1	2.40	0.52
12:L:123:LEU:HD22	12:L:150:MET:HG3	1.91	0.52
12:L:264:HIS:O	12:L:265:PRO:C	2.53	0.52
62:L:703:CDL:H741	62:L:703:CDL:H781	1.92	0.52
13:M:84:LEU:HD21	13:M:95:TYR:HB3	1.90	0.52
13:M:171:VAL:HG11	13:M:179:LEU:CD2	2.35	0.52
13:M:346:ARG:O	13:M:419:LEU:HA	2.09	0.52
14:N:175:MET:HG2	14:N:219:LEU:CD2	2.40	0.52
15:O:170:LEU:HD13	15:O:187:TYR:CG	2.44	0.52
17:Q:72:ILE:HD13	17:Q:143:TRP:NE1	2.24	0.52
25:Z:64:ASP:OD1	25:Z:65:LEU:N	2.42	0.52
28:c:47:SER:HB2	29:d:59:HIS:HD2	1.74	0.52
46:AB:70:ARG:NH2	46:AB:332:ASP:OD2	2.42	0.52
48:Ad:140:TYR:HA	48:Ad:144:GLU:OE1	2.09	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.52
5:E:240:PRO:HG3	6:F:60:GLY:HA2	1.91	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
12:L:108:MET:HB2	12:L:114:ILE:CD1	2.39	0.52
12:L:533:ILE:HG23	12:L:534:HIS:HD2	1.74	0.52
14:N:175:MET:HG2	14:N:219:LEU:HD22	1.91	0.52
15:O:172:ALA:HA	15:O:236:ASP:HB3	1.91	0.52
22:W:42:TRP:CH2	66:W:201:EHZ:O1	2.63	0.52
23:X:77:HIS:HD2	23:X:115:LEU:HD21	1.75	0.52
30:e:81:LYS:O	30:e:84:GLU:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:57:VAL:HG13	39:n:104:LEU:HG	1.92	0.52
46:AB:170:GLN:HG3	46:AB:339:TYR:OH	2.10	0.52
47:AC:21:LEU:HD22	68:AC:403:UQ6:H3M2	1.88	0.52
47:AC:148:ASN:HB2	49:Ae:220:LEU:O	2.09	0.52
48:AD:215:LEU:CD1	69:AD:401:HEC:HMB3	2.37	0.52
48:AD:228:ARG:HG2	48:AD:231:LEU:HD12	1.91	0.52
49:AE:192:VAL:HA	49:AE:195:LEU:CD1	2.37	0.52
54:AK:38:TRP:HE1	54:AK:40:LEU:HD12	1.74	0.52
50:Af:97:GLU:HA	50:Af:100:ARG:NH1	2.24	0.52
52:Ah:31:VAL:HG21	52:Ah:84:LEU:HA	1.91	0.52
1:A:104:TYR:O	1:A:105:GLU:C	2.51	0.52
3:C:114:THR:CG2	4:D:421:ARG:HH12	2.17	0.52
4:D:35:ARG:HH12	32:g:56:ASP:HB2	1.74	0.52
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:30:ASN:O	7:G:44:GLU:HA	2.09	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.52
13:M:72:LEU:HD11	13:M:233:ALA:HB1	1.92	0.52
13:M:103:GLN:O	13:M:107:ILE:HB	2.10	0.52
14:N:29:MET:HE2	14:N:141:ILE:HG12	1.92	0.52
15:O:121:PRO:HB3	15:O:178:TYR:CE1	2.45	0.52
15:O:245:PHE:HA	15:O:248:LYS:HE2	1.91	0.52
27:b:82:LYS:O	27:b:83:ASN:C	2.52	0.52
29:d:1:MET:HG3	29:d:2:MET:N	2.25	0.52
30:e:44:ALA:HA	30:e:47:ILE:HG12	1.92	0.52
37:l:169:GLU:C	37:l:171:GLY:N	2.55	0.52
39:n:37:TYR:C	39:n:39:TYR:N	2.67	0.52
45:AA:276:ARG:CG	45:AA:462:ILE:HD11	2.39	0.52
45:AA:392:LYS:HE2	45:AA:396:ARG:HH22	1.74	0.52
47:AC:245:PHE:CE1	48:AD:102:LEU:HD23	2.45	0.52
49:AE:88:PHE:HB3	49:AE:91:TYR:HD2	1.75	0.52
50:AF:97:GLU:HA	50:AF:100:ARG:HH11	1.75	0.52
48:Ad:215:LEU:HD21	69:Ad:401:HEC:C1B	2.40	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.52
5:E:192:TYR:CE2	5:E:213:PRO:HB2	2.45	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.45	0.52
7:G:671:LEU:CD1	19:S:42:VAL:HG12	2.40	0.52
10:J:106:LEU:HD12	10:J:109:TYR:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:195:PHE:CD1	16:P:198:ALA:HB2	2.45	0.52
20:T:79:ILE:CG2	20:T:145:VAL:HG13	2.40	0.52
20:U:128:PHE:CE1	20:U:148:ILE:HG23	2.45	0.52
22:W:73:ASN:O	22:W:76:VAL:HG12	2.10	0.52
23:X:47:ARG:HH12	33:h:188:ASP:HB2	1.73	0.52
23:X:129:THR:CG2	27:b:68:SER:HA	2.39	0.52
27:b:68:SER:O	27:b:69:HIS:C	2.51	0.52
29:d:62:LEU:O	29:d:66:THR:OG1	2.22	0.52
39:n:168:TRP:HD1	39:n:169:HIS:CE1	2.27	0.52
42:q:29:ARG:HD3	42:q:74:PHE:CE1	2.44	0.52
42:q:89:TRP:HB2	42:q:98:PRO:HD3	1.92	0.52
45:AA:207:ASN:O	45:AA:211:LEU:HG	2.09	0.52
52:AH:79:CYS:HA	52:AH:82:HIS:HE2	1.71	0.52
46:Ab:170:GLN:HG3	46:Ab:339:TYR:OH	2.10	0.52
3:C:124:ARG:HD2	17:Q:140:LYS:HZ2	1.75	0.51
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.74	0.51
6:F:63:TYR:H	6:F:256:ARG:HH21	1.57	0.51
7:G:47:THR:O	7:G:96:VAL:HG12	2.10	0.51
7:G:275:PRO:HB2	17:Q:86:ASN:ND2	2.25	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.51
7:G:614:GLY:O	22:W:129:HIS:NE2	2.41	0.51
8:H:51:ASP:OD2	61:H:401:UQ9:C16	2.58	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.51
13:M:115:LEU:HD21	13:M:176:LEU:CD2	2.37	0.51
13:M:139:GLN:HB3	13:M:222:GLU:CG	2.40	0.51
20:U:120:MET:HE1	39:n:24:LEU:CD1	2.40	0.51
24:Y:17:GLY:O	24:Y:81:GLN:HG2	2.09	0.51
25:Z:97:ILE:CG2	30:e:83:ARG:HB2	2.40	0.51
25:Z:97:ILE:HG21	30:e:83:ARG:HB2	1.92	0.51
39:n:143:GLU:O	39:n:143:GLU:HG2	2.10	0.51
41:p:164:LEU:O	41:p:168:LYS:N	2.42	0.51
43:r:28:TYR:O	43:r:29:GLN:C	2.53	0.51
47:AC:221:HIS:O	47:AC:225:THR:HB	2.09	0.51
48:AD:94:TYR:CE2	52:AH:84:LEU:HD23	2.45	0.51
48:AD:155:GLN:CA	48:AD:166:MET:HG2	2.40	0.51
52:AH:42:VAL:HG22	52:AH:45:ARG:HH21	1.74	0.51
54:Ak:12:GLU:HA	54:Ak:15:ARG:HH11	1.73	0.51
2:B:92:PRO:CD	2:B:121:PHE:H	2.18	0.51
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.33	0.51
4:D:106:VAL:HG21	4:D:447:VAL:CG2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:217:GLU:CD	17:Q:166:TRP:HE1	2.18	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.51
10:J:127:GLU:OE2	25:Z:120:LEU:HD23	2.11	0.51
12:L:180:ILE:HD11	13:M:400:ILE:HB	1.92	0.51
12:L:286:LEU:HG	12:L:290:ILE:CD1	2.40	0.51
13:M:422:HIS:HB3	38:m:51:TYR:CE2	2.44	0.51
20:T:130:ILE:HG23	20:T:131:PRO:CD	2.40	0.51
25:Z:61:LEU:O	25:Z:64:ASP:OD1	2.28	0.51
25:Z:65:LEU:HB2	27:b:50:PRO:HG2	1.91	0.51
45:AA:72:GLY:C	45:AA:74:TRP:CZ3	2.89	0.51
48:AD:133:ARG:HH21	49:AE:148:ALA:HB2	1.75	0.51
49:AE:196:ARG:HD2	49:AE:249:ILE:CG2	2.40	0.51
48:Ad:112:ARG:HD3	48:Ad:257:ASP:OD2	2.09	0.51
49:Ae:152:ILE:HG23	49:Ae:154:ILE:CD1	2.38	0.51
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.33	0.51
5:E:129:TYR:CE2	5:E:207:LEU:HB3	2.46	0.51
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.39	0.51
7:G:75:CYS:SG	7:G:76:ARG:N	2.84	0.51
7:G:367:CYS:HB3	7:G:533:GLY:O	2.10	0.51
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.44	0.51
8:H:51:ASP:O	8:H:54:LYS:HG2	2.10	0.51
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.51
12:L:202:MET:CE	12:L:265:PRO:HG3	2.32	0.51
12:L:556:ILE:HD11	38:m:76:ILE:CG2	2.40	0.51
14:N:168:GLY:O	14:N:172:GLN:HG2	2.10	0.51
20:U:125:GLU:OE2	35:j:44:TYR:CE1	2.63	0.51
34:i:10:LEU:HA	34:i:13:GLN:HB3	1.91	0.51
35:j:87:PRO:HG3	40:o:96:VAL:HG23	1.92	0.51
45:AA:171:GLU:O	45:AA:174:GLU:HG2	2.10	0.51
45:AA:400:VAL:O	45:AA:403:LEU:HB2	2.10	0.51
47:AC:285:PRO:O	49:Ae:253:PRO:HB3	2.10	0.51
49:AE:263:TYR:HA	49:AE:273:VAL:HA	1.93	0.51
46:Ab:43:LEU:N	46:Ab:47:LEU:O	2.44	0.51
47:Ac:346:PRO:O	47:Ac:349:ILE:HG22	2.10	0.51
48:Ad:215:LEU:CD1	69:Ad:401:HEC:HMB3	2.36	0.51
49:Ae:154:ILE:HB	49:Ae:271:VAL:O	2.11	0.51
52:Ah:31:VAL:HG13	52:Ah:83:LYS:HE2	1.93	0.51
2:B:126:ARG:HG3	8:H:214:GLU:HA	1.91	0.51
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.51
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.45	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
9:I:38:TYR:HB3	9:I:41:LYS:HB2	1.93	0.51
9:I:209:TYR:HA	9:I:212:ARG:CG	2.39	0.51
11:K:59:ILE:O	11:K:60:PRO:C	2.49	0.51
14:N:25:ASN:ND2	30:e:18:PHE:CE2	2.78	0.51
31:f:34:LEU:HD22	33:h:139:ILE:HG13	1.91	0.51
33:h:52:LYS:O	33:h:53:ARG:C	2.53	0.51
34:i:77:ILE:HD13	34:i:80:TRP:CZ3	2.46	0.51
42:q:65:THR:CG2	42:q:66:THR:N	2.72	0.51
48:AD:321:TYR:CD2	48:AD:323:PRO:HD3	2.44	0.51
47:Ac:221:HIS:O	47:Ac:225:THR:HB	2.10	0.51
49:Ae:241:SER:OG	49:Ae:253:PRO:HD2	2.10	0.51
49:Ae:263:TYR:CB	49:Ae:273:VAL:HG22	2.37	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
7:G:41:VAL:HG21	7:G:56:VAL:CB	2.41	0.51
7:G:253:VAL:O	7:G:253:VAL:HG12	2.11	0.51
7:G:304:GLU:HB2	7:G:316:TYR:HD2	1.75	0.51
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.41	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:386:LEU:HD21	7:G:523:VAL:HG13	1.91	0.51
12:L:49:LEU:HB3	12:L:50:PRO:HD3	1.91	0.51
12:L:595:ILE:O	12:L:599:ILE:HG13	2.11	0.51
13:M:129:THR:CG2	13:M:235:LEU:HD11	2.40	0.51
14:N:240:MET:HE2	14:N:326:PHE:CZ	2.45	0.51
14:N:342:GLN:HE21	29:d:30:ARG:HH11	1.59	0.51
15:O:354:LEU:HG	28:c:44:VAL:CG2	2.41	0.51
16:P:207:PHE:O	16:P:241:TYR:HA	2.10	0.51
23:X:168:PHE:C	23:X:169:PHE:CD1	2.89	0.51
24:Y:143:VAL:HG23	33:h:157:ARG:HG2	1.92	0.51
26:a:1:MET:HG3	62:q:201:CDL:CB2	2.41	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
45:AA:148:ALA:HA	45:AA:250:LEU:HD21	1.92	0.51
47:AC:107:TYR:HE1	47:AC:308:HIS:HB2	1.76	0.51
48:AD:213:SER:HB3	48:AD:236:TYR:CE2	2.45	0.51
48:AD:215:LEU:HD21	69:AD:401:HEC:C1B	2.40	0.51
50:AF:87:ASP:HB3	50:AF:89:PHE:CE1	2.45	0.51
50:AF:88:LYS:HD2	50:AF:90:TYR:HB3	1.91	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)
47:Ac:313:ARG:HB2	50:Af:39:HIS:ND1	2.25	0.51
49:Ae:248:ARG:HG2	49:Ae:257:ASN:ND2	2.25	0.51
51:Ag:31:PHE:CE1	62:Ag:102:CDL:H312	2.45	0.51
54:Ak:38:TRP:O	54:Ak:39:ARG:C	2.51	0.51
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.10	0.51
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.51
6:F:42:PHE:CE1	6:F:130:ILE:HD12	2.46	0.51
7:G:355:LYS:HA	7:G:366:LEU:CD1	2.37	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:33:LEU:HD23	43:r:25:GLN:HG2	1.92	0.51
8:H:51:ASP:OD2	61:H:401:UQ9:C15	2.56	0.51
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.46	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
12:L:530:PRO:O	12:L:534:HIS:HB2	2.11	0.51
13:M:31:SER:HA	13:M:34:ILE:CG1	2.41	0.51
13:M:251:ASP:N	13:M:252:PRO:HD2	2.26	0.51
27:b:36:SER:HB3	27:b:39:THR:OG1	2.10	0.51
36:k:34:PRO:HD2	36:k:59:TYR:CG	2.46	0.51
45:AA:51:SER:OG	45:AA:243:LEU:HD13	2.10	0.51
45:AA:73:VAL:HG23	45:AA:147:LEU:HD13	1.93	0.51
48:AD:318:LYS:CD	49:AE:86:PRO:HB2	2.41	0.51
45:Aa:148:ALA:HA	45:Aa:250:LEU:HD21	1.92	0.51
48:Ad:237:PHE:CG	48:Ad:242:ILE:HB	2.46	0.51
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
8:H:23:VAL:HG11	26:a:9:LEU:CD2	2.39	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
10:J:159:LEU:HD23	11:K:69:CYS:SG	2.51	0.51
12:L:161:ARG:NE	12:L:163:ASP:HB2	2.26	0.51
12:L:536:ILE:HD11	12:L:540:LYS:HD2	1.93	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	2.26	0.51
13:M:263:LEU:CD1	38:m:102:TYR:CD1	2.90	0.51
13:M:275:ILE:CD1	13:M:288:TYR:CG	2.84	0.51
13:M:336:ARG:HH12	13:M:433:GLU:CD	2.19	0.51
15:O:240:ALA:O	15:O:244:THR:N	2.44	0.51
16:P:305:PHE:CG	16:P:314:THR:HG22	2.46	0.51
26:a:42:GLN:O	26:a:43:TYR:C	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:28:ASP:O	29:d:29:PRO:C	2.53	0.51
33:h:57:VAL:HG13	39:n:104:LEU:HD21	1.92	0.51
36:k:42:LEU:HG	39:n:39:TYR:CD1	2.46	0.51
40:o:89:TYR:O	40:o:90:CYS:C	2.52	0.51
42:q:88:ARG:HB2	42:q:93:MET:HB2	1.91	0.51
42:q:88:ARG:HG3	42:q:89:TRP:N	2.26	0.51
45:AA:276:ARG:HH12	45:AA:278:ARG:HD2	1.75	0.51
45:AA:341:PHE:CZ	45:AA:372:LEU:HD13	2.46	0.51
47:AC:150:LEU:HD13	47:AC:164:ILE:HD12	1.92	0.51
50:AF:92:GLU:HG2	50:AF:96:LYS:HE2	1.93	0.51
52:AH:52:ASP:N	52:AH:65:CYS:SG	2.84	0.51
47:Ac:107:TYR:HE1	47:Ac:308:HIS:HB2	1.76	0.51
47:Ac:291:VAL:O	47:Ac:295:ILE:HG12	2.11	0.51
49:Ae:242:HIS:CD2	49:Ae:251:LYS:HB3	2.45	0.51
50:Af:72:ARG:O	50:Af:74:GLN:HG2	2.10	0.51
4:D:299:GLN:OE1	43:r:104:TRP:HB2	2.10	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:358:LEU:HD12	7:G:366:LEU:CD2	2.40	0.51
7:G:401:LEU:HD21	7:G:462:PHE:CE2	2.46	0.51
7:G:401:LEU:HD21	7:G:466:LEU:HD21	1.92	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:42:PRO:HB3	42:q:27:PHE:HE2	1.76	0.51
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.39	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
12:L:9:LEU:HD11	58:i:201:3PE:C2A	2.41	0.51
12:L:60:GLU:HG3	12:L:83:ASP:HA	1.93	0.51
13:M:304:GLN:HA	13:M:309:PHE:CE1	2.45	0.51
14:N:45:ILE:HA	14:N:52:SER:OG	2.11	0.51
15:O:289:TRP:HA	15:O:289:TRP:CE3	2.46	0.51
20:T:140:CYS:HB2	20:T:143:GLU:CG	2.40	0.51
21:V:31:THR:HA	21:V:88:LEU:HD13	1.92	0.51
26:a:6:LEU:O	26:a:7:PRO:C	2.52	0.51
47:AC:37:LEU:HB2	67:AC:402:HEM:HMB2	1.93	0.51
48:AD:237:PHE:CG	48:AD:242:ILE:HB	2.46	0.51
48:Ad:323:PRO:HG2	48:Ad:325:LYS:CD	2.41	0.51
49:Ae:127:TYR:HE1	53:Aj:33:GLU:HG3	1.74	0.51
52:Ah:52:ASP:OD1	52:Ah:53:ASN:N	2.44	0.51
2:B:116:ARG:O	8:H:39:ILE:HG22	2.09	0.51
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:VAL:HG22	5:E:221:ARG:HH12	1.75	0.51
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.51
8:H:172:MET:HE1	25:Z:46:GLY:HA2	1.93	0.51
12:L:451:MET:O	12:L:452:ASN:C	2.53	0.51
15:O:182:GLN:O	15:O:183:CYS:C	2.54	0.51
16:P:55:VAL:HG22	16:P:79:GLN:HB3	1.91	0.51
16:P:367:GLU:HG2	16:P:368:GLU:N	2.26	0.51
17:Q:91:VAL:HG13	17:Q:95:LYS:NZ	2.26	0.51
18:R:72:VAL:HG12	18:R:73:GLU:N	2.26	0.51
19:S:79:LEU:CA	19:S:82:LEU:HD12	2.26	0.51
20:U:79:ILE:HG13	20:U:126:PHE:CE2	2.45	0.51
32:g:140:PHE:HZ	41:p:152:ALA:HB1	1.76	0.51
40:o:4:HIS:HA	40:o:7:ARG:NH1	2.25	0.51
45:AA:226:ALA:HB2	45:AA:253:VAL:HB	1.93	0.51
46:Ab:348:GLY:HA2	46:Ab:448:PRO:HD3	1.91	0.51
48:Ad:201:VAL:HG22	48:Ad:278:SER:CB	2.41	0.51
48:Ad:227:LEU:HD12	48:Ad:227:LEU:C	2.34	0.51
48:Ad:232:TYR:HD1	48:Ad:242:ILE:O	1.93	0.51
48:Ad:248:ILE:CG2	48:Ad:263:MET:HG3	2.40	0.51
51:Ag:73:LYS:NZ	52:Ah:63:GLU:HG2	2.26	0.51
4:D:166:ARG:CZ	25:Z:8:GLN:HG2	2.41	0.51
8:H:142:TYR:CE1	8:H:285:LEU:CD2	2.94	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
10:J:25:PRO:HD2	10:J:75:THR:HG21	1.93	0.51
11:K:73:VAL:HG21	14:N:38:LEU:HD22	1.93	0.51
12:L:404:THR:HG22	12:L:405:ASN:H	1.75	0.51
13:M:4:ILE:HD11	13:M:41:LEU:HD21	1.92	0.51
17:Q:77:VAL:HG12	17:Q:101:PHE:CG	2.46	0.51
20:T:105:MET:HB2	20:T:139:MET:SD	2.51	0.51
20:U:84:LEU:HD11	20:U:100:VAL:HG12	1.93	0.51
24:Y:14:VAL:HG13	24:Y:15:PRO:HD2	1.93	0.51
27:b:11:ASN:OD1	27:b:12:ALA:N	2.44	0.51
32:g:115:TRP:HA	32:g:118:ARG:HH11	1.74	0.51
33:h:73:PHE:CE2	33:h:74:TYR:CE1	2.98	0.51
40:o:7:ARG:HH11	40:o:106:ARG:HH12	1.59	0.51
45:AA:340:SER:O	45:AA:358:PHE:HA	2.11	0.51
49:AE:184:ILE:HG21	49:AE:208:PRO:HB3	1.93	0.51
49:AE:195:LEU:HD11	49:AE:248:ARG:NH1	2.26	0.51
46:Ab:236:GLN:HG3	46:Ab:237:PHE:HD2	1.76	0.51
48:Ad:213:SER:HB3	48:Ad:236:TYR:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:196:ARG:HD2	49:Ae:249:ILE:CG2	2.41	0.51
50:Af:99:ILE:O	50:Af:103:LYS:HG2	2.11	0.51
1:A:59:ALA:O	1:A:62:PHE:HB3	2.11	0.50
4:D:49:GLY:O	14:N:173:THR:HG21	2.10	0.50
4:D:84:PHE:HB2	4:D:97:LEU:HB3	1.93	0.50
4:D:253:LEU:HB2	43:r:23:LYS:HD3	1.92	0.50
4:D:280:ALA:CB	21:V:11:LEU:CG	2.81	0.50
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.46	0.50
7:G:382:ARG:O	7:G:386:LEU:HD12	2.10	0.50
9:I:71:GLY:HA2	57:I:301:PC1:H351	1.93	0.50
11:K:93:LEU:HD13	14:N:57:THR:HG21	1.92	0.50
12:L:362:ILE:CD1	12:L:430:VAL:HG13	2.41	0.50
13:M:249:ILE:HG22	13:M:250:LEU:N	2.26	0.50
17:Q:75:ARG:HH12	17:Q:104:ARG:HG2	1.76	0.50
17:Q:167:ASN:C	17:Q:168:LYS:HG2	2.36	0.50
21:V:62:GLU:HB3	21:V:68:LEU:HD13	1.92	0.50
23:X:9:THR:HG23	23:X:12:GLU:H	1.76	0.50
23:X:25:LEU:O	23:X:29:ALA:N	2.44	0.50
24:Y:83:ARG:HH12	24:Y:90:LEU:HB3	1.76	0.50
41:p:113:CYS:O	41:p:113:CYS:SG	2.69	0.50
46:AB:425:VAL:HG12	46:AB:429:LYS:HZ1	1.76	0.50
48:AD:201:VAL:HG22	48:AD:278:SER:CB	2.41	0.50
48:AD:214:LEU:HD12	48:AD:234:ASN:CG	2.36	0.50
48:AD:242:ILE:CD1	48:AD:244:MET:HE2	2.41	0.50
47:Ac:15:ASN:OD1	47:Ac:19:ILE:HB	2.11	0.50
47:Ac:140:PHE:HE1	47:Ac:170:VAL:HG13	1.76	0.50
2:B:174:SER:HA	3:C:203:LEU:CD2	2.41	0.50
4:D:444:LEU:HD21	8:H:206:GLU:O	2.12	0.50
5:E:128:LYS:CB	5:E:167:LEU:HA	2.42	0.50
7:G:617:ARG:NH1	22:W:129:HIS:N	2.57	0.50
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.50
8:H:74:ALA:HB3	8:H:75:PRO:HD3	1.93	0.50
10:J:7:VAL:O	10:J:11:LEU:HD13	2.12	0.50
12:L:395:ILE:O	12:L:399:ILE:HG13	2.11	0.50
14:N:175:MET:O	14:N:179:MET:HG2	2.12	0.50
20:T:87:LEU:HD23	20:T:122:MET:CE	2.41	0.50
20:U:79:ILE:HG23	20:U:145:VAL:HG13	1.91	0.50
26:a:3:PHE:CE2	62:q:201:CDL:H112	2.47	0.50
41:p:49:ARG:O	41:p:52:ILE:HB	2.10	0.50
42:q:6:VAL:HG12	62:q:201:CDL:OA9	2.11	0.50
46:AB:305:THR:O	46:AB:311:GLN:HG3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:131:ALA:HB3	48:AD:133:ARG:HG3	1.91	0.50
49:AI:64:LEU:CA	49:AI:78:PHE:HA	2.34	0.50
45:Aa:101:THR:HG21	45:Aa:149:ASP:HB3	1.94	0.50
46:Ab:299:ILE:H	46:Ab:299:ILE:HD12	1.76	0.50
47:Ac:294:LEU:CG	70:Ac:405:U10:H1M3	2.42	0.50
49:Ae:127:TYR:CE1	53:Aj:33:GLU:HG3	2.46	0.50
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.26	0.50
12:L:349:SER:HB2	12:L:443:ILE:HG23	1.93	0.50
12:L:383:MET:CB	12:L:386:LEU:HD12	2.30	0.50
13:M:294:MET:HE3	13:M:319:HIS:HD2	1.76	0.50
13:M:354:LEU:O	13:M:355:MET:C	2.52	0.50
14:N:36:SER:HB2	14:N:134:GLN:HE22	1.76	0.50
14:N:248:LEU:CD1	14:N:296:LEU:HD23	2.41	0.50
16:P:68:TYR:CD1	16:P:242:VAL:HG21	2.46	0.50
16:P:172:ALA:H	16:P:202:ARG:NH2	2.08	0.50
17:Q:167:ASN:HA	44:s:64:ARG:HD3	1.94	0.50
20:U:122:MET:HA	20:U:122:MET:HE2	1.91	0.50
25:Z:120:LEU:HD21	30:e:32:ARG:HH21	1.75	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
34:i:32:GLU:HG3	39:n:115:TYR:HA	1.93	0.50
37:l:87:ASP:OD1	37:l:88:PRO:HD2	2.11	0.50
48:AD:116:VAL:HA	48:AD:253:LEU:CD2	2.41	0.50
49:AE:127:TYR:CE1	53:AJ:33:GLU:HG3	2.46	0.50
49:AI:65:VAL:HG11	49:AI:77:ARG:NH2	2.25	0.50
48:Ad:214:LEU:HD12	48:Ad:234:ASN:CG	2.36	0.50
49:Ae:145:ASP:O	49:Ae:149:MET:HG3	2.12	0.50
1:A:57:LEU:O	1:A:61:THR:HG23	2.12	0.50
5:E:43:THR:HG23	5:E:46:ASN:H	1.75	0.50
6:F:238:CYS:O	6:F:239:PRO:C	2.54	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:136:GLU:HB3	17:Q:87:MET:HB3	1.92	0.50
12:L:21:ILE:HG12	12:L:27:ILE:HG23	1.93	0.50
12:L:117:PHE:HE1	12:L:243:VAL:CG2	2.23	0.50
12:L:385:PHE:CD1	35:j:72:ARG:CG	2.95	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
18:R:55:VAL:HG22	18:R:56:ASN:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:57:ARG:HG2	24:Y:60:ARG:NH2	2.27	0.50
41:p:5:TRP:HZ3	41:p:10:TYR:O	1.93	0.50
49:AE:242:HIS:HD2	49:AE:251:LYS:HB3	1.76	0.50
53:AJ:22:ALA:HB1	54:AK:27:VAL:HG11	1.92	0.50
45:Aa:73:VAL:HG23	45:Aa:147:LEU:HD13	1.93	0.50
45:Aa:281:ALA:HB2	51:Ag:12:ARG:CZ	2.41	0.50
52:Ah:69:LEU:O	52:Ah:70:PHE:C	2.53	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.50
4:D:54:PRO:HB2	4:D:59:ALA:HB2	1.94	0.50
4:D:55:SER:HB3	4:D:58:THR:HB	1.94	0.50
4:D:266:ARG:HD3	58:H:403:3PE:O12	2.11	0.50
5:E:136:THR:HG22	5:E:137:THR:N	2.27	0.50
6:F:113:LEU:HB3	6:F:154:ALA:HB2	1.92	0.50
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.94	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
10:J:13:LEU:CD2	11:K:14:LEU:HD12	2.41	0.50
12:L:365:ILE:CD1	12:L:366:MET:HE2	2.42	0.50
12:L:441:ILE:HD13	35:j:48:PRO:HD3	1.94	0.50
13:M:118:PHE:O	13:M:122:PHE:HB2	2.11	0.50
13:M:123:GLU:HB3	14:N:255:PRO:HG2	1.93	0.50
16:P:374:THR:HG23	16:P:374:THR:O	2.10	0.50
34:i:10:LEU:HD12	34:i:13:GLN:HB3	1.94	0.50
36:k:34:PRO:CG	36:k:59:TYR:CD1	2.94	0.50
39:n:114:MET:O	39:n:115:TYR:C	2.52	0.50
47:AC:21:LEU:HD11	68:AC:403:UQ6:O2	2.11	0.50
45:Aa:273:SER:HB2	51:Ag:18:SER:O	2.11	0.50
45:Aa:393:ASN:O	45:Aa:397:ASN:ND2	2.44	0.50
48:Ad:138:VAL:HG11	48:Ad:276:TRP:NE1	2.26	0.50
48:Ad:242:ILE:CD1	48:Ad:244:MET:HE2	2.41	0.50
49:Ae:195:LEU:HD11	49:Ae:248:ARG:NH1	2.26	0.50
50:Af:76:LEU:HB2	50:Af:81:TRP:CD1	2.47	0.50
2:B:125:PRO:O	2:B:152:MET:HA	2.10	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
11:K:38:LEU:HG	11:K:42:ILE:HD11	1.93	0.50
12:L:403:ASN:OD1	37:l:153:TYR:HB3	2.11	0.50
14:N:189:TRP:HB2	14:N:204:ASN:HD21	1.77	0.50
16:P:150:ARG:O	16:P:151:ALA:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:348:LYS:HB3	16:P:351:GLU:OE2	2.11	0.50
18:R:70:ASN:HD22	18:R:111:PHE:HE1	1.60	0.50
24:Y:115:MET:SD	24:Y:119:TYR:HE2	2.34	0.50
26:a:4:GLU:O	26:a:7:PRO:HD2	2.11	0.50
37:l:108:ASP:HB3	37:l:111:MET:HE2	1.93	0.50
38:m:124:LYS:HE2	38:m:125:PHE:CE2	2.47	0.50
43:r:6:ARG:HG2	43:r:6:ARG:O	2.11	0.50
47:AC:291:VAL:O	47:AC:295:ILE:HG12	2.11	0.50
48:AD:91:PRO:HG3	48:AD:236:TYR:CD1	2.47	0.50
49:AE:212:ILE:HD12	49:AE:263:TYR:CG	2.46	0.50
46:Ab:227:HIS:HD2	46:Ab:231:LYS:HE2	1.76	0.50
46:Ab:280:ASN:O	46:Ab:283:ALA:HB3	2.12	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.50
8:H:103:LEU:HG	8:H:160:TYR:CD1	2.46	0.50
8:H:172:MET:SD	25:Z:46:GLY:HA2	2.52	0.50
12:L:60:GLU:O	12:L:61:TYR:CD1	2.65	0.50
13:M:4:ILE:HG22	13:M:107:ILE:CD1	2.32	0.50
13:M:63:THR:N	13:M:64:PRO:HD2	2.27	0.50
13:M:248:ILE:HG13	13:M:249:ILE:N	2.26	0.50
13:M:278:ARG:HH22	37:l:108:ASP:CG	2.20	0.50
13:M:328:CYS:SG	13:M:436:LEU:HD21	2.52	0.50
13:M:432:ARG:HA	13:M:435:THR:HG22	1.94	0.50
14:N:258:THR:HG23	14:N:336:THR:HG22	1.93	0.50
20:U:90:TYR:HD2	20:U:93:ILE:H	1.60	0.50
21:V:44:TYR:CD1	21:V:48:THR:HG23	2.46	0.50
22:W:95:GLU:HB3	22:W:101:LYS:HG3	1.94	0.50
27:b:35:ILE:O	27:b:35:ILE:CD1	2.59	0.50
27:b:38:TYR:HA	27:b:41:TYR:HD2	1.76	0.50
37:l:38:PRO:C	38:m:75:ASN:HD21	2.20	0.50
45:AA:101:THR:HG21	45:AA:149:ASP:HB3	1.94	0.50
45:AA:127:GLU:OE2	45:AA:348:TYR:HB3	2.11	0.50
49:AE:136:PHE:O	49:AE:137:VAL:C	2.51	0.50
49:AE:155:LYS:HZ3	49:AE:157:SER:HB3	1.77	0.50
46:Ab:64:PHE:HZ	46:Ab:394:SER:HA	1.77	0.50
47:Ac:22:PRO:HA	51:Ag:5:PHE:CZ	2.46	0.50
49:Ae:242:HIS:HD2	49:Ae:251:LYS:HB3	1.76	0.50
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.47	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:295:PRO:HD2	6:F:298:GLU:OE2	2.11	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.50
10:J:37:PHE:CE2	10:J:41:LEU:HD11	2.46	0.50
12:L:589:MET:O	12:L:592:LEU:N	2.45	0.50
15:O:319:ILE:HD12	15:O:324:GLY:HA3	1.94	0.50
16:P:157:LYS:O	16:P:158:GLU:C	2.53	0.50
19:S:36:PHE:CZ	19:S:44:LEU:HD11	2.37	0.50
20:U:142:GLN:O	20:U:145:VAL:N	2.43	0.50
21:V:12:VAL:CG1	21:V:13:GLY:H	2.22	0.50
23:X:8:PRO:HD3	23:X:54:ARG:CD	2.40	0.50
24:Y:12:HIS:NE2	24:Y:127:PHE:HZ	2.09	0.50
32:g:106:TYR:CZ	33:h:86:ILE:HD12	2.47	0.50
37:l:49:ALA:HA	37:l:59:VAL:HG13	1.93	0.50
46:AB:232:GLN:O	46:AB:235:GLU:HG3	2.11	0.50
48:AD:240:GLN:CG	52:AH:70:PHE:HZ	2.25	0.50
49:AE:184:ILE:CG2	49:AE:208:PRO:HB3	2.42	0.50
49:AE:197:ASP:HB3	49:AE:257:ASN:ND2	2.27	0.50
47:Ac:223:TYR:CE1	48:Ad:314:LEU:HG	2.46	0.50
54:Ak:23:MET:O	54:Ak:27:VAL:HG23	2.12	0.50
1:A:67:LEU:HD13	11:K:68:ALA:HB3	1.92	0.50
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.51	0.50
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.42	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.50
6:F:174:ARG:O	6:F:178:GLU:HG3	2.11	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:224:PHE:CG	61:H:401:UQ9:C20	2.93	0.50
10:J:19:LEU:CD2	11:K:32:CYS:HA	2.42	0.50
12:L:354:GLN:O	12:L:354:GLN:HG2	2.12	0.50
16:P:40:VAL:HB	16:P:53:GLY:HA2	1.93	0.50
18:R:32:THR:CG2	18:R:36:GLN:H	2.18	0.50
23:X:36:CYS:SG	23:X:36:CYS:O	2.69	0.50
23:X:170:TRP:CZ3	62:d:201:CDL:H522	2.47	0.50
33:h:57:VAL:HG13	39:n:104:LEU:CD2	2.41	0.50
46:AB:64:PHE:HZ	46:AB:394:SER:HA	1.77	0.50
46:AB:227:HIS:HD2	46:AB:231:LYS:HE2	1.76	0.50
48:AD:232:TYR:HD1	48:AD:242:ILE:O	1.93	0.50
45:Aa:127:GLU:OE2	45:Aa:348:TYR:HB3	2.11	0.50
48:Ad:116:VAL:HA	48:Ad:253:LEU:CD2	2.41	0.50
48:Ad:249:TYR:O	48:Ad:250:THR:C	2.55	0.50
4:D:105:MET:SD	4:D:441:GLY:HA2	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
5:E:130:HIS:O	5:E:132:GLN:HG3	2.12	0.49
5:E:152:GLN:HE21	5:E:159:VAL:HB	1.76	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:85:LEU:CD2	8:H:108:THR:HB	2.37	0.49
12:L:123:LEU:CD2	12:L:150:MET:HG3	2.43	0.49
12:L:217:LEU:HD13	12:L:273:ILE:HG23	1.93	0.49
12:L:306:THR:HA	12:L:336:LYS:NZ	2.27	0.49
13:M:25:THR:HG22	32:g:84:ASN:OD1	2.11	0.49
13:M:158:ILE:HG12	14:N:287:LEU:HD11	1.94	0.49
14:N:175:MET:HE1	14:N:227:ILE:HG22	1.94	0.49
14:N:190:MET:HB3	14:N:201:THR:HG23	1.94	0.49
14:N:307:THR:O	15:O:319:ILE:HG12	2.11	0.49
16:P:246:SER:O	16:P:247:LYS:C	2.55	0.49
21:V:56:LEU:C	21:V:56:LEU:CD1	2.85	0.49
21:V:56:LEU:HA	21:V:59:VAL:HB	1.94	0.49
23:X:7:LEU:CD1	25:Z:87:LEU:HB3	2.41	0.49
23:X:119:ARG:HD2	23:X:120:PRO:HD2	1.94	0.49
25:Z:140:PHE:O	25:Z:141:THR:C	2.55	0.49
28:c:55:TRP:CE2	29:d:66:THR:HG22	2.47	0.49
35:j:92:TRP:O	40:o:107:ARG:NH2	2.45	0.49
45:AA:341:PHE:CD1	45:AA:342:GLN:N	2.79	0.49
45:Aa:274:GLU:CG	45:Aa:456:VAL:HB	2.42	0.49
46:Ab:425:VAL:HG12	46:Ab:429:LYS:HZ1	1.77	0.49
48:Ad:138:VAL:C	48:Ad:140:TYR:H	2.19	0.49
50:Af:56:TYR:OH	51:Ag:10:ARG:HB3	2.12	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49
4:D:70:ASP:HB2	4:D:72:LEU:HG	1.94	0.49
5:E:233:LEU:HD13	6:F:48:ARG:HH22	1.76	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
7:G:304:GLU:HB2	7:G:316:TYR:CD2	2.46	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:12:PRO:O	26:a:15:CYS:HB3	2.13	0.49
10:J:22:LYS:HZ2	11:K:21:MET:C	2.20	0.49
10:J:68:GLY:O	10:J:69:TYR:C	2.55	0.49
11:K:66:PHE:CE1	14:N:35:PHE:CZ	2.97	0.49
12:L:445:GLU:CB	12:L:450:LEU:HD23	2.37	0.49
13:M:122:PHE:CE1	13:M:238:LEU:HG	2.46	0.49
13:M:184:HIS:CD2	13:M:249:ILE:HG23	2.47	0.49
13:M:441:MET:HG3	13:M:445:ILE:HD12	1.94	0.49
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:133:TRP:CG	14:N:133:TRP:O	2.63	0.49
15:O:170:LEU:HD21	15:O:184:VAL:HG22	1.95	0.49
20:T:90:TYR:CE2	20:T:92:LYS:HB2	2.46	0.49
20:U:132:ASP:HA	20:U:135:ALA:HB3	1.93	0.49
21:V:90:LEU:HD21	21:V:94:MET:HE3	1.94	0.49
24:Y:143:VAL:CG2	33:h:161:ARG:HD2	2.41	0.49
25:Z:129:THR:HG22	25:Z:131:GLU:H	1.77	0.49
27:b:28:LEU:HA	27:b:31:ILE:CG2	2.42	0.49
27:b:66:VAL:HG22	27:b:75:GLY:CA	2.40	0.49
28:c:40:ASN:O	28:c:43:ALA:N	2.45	0.49
46:AB:176:ASN:O	46:AB:258:ILE:HD11	2.12	0.49
46:AB:307:SER:HB2	46:AB:310:SER:HB2	1.93	0.49
47:AC:116:GLY:C	67:AC:402:HEM:CMC	2.85	0.49
47:AC:155:TYR:CZ	54:Ak:38:TRP:HZ3	2.29	0.49
48:AD:249:TYR:O	48:AD:250:THR:C	2.55	0.49
49:AE:179:ARG:HA	49:AE:183:GLU:OE1	2.12	0.49
49:AI:67:THR:HG23	46:Ab:113:THR:HB	1.93	0.49
45:Aa:226:ALA:HB2	45:Aa:253:VAL:HB	1.93	0.49
46:Ab:278:ILE:HB	46:Ab:329:SER:C	2.37	0.49
49:Ae:204:ARG:O	49:Ae:260:VAL:HG11	2.12	0.49
2:B:170:TYR:OH	4:D:131:GLN:O	2.30	0.49
3:C:100:ARG:HH12	21:V:86:LYS:NZ	2.10	0.49
3:C:216:LYS:HG3	16:P:209:ARG:HH11	1.76	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
5:E:135:THR:O	6:F:369:ARG:NE	2.41	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
7:G:298:LYS:O	42:q:134:ILE:HA	2.12	0.49
8:H:202:GLU:OE2	8:H:211:PHE:HB3	2.12	0.49
12:L:393:ASP:OD1	12:L:393:ASP:C	2.56	0.49
13:M:88:ASN:O	13:M:89:ASN:HB3	2.12	0.49
13:M:207:MET:SD	13:M:240:SER:HA	2.52	0.49
13:M:388:TRP:CD1	38:m:109:ARG:HD2	2.47	0.49
13:M:422:HIS:CE1	38:m:56:ARG:HH22	2.29	0.49
14:N:342:GLN:NE2	29:d:30:ARG:HH11	2.09	0.49
15:O:136:TYR:OH	15:O:191:LYS:HA	2.11	0.49
15:O:259:ASP:O	15:O:260:SER:C	2.54	0.49
23:X:165:THR:OG1	23:X:172:VAL:HG11	2.12	0.49
30:e:41:ILE:HG12	33:h:174:PRO:HB2	1.93	0.49
39:n:96:CYS:SG	39:n:97:TYR:CZ	3.05	0.49
39:n:163:LEU:O	39:n:164:PRO:C	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:74:ILE:O	41:p:75:THR:C	2.54	0.49
42:q:97:PRO:C	42:q:99:THR:N	2.70	0.49
46:AB:299:ILE:HD12	46:AB:299:ILE:N	2.27	0.49
47:AC:218:ILE:HB	47:AC:219:PRO:HD2	1.94	0.49
48:AD:323:PRO:HG2	48:AD:325:LYS:CD	2.41	0.49
49:AE:178:HIS:HD2	49:AE:179:ARG:N	2.11	0.49
52:AH:87:ASN:OD1	52:AH:87:ASN:C	2.55	0.49
48:Ad:255:TYR:HH	48:Ad:266:VAL:HA	1.76	0.49
49:Ae:184:ILE:CG2	49:Ae:208:PRO:HB3	2.42	0.49
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.77	0.49
57:B:303:PC1:H232	57:B:303:PC1:C32	2.37	0.49
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.48	0.49
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.13	0.49
10:J:66:VAL:O	10:J:67:PHE:C	2.55	0.49
10:J:124:LEU:HD23	10:J:125:MET:HG2	1.95	0.49
12:L:399:ILE:HG22	12:L:409:LEU:HD13	1.93	0.49
12:L:564:LYS:HG2	38:m:77:TYR:CZ	2.47	0.49
15:O:276:LEU:HD11	15:O:278:TYR:CE2	2.47	0.49
23:X:7:LEU:HD13	25:Z:87:LEU:HB3	1.93	0.49
30:e:20:PHE:CZ	33:h:178:PHE:HB2	2.47	0.49
38:m:45:ARG:CZ	39:n:140:LEU:HD11	2.43	0.49
45:AA:313:HIS:HB3	45:AA:341:PHE:HB3	1.94	0.49
46:Ab:176:ASN:CA	46:Ab:258:ILE:HD11	2.43	0.49
47:Ac:270:PRO:HG3	70:Ac:405:U10:O3	2.13	0.49
49:Ae:142:ALA:HB1	49:Ae:146:VAL:HG23	1.94	0.49
49:Ae:178:HIS:HD2	49:Ae:179:ARG:N	2.11	0.49
49:Ae:197:ASP:HB3	49:Ae:257:ASN:ND2	2.27	0.49
50:Af:97:GLU:HA	50:Af:100:ARG:HH12	1.77	0.49
52:Ah:32:ARG:HD3	52:Ah:76:ARG:HH22	1.77	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.30	0.49
5:E:244:VAL:HG23	6:F:256:ARG:CG	2.42	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.49
8:H:63:PRO:O	8:H:66:THR:HG22	2.12	0.49
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.49
12:L:553:LEU:HD21	38:m:93:ALA:O	2.12	0.49
13:M:348:LEU:HD12	13:M:415:GLN:HE22	1.77	0.49
13:M:420:THR:HG21	13:M:423:MET:HG2	1.93	0.49
15:O:143:TYR:CZ	15:O:164:TYR:HE2	2.30	0.49
16:P:178:SER:O	16:P:179:LYS:C	2.55	0.49
16:P:208:GLY:N	16:P:211:ASP:HB3	2.20	0.49
23:X:59:GLU:O	23:X:63:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:90:MET:O	34:i:91:ALA:C	2.53	0.49
37:l:81:ARG:HD3	37:l:85:GLU:OE2	2.13	0.49
48:AD:160:ASP:HA	48:Ad:183:GLU:HG2	1.95	0.49
52:AH:80:VAL:O	52:AH:84:LEU:HB2	2.12	0.49
1:A:90:MET:HG2	10:J:152:MET:CE	2.41	0.49
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.38	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.12	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:171:VAL:O	6:F:175:GLU:HG2	2.12	0.49
6:F:225:LEU:HB2	17:Q:160:TYR:CD2	2.45	0.49
7:G:43:VAL:CG1	7:G:55:LYS:HD3	2.41	0.49
8:H:93:HIS:O	26:a:23:THR:HG22	2.13	0.49
8:H:222:LEU:O	8:H:223:PHE:C	2.51	0.49
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.49
12:L:316:THR:CG2	12:L:325:ALA:CB	2.89	0.49
13:M:178:ILE:HD12	33:h:143:GLU:HG3	1.94	0.49
13:M:285:LEU:HD22	13:M:410:MET:SD	2.53	0.49
14:N:230:ILE:HG21	14:N:296:LEU:HD11	1.94	0.49
14:N:231:SER:HA	14:N:300:THR:HA	1.93	0.49
16:P:168:SER:O	16:P:202:ARG:HA	2.13	0.49
19:S:42:VAL:O	19:S:46:LYS:HG3	2.12	0.49
21:V:39:PRO:HB2	21:V:42:ALA:HB2	1.94	0.49
25:Z:110:VAL:HG11	30:e:72:THR:N	2.27	0.49
45:AA:50:VAL:HG22	45:AA:60:ALA:HB2	1.93	0.49
45:AA:235:GLY:HA3	45:AA:406:THR:HG22	1.95	0.49
46:AB:176:ASN:CA	46:AB:258:ILE:HD11	2.43	0.49
47:AC:94:LEU:CD1	67:AC:402:HEM:HAB	2.42	0.49
45:Aa:51:SER:OG	45:Aa:243:LEU:HD13	2.13	0.49
47:Ac:278:TYR:CZ	47:Ac:282:ARG:HD2	2.48	0.49
49:Ae:165:MET:O	49:Ae:176:VAL:N	2.44	0.49
52:Ah:42:VAL:O	52:Ah:46:GLU:HG3	2.13	0.49
52:Ah:58:ARG:CG	52:Ah:61:THR:HB	2.43	0.49
53:Aj:23:LEU:HD22	54:Ak:23:MET:SD	2.52	0.49
2:B:91:TRP:N	2:B:91:TRP:CD1	2.80	0.49
4:D:47:PHE:CD1	14:N:227:ILE:HD11	2.48	0.49
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.38	0.49
7:G:117:MET:HE3	7:G:143:SER:N	2.27	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:66:THR:HA	8:H:124:ASN:OD1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
8:H:224:PHE:CB	61:H:401:UQ9:C20	2.89	0.49
10:J:123:TRP:CZ2	30:e:76:MET:SD	3.05	0.49
12:L:68:TRP:CE3	12:L:76:LEU:HD21	2.47	0.49
12:L:491:LEU:HD13	35:j:80:VAL:HG22	1.94	0.49
12:L:496:LEU:HA	12:L:499:LEU:HB2	1.94	0.49
13:M:193:ASN:HA	13:M:253:LEU:HD23	1.94	0.49
15:O:260:SER:O	15:O:263:ALA:HB3	2.13	0.49
16:P:211:ASP:O	16:P:215:ASN:HB2	2.12	0.49
16:P:298:TYR:HA	16:P:301:ILE:HG12	1.95	0.49
23:X:73:GLN:OE1	23:X:117:TRP:HZ2	1.96	0.49
23:X:115:LEU:HD13	23:X:117:TRP:CZ3	2.48	0.49
23:X:168:PHE:O	23:X:170:TRP:NE1	2.45	0.49
25:Z:66:GLU:HA	25:Z:69:ILE:HG12	1.93	0.49
25:Z:126:GLY:HA3	30:e:76:MET:HE1	1.94	0.49
31:f:38:ARG:O	33:h:134:GLU:OE2	2.30	0.49
37:l:158:PRO:CD	40:o:22:ILE:HB	2.31	0.49
40:o:22:ILE:HD12	40:o:102:PHE:HD1	1.77	0.49
45:AA:193:GLN:NE2	49:AE:85:VAL:HG11	2.28	0.49
46:AB:375:LYS:NZ	46:AB:419:VAL:O	2.36	0.49
48:AD:167:ARG:NH1	48:AD:169:GLY:HA2	2.28	0.49
45:Aa:338:CYS:SG	45:Aa:359:VAL:C	2.96	0.49
47:Ac:281:LEU:HD12	47:Ac:290:GLY:HA3	1.95	0.49
49:Ae:155:LYS:HZ3	49:Ae:157:SER:HB3	1.76	0.49
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.95	0.49
1:A:105:GLU:HG3	1:A:111:LEU:HD22	1.95	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.11	0.49
5:E:235:GLU:HB2	6:F:37:ASP:CB	2.43	0.49
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.93	0.49
6:F:146:GLY:O	6:F:150:GLY:N	2.46	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:224:ARG:HD2	17:Q:164:PHE:CE1	2.48	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.49
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.49
8:H:274:ARG:HH22	61:H:401:UQ9:C1M	2.23	0.49
12:L:67:HIS:HE2	12:L:69:VAL:C	2.21	0.49
13:M:5:ILE:HG13	13:M:6:LEU:N	2.28	0.49
13:M:139:GLN:HG3	13:M:140:THR:N	2.27	0.49
13:M:248:ILE:CG1	13:M:249:ILE:HD12	2.39	0.49
16:P:166:HIS:CE1	16:P:168:SER:HB2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:67:GLN:HG2	18:R:109:LEU:HD21	1.94	0.49
19:S:24:CYS:N	19:S:58:CYS:SG	2.85	0.49
20:T:138:LEU:HD13	20:T:144:ILE:CD1	2.42	0.49
20:T:140:CYS:O	20:T:144:ILE:HG13	2.12	0.49
23:X:166:ARG:HH22	29:d:87:ASP:CG	2.20	0.49
28:c:70:LYS:O	28:c:75:LEU:HA	2.13	0.49
31:f:24:CYS:SG	31:f:28:ARG:NH1	2.86	0.49
32:g:53:TRP:H	32:g:53:TRP:HE3	1.58	0.49
38:m:75:ASN:OD1	38:m:79:ASN:ND2	2.46	0.49
48:AD:114:PHE:HD2	48:AD:140:TYR:CZ	2.31	0.49
50:AF:95:LEU:O	50:AF:99:ILE:HG12	2.12	0.49
45:Aa:107:ASN:HB2	46:Ab:305:THR:HG21	1.94	0.49
45:Aa:197:LEU:HD21	45:Aa:348:TYR:CD2	2.48	0.49
46:Ab:176:ASN:O	46:Ab:258:ILE:HD11	2.12	0.49
52:Ah:32:ARG:HB3	52:Ah:76:ARG:NH2	2.27	0.49
1:A:89:ILE:O	1:A:93:ILE:HG12	2.13	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.94	0.49
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
7:G:344:GLY:O	7:G:345:LEU:HB2	2.12	0.49
7:G:386:LEU:HD21	7:G:523:VAL:HG11	1.95	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
8:H:70:LEU:HD22	8:H:121:TRP:CZ3	2.48	0.49
13:M:348:LEU:HB2	13:M:415:GLN:OE1	2.13	0.49
14:N:309:ASN:HA	15:O:319:ILE:CG2	2.42	0.49
15:O:256:LEU:CD2	15:O:276:LEU:HD23	2.42	0.49
20:T:88:LYS:NZ	20:T:96:GLU:H	2.11	0.49
20:T:104:PHE:CZ	20:T:118:ILE:HG21	2.48	0.49
23:X:112:LEU:HD13	23:X:118:VAL:HG22	1.94	0.49
62:h:201:CDL:H181	62:h:201:CDL:H221	1.95	0.49
34:i:4:TYR:HE1	39:n:4:CYS:SG	2.35	0.49
36:k:55:GLU:OE1	39:n:38:ARG:HB2	2.13	0.49
45:AA:191:ALA:O	45:AA:271:THR:N	2.46	0.49
46:AB:388:THR:HG23	46:AB:391:GLY:H	1.77	0.49
47:Ac:361:ILE:HA	47:Ac:365:LEU:HB2	1.95	0.49
1:A:97:ILE:HG13	1:A:98:LEU:HD22	1.93	0.49
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.48	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:66:LYS:HG2	6:F:189:SER:HB3	1.95	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:116:ILE:HA	8:H:211:PHE:HE1	1.75	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
11:K:59:ILE:HD12	14:N:27:MET:HG2	1.95	0.49
12:L:141:PHE:HE2	13:M:370:PRO:HG3	1.60	0.49
12:L:227:PHE:CD2	12:L:283:LEU:HD23	2.48	0.49
12:L:316:THR:HG23	12:L:325:ALA:CB	2.32	0.49
13:M:134:THR:O	13:M:142:ARG:CD	2.59	0.49
13:M:216:LEU:HD12	13:M:236:LEU:CD2	2.38	0.49
13:M:227:GLY:HA2	13:M:230:ILE:HG22	1.95	0.49
15:O:78:ALA:HB2	15:O:85:HIS:HB2	1.95	0.49
16:P:354:ARG:NH2	22:W:56:ASP:OD1	2.45	0.49
20:T:90:TYR:HE2	20:T:92:LYS:HB3	1.78	0.49
20:U:118:ILE:O	20:U:119:ILE:C	2.55	0.49
25:Z:92:GLU:OE2	30:e:97:HIS:CE1	2.66	0.49
29:d:103:GLU:HG3	29:d:105:GLU:OE2	2.13	0.49
37:l:167:TYR:OH	37:l:176:LYS:O	2.14	0.49
39:n:20:TYR:OH	39:n:45:ARG:HB2	2.12	0.49
39:n:114:MET:HG3	39:n:115:TYR:HD2	1.78	0.49
47:AC:278:TYR:CZ	47:AC:282:ARG:HD2	2.48	0.49
48:AD:200:ILE:HG12	69:AD:401:HEC:HMA3	1.95	0.49
45:Aa:48:THR:OG1	45:Aa:423:ARG:HG2	2.12	0.49
46:Ab:278:ILE:HB	46:Ab:329:SER:O	2.12	0.49
1:A:24:LEU:N	1:A:25:PRO:CD	2.76	0.48
2:B:194:CYS:HB2	9:I:153:ILE:O	2.12	0.48
5:E:134:CYS:SG	5:E:139:CYS:SG	3.11	0.48
5:E:227:ALA:H	6:F:284:HIS:HB3	1.76	0.48
7:G:357:LEU:HD13	7:G:627:SER:OG	2.12	0.48
8:H:311:THR:O	8:H:312:ALA:C	2.56	0.48
10:J:125:MET:HE3	10:J:128:VAL:HG21	1.94	0.48
23:X:69:ASN:O	23:X:70:PHE:C	2.56	0.48
26:a:18:ILE:N	26:a:19:PRO:CD	2.76	0.48
26:a:37:ARG:CB	26:a:48:MET:HE2	2.43	0.48
32:g:109:ASP:HB2	32:g:114:GLU:HB3	1.94	0.48
39:n:81:ILE:HD12	39:n:87:GLY:O	2.12	0.48
45:AA:182:VAL:HG22	49:AE:80:HIS:CE1	2.48	0.48
45:AA:280:ASP:OD2	51:AG:10:ARG:HA	2.12	0.48
46:AB:177:LEU:HD11	46:AB:272:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:185:LEU:HD23	47:AC:188:ILE:HD12	1.95	0.48
49:AE:92:ARG:HA	51:AG:24:GLN:HA	1.94	0.48
52:AH:51:CYS:O	52:AH:54:ARG:HB3	2.13	0.48
46:Ab:426:LYS:HA	46:Ab:429:LYS:HZ3	1.78	0.48
47:Ac:17:SER:HA	47:Ac:21:LEU:HD12	1.95	0.48
48:Ad:167:ARG:NH1	48:Ad:169:GLY:HA2	2.28	0.48
49:Ae:184:ILE:HG21	49:Ae:208:PRO:HB3	1.93	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
4:D:72:LEU:HD11	14:N:50:PRO:HB3	1.93	0.48
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.48
8:H:179:TRP:CZ3	9:I:62:MET:HE1	2.48	0.48
13:M:1:MET:HB2	13:M:52:PHE:CE2	2.48	0.48
13:M:313:THR:HA	13:M:316:MET:CE	2.43	0.48
16:P:346:GLU:H	16:P:346:GLU:CD	2.20	0.48
17:Q:72:ILE:HD13	17:Q:143:TRP:HE1	1.76	0.48
22:W:46:VAL:N	22:W:47:PRO:HD2	2.28	0.48
23:X:44:MET:HE2	25:Z:73:PRO:HA	1.95	0.48
23:X:139:GLU:O	23:X:140:ASN:C	2.55	0.48
28:c:62:HIS:O	28:c:66:VAL:HG23	2.12	0.48
32:g:108:PRO:HB3	33:h:118:SER:OG	2.12	0.48
35:j:97:LEU:HD13	40:o:104:ARG:N	2.28	0.48
35:j:99:ILE:CD1	40:o:107:ARG:HB2	2.42	0.48
38:m:122:ASP:O	38:m:123:ARG:C	2.54	0.48
41:p:5:TRP:CZ3	41:p:10:TYR:O	2.66	0.48
43:r:12:ARG:HE	43:r:20:LEU:HD21	1.78	0.48
45:AA:182:VAL:HA	49:AE:80:HIS:NE2	2.28	0.48
45:AA:409:VAL:O	45:AA:413:ILE:HG13	2.12	0.48
49:AE:83:VAL:C	49:AE:84:LYS:HD2	2.38	0.48
52:AH:39:GLU:O	52:AH:42:VAL:HG12	2.12	0.48
46:Ab:64:PHE:CZ	46:Ab:394:SER:HA	2.49	0.48
52:Ah:31:VAL:HG13	52:Ah:83:LYS:HG3	1.95	0.48
52:Ah:39:GLU:HG2	52:Ah:43:LYS:HE2	1.95	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.48
5:E:201:GLU:HA	5:E:204:ILE:HD12	1.96	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
10:J:52:GLY:O	10:J:55:VAL:HG12	2.13	0.48
11:K:70:GLU:HA	14:N:38:LEU:HD21	1.94	0.48
12:L:101:MET:HE1	12:L:121:LEU:CB	2.43	0.48
12:L:144:TRP:HH2	12:L:256:GLY:HA2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.47	0.48
14:N:31:VAL:HB	14:N:35:PHE:CE2	2.48	0.48
15:O:256:LEU:HB3	15:O:258:TYR:HE1	1.73	0.48
16:P:122:HIS:HB3	18:R:46:VAL:CG1	2.43	0.48
16:P:265:PHE:HZ	16:P:338:LEU:HD12	1.78	0.48
17:Q:99:MET:SD	17:Q:128:PHE:HE2	2.36	0.48
21:V:90:LEU:HD23	21:V:94:MET:HG2	1.94	0.48
22:W:103:ARG:O	22:W:104:THR:C	2.55	0.48
23:X:17:GLU:HG2	30:e:104:PRO:HD2	1.95	0.48
33:h:73:PHE:O	33:h:77:LEU:N	2.46	0.48
46:Ab:388:THR:HG23	46:Ab:391:GLY:H	1.78	0.48
47:Ac:185:LEU:HD23	47:Ac:188:ILE:HD12	1.95	0.48
49:Ae:179:ARG:HA	49:Ae:183:GLU:OE1	2.12	0.48
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
4:D:42:GLU:HA	4:D:45:GLU:HG2	1.96	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.94	0.48
6:F:288:VAL:O	6:F:289:GLU:HB3	2.13	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:30:TYR:HE1	26:a:1:MET:O	1.87	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.48
10:J:151:MET:O	10:J:154:VAL:HG12	2.13	0.48
12:L:41:LYS:HG3	12:L:98:TRP:CH2	2.44	0.48
12:L:402:CYS:SG	12:L:403:ASN:N	2.87	0.48
12:L:550:LEU:HD12	13:M:275:ILE:CB	2.30	0.48
13:M:114:GLU:HG3	23:X:169:PHE:HB3	1.94	0.48
13:M:166:LEU:HD21	13:M:170:HIS:CE1	2.48	0.48
14:N:321:LYS:HD2	29:d:49:ARG:NE	2.29	0.48
39:n:44:MET:O	39:n:45:ARG:C	2.54	0.48
39:n:51:HIS:HB3	39:n:63:LEU:HD13	1.95	0.48
45:AA:50:VAL:HG22	45:AA:60:ALA:CB	2.43	0.48
45:AA:469:ASN:ND2	47:AC:223:TYR:CZ	2.81	0.48
47:AC:361:ILE:HA	47:AC:365:LEU:HB2	1.95	0.48
49:AI:72:VAL:HG21	46:Ab:111:SER:HB3	1.95	0.48
45:Aa:273:SER:HB2	51:Ag:19:LEU:HA	1.95	0.48
49:Ae:176:VAL:HG13	49:Ae:212:ILE:HG12	1.95	0.48
49:Ae:231:PHE:HD2	49:Ae:250:ARG:NH1	2.12	0.48
50:Af:98:VAL:HA	50:Af:101:GLU:OE1	2.14	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ASP:O	2:B:116:ARG:C	2.54	0.48
6:F:116:ASN:O	6:F:245:VAL:HG13	2.13	0.48
6:F:289:GLU:O	6:F:289:GLU:CD	2.56	0.48
7:G:662:THR:HB	19:S:25:GLN:NE2	2.28	0.48
8:H:91:MET:O	8:H:92:PRO:C	2.54	0.48
10:J:39:GLY:HA2	10:J:42:MET:HE2	1.94	0.48
12:L:316:THR:HG21	12:L:325:ALA:HA	1.95	0.48
12:L:361:ASN:O	12:L:361:ASN:CG	2.54	0.48
12:L:433:THR:HG21	12:L:436:ARG:NH2	2.29	0.48
13:M:178:ILE:HG12	41:p:82:VAL:HG11	1.95	0.48
15:O:323:GLN:HE22	32:g:54:GLN:C	2.20	0.48
20:U:94:ASP:OD1	20:U:95:PRO:HD2	2.13	0.48
21:V:11:LEU:HD23	21:V:14:LEU:HD13	1.95	0.48
23:X:5:VAL:O	23:X:6:GLU:C	2.54	0.48
30:e:101:ARG:NH1	30:e:102:GLU:O	2.47	0.48
33:h:73:PHE:HE2	33:h:74:TYR:HE1	1.62	0.48
33:h:86:ILE:HG21	62:h:201:CDL:HA61	1.95	0.48
36:k:41:LYS:C	36:k:43:ALA:N	2.64	0.48
39:n:155:PRO:HG2	39:n:165:PRO:HG2	1.95	0.48
42:q:60:ARG:HH12	42:q:95:ASP:HA	1.78	0.48
44:s:64:ARG:HD2	44:s:64:ARG:N	2.29	0.48
45:AA:50:VAL:HA	45:AA:60:ALA:HA	1.96	0.48
45:AA:403:LEU:HG	45:AA:405:GLY:H	1.78	0.48
46:AB:286:PHE:CZ	46:AB:427:ALA:HB1	2.49	0.48
45:Aa:136:LEU:HD21	46:Ab:380:ALA:HA	1.95	0.48
47:Ac:32:ASN:ND2	47:Ac:228:ASP:OD1	2.47	0.48
47:Ac:312:GLN:HE21	50:Af:37:THR:HB	1.78	0.48
52:Ah:43:LYS:HA	52:Ah:46:GLU:CD	2.38	0.48
2:B:97:LEU:CD2	4:D:94:VAL:HG11	2.44	0.48
2:B:224:ARG:HG3	16:P:85:ARG:HH12	1.77	0.48
3:C:134:LEU:H	3:C:134:LEU:HD12	1.79	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:32:ILE:N	7:G:43:VAL:O	2.46	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
8:H:85:LEU:HB3	8:H:233:LEU:CD2	2.42	0.48
10:J:92:LEU:O	10:J:96:VAL:HG23	2.14	0.48
12:L:141:PHE:HD1	12:L:182:PHE:CD2	2.31	0.48
12:L:264:HIS:HA	12:L:267:THR:OG1	2.13	0.48
12:L:274:LEU:O	12:L:277:MET:HG2	2.14	0.48
12:L:358:LYS:CG	39:n:80:TYR:CE2	2.92	0.48
12:L:542:LEU:HD11	58:L:702:3PE:H261	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:311:GLY:HA2	13:M:314:MET:CE	2.42	0.48
14:N:4:ILE:HG23	14:N:5:THR:N	2.29	0.48
16:P:66:GLY:O	16:P:67:ARG:C	2.54	0.48
16:P:79:GLN:NE2	16:P:102:GLN:O	2.47	0.48
16:P:197:GLU:HA	16:P:260:GLY:HA2	1.96	0.48
20:T:133:ILE:O	20:T:136:GLU:N	2.46	0.48
22:W:120:ASP:OD1	22:W:121:PHE:N	2.46	0.48
27:b:78:LEU:HA	27:b:80:TRP:CD1	2.49	0.48
30:e:47:ILE:HG13	30:e:47:ILE:O	2.12	0.48
33:h:96:ALA:O	41:p:63:TYR:CE1	2.66	0.48
33:h:159:LEU:HB3	33:h:163:ARG:NH1	2.22	0.48
36:k:38:VAL:HG13	39:n:39:TYR:HB2	1.96	0.48
37:l:48:ARG:CZ	37:l:64:PRO:HD2	2.44	0.48
46:AB:109:LYS:O	46:AB:123:VAL:HA	2.14	0.48
48:AD:155:GLN:HG3	48:AD:165:PHE:O	2.13	0.48
52:AH:33:GLU:O	52:AH:37:GLN:HG2	2.14	0.48
46:Ab:109:LYS:O	46:Ab:123:VAL:HA	2.14	0.48
46:Ab:286:PHE:CZ	46:Ab:427:ALA:HB1	2.49	0.48
50:Af:59:ARG:HA	50:Af:62:ARG:CZ	2.43	0.48
1:A:84:THR:HG23	27:b:46:ASN:HD21	1.78	0.48
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.44	0.48
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.67	0.48
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.48
6:F:227:PRO:HG3	7:G:94:MET:SD	2.54	0.48
7:G:53:CYS:O	7:G:56:VAL:HG12	2.13	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:432:ILE:CG2	7:G:451:ILE:HD11	2.39	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.48
9:I:80:GLU:CB	43:r:26:LEU:HD11	2.43	0.48
12:L:496:LEU:HD12	12:L:497:GLY:CA	2.44	0.48
13:M:173:THR:HG22	33:h:150:ARG:NH1	2.29	0.48
13:M:307:TRP:CE3	13:M:383:MET:CE	2.97	0.48
14:N:227:ILE:CA	14:N:230:ILE:HG22	2.38	0.48
15:O:314:LEU:HD12	15:O:315:PRO:HD3	1.93	0.48
16:P:328:MET:O	16:P:330:THR:HG23	2.13	0.48
20:U:132:ASP:O	20:U:136:GLU:HG3	2.14	0.48
23:X:17:GLU:HB3	23:X:19:LYS:HG3	1.96	0.48
31:f:25:TYR:CE1	31:f:29:LYS:HD3	2.48	0.48
34:i:108:ASP:OD2	41:p:18:PRO:HB2	2.13	0.48
37:l:48:ARG:HH21	37:l:63:GLU:HA	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:m:201:3PE:H242	58:m:201:3PE:H3B1	1.95	0.48
40:o:87:TRP:NE1	40:o:91:GLU:OE1	2.45	0.48
49:AE:204:ARG:O	49:AE:260:VAL:HG11	2.12	0.48
49:AE:231:PHE:HD2	49:AE:250:ARG:NH1	2.12	0.48
49:AE:246:SER:HB3	49:AE:248:ARG:HE	1.79	0.48
52:AH:42:VAL:O	52:AH:46:GLU:HG3	2.13	0.48
49:AI:61:ALA:C	46:Ab:326:PHE:HD1	2.21	0.48
49:Ae:93:ARG:HA	51:Ag:25:ARG:CG	2.44	0.48
50:Af:29:LYS:HA	50:Af:81:TRP:CD1	2.48	0.48
1:A:4:TYR:CE1	58:H:402:3PE:H282	2.48	0.48
57:B:303:PC1:H132	42:q:29:ARG:HA	1.96	0.48
7:G:66:HIS:HB3	7:G:69:LEU:HB2	1.96	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
8:H:64:LEU:H	8:H:64:LEU:CD2	2.24	0.48
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.48	0.48
8:H:130:PHE:O	8:H:134:ARG:HG3	2.14	0.48
58:H:403:3PE:H3E1	58:H:403:3PE:H3I2	1.95	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
9:I:180:HIS:CE1	16:P:100:LEU:HD21	2.48	0.48
10:J:104:CYS:HA	10:J:107:ASN:HB2	1.96	0.48
10:J:123:TRP:CH2	30:e:72:THR:C	2.91	0.48
12:L:308:SER:O	12:L:311:GLY:N	2.47	0.48
12:L:319:MET:O	12:L:319:MET:HG2	2.13	0.48
13:M:269:MET:HE3	13:M:399:ASN:HB3	1.96	0.48
13:M:422:HIS:CE1	13:M:425:ASN:OD1	2.66	0.48
14:N:146:TYR:CE1	14:N:198:PRO:HG2	2.49	0.48
15:O:76:GLU:HB2	15:O:266:PRO:HB3	1.95	0.48
16:P:235:THR:HB	16:P:273:LEU:HB2	1.95	0.48
24:Y:143:VAL:HG22	33:h:161:ARG:CD	2.40	0.48
36:k:69:PHE:CE1	36:k:73:ILE:HD11	2.48	0.48
40:o:111:ARG:O	40:o:115:ARG:HG3	2.14	0.48
47:AC:32:ASN:ND2	47:AC:228:ASP:OD1	2.47	0.48
47:AC:304:MET:HA	47:AC:307:LEU:HD12	1.96	0.48
48:AD:242:ILE:HD11	48:AD:244:MET:HE2	1.95	0.48
46:Ab:90:THR:HG23	46:Ab:95:SER:HA	1.95	0.48
47:Ac:311:LYS:O	50:Af:39:HIS:N	2.41	0.48
48:Ad:88:GLU:HA	52:Ah:70:PHE:CE1	2.49	0.48
4:D:72:LEU:HD12	14:N:50:PRO:HG2	1.90	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.96	0.48
5:E:221:ARG:HH22	6:F:285:PRO:HB2	1.78	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.40	0.48
16:P:360:ARG:HD3	16:P:360:ARG:O	2.14	0.48
22:W:46:VAL:O	22:W:50:VAL:HG23	2.14	0.48
23:X:80:GLU:O	23:X:81:PRO:C	2.56	0.48
28:c:65:ASP:O	28:c:66:VAL:C	2.56	0.48
30:e:38:LYS:HG2	33:h:179:ILE:HG23	1.95	0.48
30:e:102:GLU:HG2	30:e:103:GLU:H	1.79	0.48
31:f:39:ASN:ND2	31:f:46:ARG:O	2.47	0.48
34:i:90:MET:SD	34:i:97:ILE:HD11	2.53	0.48
36:k:41:LYS:O	36:k:42:LEU:C	2.50	0.48
37:l:167:TYR:HD2	37:l:168:LEU:CD1	2.19	0.48
42:q:23:LEU:HD11	42:q:33:ILE:HG12	1.96	0.48
46:AB:92:LYS:HG3	46:AB:145:GLU:HG3	1.95	0.48
47:AC:268:ILE:CD1	49:Ae:238:CYS:SG	3.00	0.48
47:AC:287:LYS:NZ	49:Ae:219:HIS:CA	2.60	0.48
47:AC:297:SER:O	47:AC:300:ILE:HG22	2.13	0.48
49:AE:192:VAL:O	49:AE:195:LEU:HB2	2.13	0.48
45:Aa:65:SER:O	45:Aa:66:HIS:C	2.55	0.48
47:Ac:218:ILE:HB	47:Ac:219:PRO:HD2	1.94	0.48
47:Ac:304:MET:HA	47:Ac:307:LEU:HD12	1.96	0.48
48:Ad:242:ILE:HD11	48:Ad:244:MET:HE2	1.95	0.48
49:Ae:153:GLU:C	49:Ae:154:ILE:HD12	2.38	0.48
50:Af:108:TRP:HA	50:Af:111:LYS:HZ3	1.79	0.48
2:B:131:MET:HE3	2:B:152:MET:HE2	1.95	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.48
5:E:43:THR:OG1	5:E:44:PRO:CD	2.61	0.48
6:F:146:GLY:HA3	6:F:193:PHE:CE2	2.48	0.48
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.49	0.48
8:H:96:ILE:HG12	25:Z:143:TYR:OH	2.14	0.48
8:H:116:ILE:HG13	8:H:117:LEU:H	1.75	0.48
15:O:76:GLU:O	15:O:77:ILE:C	2.57	0.48
16:P:294:PRO:HB3	16:P:296:PHE:HD1	1.79	0.48
20:T:117:GLU:HG2	22:W:43:TYR:CZ	2.49	0.48
20:U:86:VAL:HG13	36:k:54:ASN:ND2	2.29	0.48
20:U:102:SER:C	20:U:141:PRO:HD3	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:128:PHE:HZ	20:U:148:ILE:HD12	1.76	0.48
33:h:96:ALA:CB	41:p:63:TYR:HD1	2.26	0.48
49:AE:143:SER:HB2	49:AE:145:ASP:OD1	2.14	0.48
49:AE:176:VAL:HG13	49:AE:212:ILE:HG12	1.95	0.48
47:Ac:137:GLN:NE2	47:Ac:141:TRP:NE1	2.61	0.48
49:Ae:217:CYS:O	49:Ae:218:THR:C	2.56	0.48
1:A:56:PHE:HB2	10:J:73:MET:HE1	1.95	0.47
2:B:126:ARG:HB2	2:B:127:GLN:NE2	2.29	0.47
2:B:141:MET:HE1	4:D:86:PRO:CB	2.44	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
12:L:31:ASN:HD22	12:L:34:LEU:HB2	1.79	0.47
12:L:145:GLU:HB3	13:M:370:PRO:HG2	1.96	0.47
12:L:513:MET:HE1	39:n:30:TRP:CB	2.44	0.47
13:M:42:LEU:HG	13:M:67:ILE:CD1	2.42	0.47
13:M:176:LEU:HD13	13:M:245:ARG:HH11	1.79	0.47
13:M:310:MET:CE	13:M:459:MET:SD	3.02	0.47
14:N:189:TRP:CZ3	14:N:282:MET:HE3	2.49	0.47
15:O:250:SER:HA	15:O:255:VAL:HG23	1.96	0.47
15:O:343:TYR:CE1	15:O:355:LYS:CB	2.96	0.47
16:P:44:GLY:HA2	17:Q:107:TRP:CE3	2.49	0.47
18:R:36:GLN:HG2	42:q:127:TYR:HD2	1.78	0.47
18:R:79:CYS:O	18:R:88:HIS:CE1	2.67	0.47
19:S:50:ASN:O	19:S:51:LEU:C	2.57	0.47
39:n:37:TYR:O	39:n:39:TYR:N	2.47	0.47
39:n:81:ILE:HD11	39:n:87:GLY:O	2.14	0.47
39:n:156:PRO:HD2	39:n:158:ARG:NH1	2.29	0.47
45:AA:102:LYS:HZ3	45:AA:153:ASN:HA	1.77	0.47
45:AA:361:ASP:O	45:AA:365:ILE:HG13	2.13	0.47
46:AB:64:PHE:CZ	46:AB:394:SER:HA	2.48	0.47
47:Ac:272:TRP:HA	47:Ac:275:LEU:HG	1.96	0.47
47:Ac:296:LEU:O	47:Ac:300:ILE:N	2.45	0.47
48:Ad:200:ILE:HG12	69:Ad:401:HEC:HMA3	1.95	0.47
49:Ae:192:VAL:O	49:Ae:195:LEU:HB2	2.13	0.47
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.96	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.47
7:G:136:GLU:OE1	17:Q:87:MET:HG3	2.15	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
12:L:3:ILE:HG22	12:L:49:LEU:HD21	1.96	0.47
12:L:483:PRO:HG2	12:L:486:LEU:HD12	1.96	0.47
13:M:49:TYR:CD1	13:M:59:ASP:HB2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:192:ASN:C	13:M:194:LEU:N	2.72	0.47
16:P:97:MET:O	16:P:103:LEU:HD11	2.15	0.47
30:e:83:ARG:HD3	30:e:92:TYR:CD2	2.48	0.47
36:k:52:ALA:O	36:k:53:ARG:C	2.56	0.47
36:k:84:PHE:CZ	36:k:88:LEU:HD22	2.49	0.47
41:p:6:ASP:C	41:p:8:ASP:N	2.69	0.47
42:q:14:VAL:HG13	42:q:23:LEU:HD22	1.95	0.47
42:q:68:MET:SD	42:q:81:MET:HG2	2.55	0.47
46:AB:173:ILE:HD11	46:AB:439:ALA:C	2.38	0.47
47:AC:281:LEU:HD12	47:AC:290:GLY:HA3	1.95	0.47
67:AC:402:HEM:HAA2	68:AC:403:UQ6:O5	2.13	0.47
49:AE:188:ALA:HA	49:AE:200:HIS:HE2	1.79	0.47
49:AE:218:THR:OG1	49:AE:254:ALA:HB1	2.13	0.47
54:AK:41:ILE:HD12	54:AK:41:ILE:N	2.29	0.47
45:Aa:361:ASP:OD1	45:Aa:361:ASP:N	2.45	0.47
45:Aa:405:GLY:C	45:Aa:408:PRO:HD2	2.39	0.47
50:Af:42:GLU:O	50:Af:46:GLU:HG2	2.15	0.47
51:Ag:78:TYR:CZ	52:Ah:62:GLU:HB2	2.49	0.47
54:Ak:38:TRP:HB2	54:Ak:41:ILE:HB	1.96	0.47
1:A:73:LEU:N	1:A:74:PRO:CD	2.77	0.47
1:A:83:LYS:HZ3	10:J:146:SER:HB2	1.76	0.47
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.49	0.47
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.47
6:F:57:LEU:HD23	6:F:61:ASP:OD1	2.13	0.47
7:G:284:GLU:OE2	17:Q:84:ARG:NH2	2.48	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
8:H:127:TYR:HD2	8:H:207:LEU:HG	1.78	0.47
11:K:95:LEU:HG	14:N:54:GLU:OE2	2.15	0.47
12:L:54:PHE:CZ	12:L:84:PHE:HB2	2.49	0.47
12:L:466:PHE:HE2	58:L:701:3PE:H331	1.79	0.47
12:L:482:MET:HE2	12:L:486:LEU:HB3	1.96	0.47
12:L:598:ILE:HD13	14:N:153:ILE:HG23	1.97	0.47
13:M:94:LEU:O	13:M:98:MET:HG2	2.14	0.47
13:M:391:PHE:HE1	58:M:502:3PE:H12	1.79	0.47
14:N:26:LEU:O	14:N:29:MET:N	2.47	0.47
16:P:221:ARG:HD2	16:P:286:ARG:HD3	1.91	0.47
17:Q:82:PRO:HG2	17:Q:93:ASN:O	2.14	0.47
20:T:117:GLU:HA	20:T:120:MET:CE	2.41	0.47
20:U:93:ILE:HD11	20:U:118:ILE:HD11	1.97	0.47
20:U:130:ILE:HD12	20:U:147:TYR:CE2	2.50	0.47
23:X:133:THR:OG1	23:X:135:ARG:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:8:HIS:O	29:d:10:PRO:HD3	2.14	0.47
33:h:98:LEU:HA	41:p:63:TYR:O	2.15	0.47
34:i:79:MET:O	34:i:80:TRP:C	2.57	0.47
38:m:124:LYS:C	38:m:126:ASN:H	2.21	0.47
45:AA:68:THR:HG22	45:AA:136:LEU:CD2	2.43	0.47
51:AG:79:GLU:HA	52:AH:58:ARG:HD2	1.95	0.47
47:Ac:128:PHE:CD1	70:Ac:405:U10:H4M2	2.50	0.47
47:Ac:346:PRO:HG3	51:Ag:66:GLU:HG2	1.95	0.47
49:Ae:156:LEU:HB2	49:Ae:269:ASP:CA	2.43	0.47
49:Ae:218:THR:OG1	49:Ae:254:ALA:HB1	2.13	0.47
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:209:GLU:OE2	6:F:230:PRO:HG2	2.15	0.47
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:20:LEU:HA	26:a:12:MET:SD	2.53	0.47
8:H:210:GLY:HA2	8:H:213:VAL:CG2	2.44	0.47
12:L:277:MET:SD	12:L:318:GLY:HA2	2.54	0.47
13:M:421:ASN:HB2	38:m:51:TYR:OH	2.15	0.47
13:M:421:ASN:ND2	38:m:47:TYR:OH	2.47	0.47
14:N:89:GLN:H	14:N:89:GLN:CD	2.22	0.47
14:N:309:ASN:N	15:O:319:ILE:HG23	2.30	0.47
16:P:157:LYS:HD3	16:P:194:VAL:O	2.14	0.47
27:b:46:ASN:OD1	27:b:47:LYS:N	2.47	0.47
45:AA:48:THR:HG22	45:AA:60:ALA:HB1	1.97	0.47
45:AA:383:ALA:O	45:AA:442:ARG:NH1	2.48	0.47
47:AC:272:TRP:HA	47:AC:275:LEU:HG	1.97	0.47
45:Aa:64:SER:OG	45:Aa:235:GLY:HA2	2.13	0.47
46:Ab:177:LEU:HD11	46:Ab:272:VAL:HG22	1.94	0.47
47:Ac:271:GLU:OE1	47:Ac:273:TYR:OH	2.32	0.47
47:Ac:297:SER:O	47:Ac:300:ILE:HG22	2.13	0.47
48:Ad:156:ASP:HB2	48:Ad:167:ARG:HG2	1.96	0.47
49:Ae:89:SER:HA	49:Ae:92:ARG:HD3	1.95	0.47
2:B:210:ARG:CD	42:q:76:ASP:HB2	2.44	0.47
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.76	0.47
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.78	0.47
4:D:235:ASP:OD2	25:Z:8:GLN:NE2	2.42	0.47
6:F:230:PRO:HA	6:F:233:VAL:O	2.15	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
9:I:188:GLU:HG3	18:R:55:VAL:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:69:CYS:O	11:K:70:GLU:C	2.57	0.47
12:L:433:THR:CG2	12:L:434:LYS:N	2.78	0.47
13:M:122:PHE:HZ	13:M:206:LYS:HD3	1.75	0.47
13:M:159:PRO:CG	58:M:501:3PE:H391	2.44	0.47
16:P:304:LEU:O	16:P:307:LEU:HB3	2.14	0.47
16:P:340:VAL:HG13	16:P:340:VAL:O	2.14	0.47
23:X:20:VAL:CG2	23:X:24:VAL:HG21	2.40	0.47
34:i:83:HIS:HD2	41:p:37:TYR:CE2	2.31	0.47
35:j:45:ARG:HD3	36:k:57:TRP:CD1	2.50	0.47
45:AA:285:ALA:O	45:AA:359:VAL:HG13	2.14	0.47
49:AE:155:LYS:HA	49:AE:270:VAL:HA	1.96	0.47
49:AE:204:ARG:HB3	49:AE:260:VAL:CG2	2.25	0.47
45:Aa:362:ALA:HB2	45:Aa:461:PRO:HB2	1.95	0.47
48:Ad:242:ILE:HG12	48:Ad:244:MET:H	1.80	0.47
48:Ad:321:TYR:HB2	50:Af:61:PHE:CE1	2.49	0.47
4:D:254:ARG:NH1	43:r:25:GLN:N	2.62	0.47
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.43	0.47
7:G:651:PRO:CD	19:S:56:ARG:HB3	2.45	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
12:L:340:PHE:O	12:L:343:SER:OG	2.32	0.47
12:L:420:ALA:HB1	12:L:498:PHE:CD2	2.50	0.47
13:M:9:LEU:HD13	62:M:503:CDL:H631	1.96	0.47
13:M:78:MET:HG2	13:M:432:ARG:HG3	1.97	0.47
13:M:370:PRO:CA	13:M:375:LEU:HD23	2.42	0.47
14:N:1:MET:HE1	14:N:43:MET:SD	2.54	0.47
14:N:1:MET:O	14:N:2:ASN:C	2.54	0.47
17:Q:85:ASN:N	17:Q:85:ASN:OD1	2.48	0.47
19:S:58:CYS:HB2	19:S:61:VAL:CG1	2.43	0.47
20:T:119:ILE:HG13	20:T:135:ALA:HB1	1.95	0.47
23:X:154:ILE:CG1	33:h:167:PRO:HG2	2.44	0.47
40:o:24:SER:OG	40:o:109:LEU:HD21	2.14	0.47
45:AA:152:GLN:O	45:AA:153:ASN:HB2	2.15	0.47
45:AA:276:ARG:NH1	45:AA:278:ARG:CD	2.76	0.47
46:AB:312:SER:OG	46:AB:357:GLN:NE2	2.40	0.47
49:AE:91:TYR:O	51:AG:25:ARG:N	2.43	0.47
50:AF:35:ASP:HB2	50:AF:90:TYR:CE1	2.48	0.47
46:Ab:173:ILE:HD11	46:Ab:439:ALA:C	2.38	0.47
48:Ad:207:GLY:O	48:Ad:208:GLU:C	2.58	0.47
1:A:71:LEU:HD21	11:K:65:VAL:CG2	2.43	0.47
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:45:GLU:HB3	5:E:91:TRP:HH2	1.78	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.44	0.47
10:J:24:SER:HB2	10:J:27:TYR:CD1	2.43	0.47
11:K:75:LEU:O	11:K:79:VAL:HG23	2.15	0.47
12:L:121:LEU:HD22	12:L:246:LEU:CD2	2.24	0.47
12:L:174:TYR:HE1	58:L:702:3PE:H362	1.78	0.47
12:L:237:MET:HE1	12:L:248:HIS:HB2	1.96	0.47
12:L:386:LEU:HA	35:j:68:TRP:HZ3	1.80	0.47
12:L:390:TYR:HE2	35:j:68:TRP:CH2	2.33	0.47
12:L:424:MET:HE2	12:L:502:LEU:CB	2.45	0.47
12:L:524:THR:HG21	39:n:77:PRO:HG2	1.96	0.47
12:L:552:LEU:HD22	12:L:553:LEU:HD12	1.97	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
14:N:120:GLN:O	14:N:176:ARG:NH2	2.48	0.47
15:O:116:LYS:HA	15:O:119:ASP:OD1	2.14	0.47
15:O:232:ALA:O	15:O:235:GLN:HB3	2.14	0.47
15:O:350:LYS:O	15:O:351:TRP:HB2	2.13	0.47
16:P:85:ARG:HE	65:P:401:NDP:C2A	2.27	0.47
16:P:210:GLU:HG3	16:P:210:GLU:O	2.15	0.47
19:S:19:ILE:HD12	19:S:94:VAL:CG1	2.44	0.47
23:X:120:PRO:CB	23:X:125:LEU:CD1	2.91	0.47
24:Y:142:LYS:O	24:Y:143:VAL:C	2.57	0.47
29:d:73:TYR:O	29:d:77:LYS:HB2	2.14	0.47
29:d:100:ASP:HB3	33:h:159:LEU:CD2	2.45	0.47
30:e:41:ILE:HD11	33:h:174:PRO:HB2	1.96	0.47
30:e:102:GLU:HG2	30:e:103:GLU:HG2	1.95	0.47
31:f:41:SER:O	31:f:42:MET:C	2.58	0.47
37:l:44:THR:CG2	37:l:47:GLU:HG3	2.45	0.47
38:m:84:PRO:HG3	58:m:201:3PE:H331	1.97	0.47
42:q:55:PHE:CZ	42:q:58:ARG:HG3	2.50	0.47
43:r:12:ARG:HB3	43:r:20:LEU:CD2	2.44	0.47
44:s:49:ASN:HA	44:s:52:LEU:HD12	1.97	0.47
45:AA:368:MET:O	45:AA:371:PHE:HB3	2.15	0.47
48:AD:242:ILE:HG12	48:AD:244:MET:H	1.80	0.47
48:AD:284:HIS:HE2	48:AD:288:MET:HE3	1.80	0.47
51:AG:11:ILE:CG2	51:AG:12:ARG:N	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Aa:341:PHE:HZ	45:Aa:372:LEU:CD1	2.28	0.47
47:Ac:206:ASN:N	67:Ac:403:HEM:O2D	2.40	0.47
49:Ae:204:ARG:HB3	49:Ae:260:VAL:CG2	2.25	0.47
49:Ae:246:SER:HB3	49:Ae:248:ARG:HE	1.79	0.47
52:Ah:51:CYS:HA	52:Ah:54:ARG:CB	2.37	0.47
2:B:95:PHE:CE2	2:B:97:LEU:HD11	2.50	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.30	0.47
6:F:382:CYS:HA	7:G:74:ASN:O	2.15	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:611:THR:HG21	17:Q:105:GLU:CA	2.30	0.47
12:L:142:ILE:HA	13:M:370:PRO:HB2	1.96	0.47
12:L:474:PRO:HD2	40:o:67:LEU:HD21	1.97	0.47
12:L:556:ILE:HG21	38:m:80:PHE:CZ	2.45	0.47
13:M:305:THR:O	13:M:306:PRO:C	2.58	0.47
15:O:205:ILE:HD13	15:O:256:LEU:HB2	1.96	0.47
15:O:243:LYS:O	15:O:247:PRO:CG	2.63	0.47
17:Q:99:MET:SD	17:Q:128:PHE:CE2	3.08	0.47
23:X:120:PRO:HB3	23:X:125:LEU:HD11	1.94	0.47
28:c:46:LEU:O	28:c:50:ALA:CB	2.63	0.47
29:d:51:ARG:O	29:d:52:PRO:C	2.55	0.47
39:n:50:GLU:O	39:n:51:HIS:C	2.56	0.47
39:n:96:CYS:SG	39:n:97:TYR:CE1	3.04	0.47
45:AA:342:GLN:HE22	45:AA:344:PHE:HD2	1.62	0.47
47:AC:16:HIS:NE2	47:AC:201:HIS:CD2	2.82	0.47
47:AC:312:GLN:HE21	50:AF:37:THR:HB	1.79	0.47
48:AD:183:GLU:HG2	48:Ad:160:ASP:HA	1.96	0.47
49:AE:156:LEU:HD23	49:AE:156:LEU:HA	1.62	0.47
49:AE:166:ALA:HA	49:AE:174:LEU:O	2.15	0.47
49:AE:217:CYS:O	49:AE:218:THR:C	2.57	0.47
47:Ac:294:LEU:O	47:Ac:297:SER:HB3	2.15	0.47
48:Ad:103:SER:HA	53:Aj:48:ASN:OD1	2.15	0.47
48:Ad:163:GLU:O	48:Ad:164:MET:C	2.57	0.47
48:Ad:235:PRO:HB3	52:Ah:73:LEU:HD13	1.95	0.47
49:Ae:156:LEU:HD12	49:Ae:268:ASP:HA	1.97	0.47
49:Ae:188:ALA:HA	49:Ae:200:HIS:HE2	1.79	0.47
50:Af:47:ALA:CB	50:Af:91:LEU:HD11	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:HE2	10:J:167:ILE:HD12	1.80	0.47
4:D:47:PHE:CD1	14:N:227:ILE:CD1	2.98	0.47
4:D:259:GLU:O	4:D:260:GLU:C	2.55	0.47
5:E:47:ASN:H	5:E:50:THR:HG23	1.79	0.47
5:E:226:PRO:HD2	5:E:230:LEU:HB3	1.97	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
8:H:1:MET:HE3	26:a:29:PHE:CE1	2.50	0.47
10:J:9:SER:HB2	11:K:7:ASN:ND2	2.20	0.47
13:M:196:TRP:HD1	13:M:250:LEU:HB2	1.80	0.47
13:M:232:ALA:HA	13:M:236:LEU:HD12	1.97	0.47
15:O:129:TYR:CE2	15:O:183:CYS:HB3	2.50	0.47
21:V:56:LEU:HD12	21:V:57:ASP:CA	2.44	0.47
22:W:32:LYS:O	22:W:36:ARG:HG3	2.15	0.47
23:X:129:THR:HG23	27:b:68:SER:CA	2.44	0.47
26:a:22:SER:O	26:a:23:THR:C	2.57	0.47
27:b:55:VAL:HG13	27:b:56:PRO:HD2	1.97	0.47
30:e:85:LYS:O	30:e:89:GLU:HG2	2.15	0.47
48:AD:148:LEU:HA	48:AD:151:GLU:CD	2.40	0.47
45:Aa:99:LYS:HD2	45:Aa:160:GLN:HE21	1.80	0.47
47:Ac:140:PHE:CE1	47:Ac:170:VAL:CG1	2.98	0.47
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47
2:B:138:THR:HG21	4:D:116:LEU:HA	1.97	0.47
3:C:149:LEU:CD1	22:W:80:ARG:HH21	2.23	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
5:E:135:THR:OG1	5:E:172:GLU:OE2	2.31	0.47
6:F:46:TYR:O	6:F:48:ARG:HG3	2.15	0.47
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.47
7:G:382:ARG:NH1	7:G:386:LEU:HD11	2.30	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.47
11:K:57:MET:C	11:K:60:PRO:HD2	2.39	0.47
15:O:78:ALA:CB	15:O:85:HIS:HB2	2.45	0.47
15:O:125:ASP:C	32:g:51:MET:HE3	2.40	0.47
15:O:135:LEU:HB3	15:O:139:ARG:NH1	2.25	0.47
16:P:209:ARG:O	16:P:210:GLU:HB3	2.15	0.47
17:Q:166:TRP:CZ3	44:s:67:PRO:HG2	2.50	0.47
18:R:72:VAL:HG21	18:R:77:ILE:HG21	1.97	0.47
21:V:22:GLU:O	21:V:26:ILE:HG12	2.15	0.47
23:X:41:LYS:HB2	23:X:131:VAL:HG11	1.96	0.47
24:Y:116:GLY:O	24:Y:120:MET:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:92:GLU:OE1	30:e:97:HIS:CD2	2.68	0.47
29:d:78:ARG:O	29:d:81:TYR:N	2.48	0.47
29:d:93:TYR:CD2	33:h:156:VAL:HG13	2.50	0.47
32:g:123:LEU:CD1	41:p:98:VAL:HG11	2.45	0.47
38:m:14:LEU:HD12	38:m:15:PRO:HD2	1.96	0.47
39:n:57:MET:O	39:n:58:MET:C	2.58	0.47
41:p:29:PRO:O	41:p:33:LEU:HD13	2.14	0.47
46:AB:284:ASN:HB3	46:AB:419:VAL:CG2	2.45	0.47
49:AE:155:LYS:HZ3	49:AE:157:SER:CB	2.28	0.47
49:AE:263:TYR:HA	49:AE:274:GLY:H	1.80	0.47
50:AF:29:LYS:HA	50:AF:81:TRP:CD1	2.50	0.47
45:Aa:152:GLN:O	45:Aa:153:ASN:HB2	2.15	0.47
49:Ae:156:LEU:HD11	49:Ae:265:PHE:CE1	2.50	0.47
51:Ag:29:SER:CB	51:Ag:32:SER:HB2	2.38	0.47
2:B:121:PHE:CB	56:B:302:UQ1:H8	2.35	0.46
4:D:83:ASN:O	4:D:84:PHE:C	2.55	0.46
4:D:198:THR:HG23	8:H:275:ALA:O	2.15	0.46
5:E:141:LEU:HD22	6:F:281:HIS:NE2	2.30	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
8:H:306:SER:OG	27:b:33:PRO:HG3	2.15	0.46
10:J:5:ILE:HG13	10:J:124:LEU:HD13	1.97	0.46
12:L:277:MET:CG	12:L:318:GLY:HA2	2.44	0.46
12:L:482:MET:HE2	12:L:486:LEU:CB	2.45	0.46
62:L:703:CDL:H322	62:L:703:CDL:H161	1.97	0.46
15:O:62:VAL:HG13	15:O:62:VAL:O	2.15	0.46
16:P:116:ILE:HG21	16:P:152:ILE:HA	1.96	0.46
20:T:87:LEU:CD2	20:T:104:PHE:CE1	2.94	0.46
23:X:4:ILE:CG2	23:X:5:VAL:N	2.50	0.46
23:X:51:LYS:CE	23:X:142:TYR:HD1	2.28	0.46
23:X:115:LEU:HD13	23:X:117:TRP:CZ2	2.51	0.46
37:l:127:ASP:O	37:l:128:VAL:C	2.58	0.46
45:AA:169:LEU:HD11	45:AA:209:ARG:HG2	1.97	0.46
46:AB:159:LYS:HE2	49:AI:37:ALA:O	2.15	0.46
49:Ae:263:TYR:HA	49:Ae:273:VAL:HA	1.97	0.46
1:A:70:ALA:HB2	10:J:58:ILE:HD11	1.96	0.46
1:A:75:LEU:O	1:A:79:ILE:HG12	2.16	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.46
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.46
7:G:401:LEU:HD12	7:G:474:VAL:HG22	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.46
11:K:30:LEU:HD22	11:K:78:LEU:CD1	2.44	0.46
11:K:57:MET:N	11:K:58:PRO:CD	2.78	0.46
12:L:42:PHE:CD2	34:i:74:HIS:HE1	2.33	0.46
12:L:203:PHE:CE1	41:p:114:GLN:HG3	2.50	0.46
12:L:305:SER:C	12:L:336:LYS:HZ3	2.24	0.46
12:L:373:LEU:CD2	12:L:427:ILE:HG22	2.45	0.46
12:L:385:PHE:CE1	35:j:72:ARG:HG3	2.50	0.46
12:L:390:TYR:CE2	35:j:68:TRP:CH2	3.03	0.46
12:L:556:ILE:HG23	38:m:80:PHE:CZ	2.50	0.46
13:M:263:LEU:HD13	38:m:102:TYR:HB2	1.97	0.46
13:M:388:TRP:NE1	38:m:109:ARG:CD	2.78	0.46
62:M:503:CDL:H382	14:N:242:THR:HG23	1.97	0.46
14:N:17:PRO:HG2	14:N:133:TRP:NE1	2.30	0.46
21:V:116:ILE:O	21:V:116:ILE:CG2	2.61	0.46
23:X:35:GLN:HG3	23:X:70:PHE:HE1	1.80	0.46
23:X:53:PRO:HD2	23:X:54:ARG:H	1.80	0.46
25:Z:72:MET:N	25:Z:73:PRO:CD	2.78	0.46
29:d:11:LEU:HB2	30:e:9:LYS:HB2	1.96	0.46
29:d:59:HIS:CE1	29:d:60:ARG:HG3	2.50	0.46
45:AA:399:LEU:C	45:AA:401:SER:N	2.73	0.46
47:AC:294:LEU:O	47:AC:297:SER:HB3	2.15	0.46
49:AE:223:VAL:HG23	47:Ac:141:TRP:CH2	2.50	0.46
45:Aa:68:THR:OG1	46:Ab:387:GLU:OE1	2.33	0.46
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.46
9:I:105:ARG:NH2	18:R:56:ASN:ND2	2.63	0.46
12:L:86:SER:OG	12:L:133:SER:HB3	2.15	0.46
12:L:172:ILE:O	12:L:176:ARG:HG2	2.16	0.46
12:L:225:ALA:CB	12:L:233:LEU:HD12	2.45	0.46
12:L:390:TYR:OH	35:j:72:ARG:HG2	2.15	0.46
12:L:480:LEU:HD22	35:j:84:PHE:HD2	1.78	0.46
12:L:581:LYS:HB2	12:L:586:LEU:HD22	1.97	0.46
13:M:213:HIS:O	13:M:217:PRO:CD	2.63	0.46
15:O:258:TYR:OH	15:O:272:ASP:HB2	2.15	0.46
18:R:38:TYR:CD1	18:R:44:ARG:HB2	2.50	0.46
21:V:56:LEU:HD13	21:V:60:LYS:HE2	1.98	0.46
22:W:50:VAL:HA	22:W:55:LEU:HD12	1.97	0.46
23:X:8:PRO:HB3	23:X:12:GLU:CD	2.40	0.46
23:X:120:PRO:HB2	23:X:125:LEU:CD1	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:41:TYR:HD1	27:b:80:TRP:CZ3	2.33	0.46
36:k:57:TRP:O	36:k:58:ARG:C	2.58	0.46
38:m:91:ALA:HB2	58:m:201:3PE:H261	1.98	0.46
41:p:6:ASP:OD1	41:p:8:ASP:HB2	2.16	0.46
41:p:43:TRP:O	41:p:44:PRO:C	2.58	0.46
45:AA:368:MET:O	45:AA:369:VAL:C	2.58	0.46
46:AB:307:SER:O	46:AB:308:LEU:C	2.58	0.46
48:AD:244:MET:HB2	69:AD:401:HEC:C4D	2.46	0.46
54:AK:3:SER:O	50:Af:110:LYS:HG2	2.16	0.46
45:Aa:310:ILE:HG21	45:Aa:379:LEU:HD21	1.96	0.46
46:Ab:142:THR:HG21	46:Ab:238:LEU:N	2.22	0.46
46:Ab:225:VAL:HG22	46:Ab:229:VAL:CG2	2.46	0.46
48:Ad:142:GLU:HG2	48:Ad:171:LEU:HD11	1.97	0.46
49:Ae:226:ALA:HB2	49:Ae:234:TYR:HE1	1.80	0.46
54:Ak:15:ARG:HA	54:Ak:18:ILE:HG12	1.97	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
5:E:45:GLU:CD	5:E:45:GLU:H	2.23	0.46
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.97	0.46
6:F:168:ASN:ND2	44:s:40:TYR:HE2	2.13	0.46
6:F:278:ILE:CG2	6:F:282:VAL:HG21	2.46	0.46
7:G:140:GLN:HG3	7:G:141:ASP:N	2.30	0.46
7:G:360:LYS:CE	7:G:632:ILE:HB	2.41	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
8:H:249:ILE:HG13	26:a:35:GLU:OE2	2.15	0.46
10:J:32:LEU:HD23	10:J:64:LEU:HD11	1.96	0.46
11:K:12:PHE:CD1	14:N:72:LEU:HD22	2.50	0.46
12:L:21:ILE:HG12	12:L:27:ILE:CG2	2.45	0.46
12:L:226:GLN:OE1	12:L:284:THR:HG21	2.14	0.46
12:L:605:ASN:HA	24:Y:5:LYS:HZ2	1.80	0.46
13:M:4:ILE:HD12	13:M:4:ILE:N	2.30	0.46
13:M:139:GLN:HG3	13:M:141:GLU:H	1.80	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
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
13:M:435:THR:O	13:M:436:LEU:C	2.58	0.46
15:O:38:TYR:CE1	15:O:292:HIS:HD2	2.34	0.46
15:O:50:THR:OG1	15:O:288:ASP:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:133:ILE:HD11	39:n:7:PRO:HD3	1.98	0.46
23:X:94:MET:O	23:X:95:GLN:C	2.59	0.46
27:b:28:LEU:O	27:b:32:MET:HG2	2.15	0.46
39:n:133:TRP:O	39:n:137:VAL:HG22	2.15	0.46
39:n:136:GLU:O	39:n:139:GLN:N	2.49	0.46
42:q:76:ASP:OD1	42:q:76:ASP:C	2.57	0.46
43:r:109:ASP:O	43:r:110:GLN:OE1	2.32	0.46
48:Ad:131:ALA:HB3	48:Ad:133:ARG:HG2	1.98	0.46
49:Ae:155:LYS:HZ3	49:Ae:157:SER:CB	2.28	0.46
53:Aj:11:TYR:HA	53:Aj:15:PHE:HB2	1.97	0.46
54:Ak:43:ASP:HA	54:Ak:49:ASN:OD1	2.15	0.46
1:A:60:ILE:O	1:A:64:LEU:HG	2.16	0.46
1:A:104:TYR:CE2	10:J:167:ILE:HD12	2.50	0.46
2:B:164:CYS:SG	55:B:301:SF4:S4	3.14	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
4:D:260:GLU:HG2	25:Z:25:LEU:HD22	1.97	0.46
12:L:573:MET:O	12:L:576:LEU:HG	2.15	0.46
13:M:151:PHE:CE2	14:N:291:PHE:HB2	2.49	0.46
14:N:154:ILE:HG12	14:N:195:PRO:CG	2.45	0.46
16:P:163:ARG:HH11	16:P:199:ILE:HD11	1.80	0.46
16:P:328:MET:HB2	16:P:329:PRO:HD2	1.98	0.46
18:R:39:ASP:CG	18:R:40:GLU:N	2.74	0.46
23:X:36:CYS:CB	23:X:66:CYS:HG	2.21	0.46
23:X:135:ARG:HH12	23:X:138:PRO:CD	2.11	0.46
24:Y:110:TYR:HD2	58:m:201:3PE:H112	1.79	0.46
45:AA:168:ILE:HA	45:AA:171:GLU:HG2	1.98	0.46
48:AD:308:ARG:HD3	51:AG:27:PHE:CZ	2.51	0.46
49:AE:165:MET:O	49:AE:176:VAL:N	2.44	0.46
49:AE:231:PHE:CD2	49:AE:250:ARG:HG3	2.50	0.46
49:AE:255:PRO:HG2	47:Ac:287:LYS:HZ1	1.81	0.46
50:Af:75:ILE:HD11	51:Ag:40:ARG:HD2	1.96	0.46
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.46
2:B:154:GLU:O	16:P:89:TYR:OH	2.33	0.46
4:D:58:THR:HA	4:D:61:TRP:CE2	2.50	0.46
4:D:238:LEU:HA	25:Z:9:ASP:HB2	1.97	0.46
58:D:501:3PE:H272	14:N:288:LEU:CD1	2.46	0.46
6:F:270:ASN:C	6:F:292:MET:HE3	2.40	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
9:I:48:VAL:O	27:b:10:LYS:NZ	2.48	0.46
9:I:89:GLU:HG3	42:q:61:TRP:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:ASN:ND2	12:L:34:LEU:HB2	2.31	0.46
13:M:10:MET:C	13:M:13:PRO:HD2	2.41	0.46
13:M:388:TRP:CD2	38:m:109:ARG:HD2	2.51	0.46
18:R:97:LYS:CE	18:R:100:LYS:HD3	2.45	0.46
23:X:49:GLU:HB3	23:X:135:ARG:HH22	1.81	0.46
28:c:55:TRP:NE1	29:d:66:THR:CG2	2.79	0.46
29:d:13:PHE:O	29:d:78:ARG:NE	2.43	0.46
40:o:71:ARG:HB3	40:o:71:ARG:NH1	2.27	0.46
41:p:6:ASP:O	41:p:8:ASP:N	2.49	0.46
62:q:201:CDL:OB7	43:r:8:ILE:HD11	2.16	0.46
45:AA:61:SER:HB3	45:AA:242:LEU:CD2	2.46	0.46
45:AA:193:GLN:CD	49:AE:85:VAL:HG11	2.41	0.46
46:AB:43:LEU:HB2	46:AB:45:ASN:OD1	2.15	0.46
46:AB:278:ILE:HB	46:AB:331:SER:HA	1.98	0.46
47:AC:296:LEU:O	47:AC:300:ILE:N	2.45	0.46
48:AD:213:SER:O	48:AD:217:GLY:N	2.49	0.46
49:AE:217:CYS:C	49:AE:219:HIS:N	2.72	0.46
52:AH:48:LEU:HA	52:AH:51:CYS:SG	2.55	0.46
50:Af:29:LYS:HA	50:Af:81:TRP:NE1	2.31	0.46
4:D:36:GLN:HE22	13:M:135:ARG:HH22	1.64	0.46
4:D:47:PHE:CE2	14:N:305:PHE:HZ	2.32	0.46
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
8:H:316:PRO:HA	25:Z:58:ARG:HH11	1.80	0.46
13:M:44:GLN:HG2	13:M:46:ASP:O	2.15	0.46
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.98	0.46
58:M:501:3PE:H321	58:M:501:3PE:C21	2.46	0.46
14:N:37:LEU:HD21	14:N:60:PHE:CD1	2.51	0.46
15:O:40:LEU:O	15:O:44:ILE:HG13	2.16	0.46
15:O:231:SER:O	15:O:234:LEU:N	2.48	0.46
15:O:243:LYS:O	15:O:247:PRO:HG3	2.16	0.46
18:R:33:HIS:HE1	18:R:56:ASN:HD22	1.64	0.46
23:X:143:HIS:CG	25:Z:114:THR:HG1	2.33	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
37:l:155:PRO:HG3	40:o:4:HIS:CD2	2.51	0.46
37:l:158:PRO:HD3	40:o:22:ILE:CG1	2.45	0.46
38:m:9:ALA:O	38:m:10:PRO:C	2.56	0.46
45:AA:51:SER:N	45:AA:59:VAL:O	2.45	0.46
45:AA:357:HIS:O	45:AA:357:HIS:CG	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AC:150:LEU:O	47:AC:153:ILE:HG13	2.15	0.46
47:AC:378:LYS:HE3	50:AF:89:PHE:HE2	1.81	0.46
48:AD:137:GLY:N	48:AD:140:TYR:O	2.47	0.46
49:AE:226:ALA:HB2	49:AE:234:TYR:HE1	1.80	0.46
45:Aa:383:ALA:O	45:Aa:442:ARG:NH1	2.48	0.46
49:Ae:166:ALA:HA	49:Ae:174:LEU:O	2.15	0.46
49:Ae:231:PHE:CD2	49:Ae:250:ARG:HG3	2.50	0.46
53:Aj:9:ARG:O	53:Aj:13:LEU:HD23	2.15	0.46
1:A:63:LEU:O	1:A:67:LEU:HG	2.15	0.46
1:A:109:LYS:HG2	1:A:112:GLU:HB2	1.98	0.46
2:B:104:MET:HE3	2:B:132:ILE:HD12	1.97	0.46
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.46
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.46
4:D:381:HIS:HE1	9:I:161:ALA:O	1.99	0.46
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.98	0.46
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.98	0.46
10:J:49:SER:O	10:J:50:PHE:C	2.57	0.46
12:L:475:THR:O	12:L:476:SER:HB2	2.15	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:116:ILE:HD12	13:M:119:TYR:HB3	1.97	0.46
13:M:319:HIS:CA	13:M:322:THR:HG22	2.41	0.46
16:P:157:LYS:O	16:P:160:GLY:N	2.49	0.46
17:Q:77:VAL:HG21	17:Q:99:MET:HE3	1.97	0.46
22:W:45:GLU:O	22:W:46:VAL:C	2.58	0.46
23:X:122:LEU:HD21	27:b:81:LEU:HD23	1.98	0.46
25:Z:110:VAL:CG2	30:e:72:THR:HG23	2.44	0.46
27:b:38:TYR:O	27:b:39:THR:C	2.58	0.46
33:h:95:GLU:OE1	33:h:114:LYS:HD3	2.15	0.46
42:q:86:TRP:HA	42:q:98:PRO:HG2	1.98	0.46
45:AA:99:LYS:HD2	45:AA:160:GLN:HE21	1.80	0.46
48:AD:149:ALA:O	48:AD:152:VAL:HG22	2.16	0.46
49:AI:64:LEU:HD23	46:Ab:171:THR:HG23	1.97	0.46
53:AJ:11:TYR:HA	53:AJ:15:PHE:HB2	1.97	0.46
49:Ae:168:LYS:HZ3	49:Ae:171:GLY:HA2	1.80	0.46
49:Ae:264:GLU:N	49:Ae:272:VAL:O	2.49	0.46
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.46
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.46
2:B:123:ALA:HB3	8:H:204:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.46
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:141:LEU:O	5:E:142:ARG:HB2	2.15	0.46
5:E:204:ILE:O	5:E:208:LYS:HG3	2.16	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CZ	2.51	0.46
6:F:102:MET:HE3	6:F:102:MET:HB2	1.73	0.46
6:F:111:LYS:HG2	6:F:239:PRO:HB2	1.97	0.46
6:F:146:GLY:HA3	6:F:193:PHE:HE2	1.81	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:111:LEU:HD11	10:J:56:PHE:HZ	1.81	0.46
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.46
9:I:80:GLU:N	26:a:1:MET:HE1	2.31	0.46
10:J:3:ASN:OD1	10:J:6:PHE:HB3	2.16	0.46
10:J:17:LEU:O	10:J:21:LEU:HG	2.16	0.46
10:J:136:GLU:HG2	10:J:139:ILE:HG13	1.98	0.46
11:K:57:MET:O	11:K:58:PRO:C	2.58	0.46
12:L:101:MET:HE1	12:L:121:LEU:HB2	1.98	0.46
12:L:324:LEU:HA	12:L:327:LEU:HD12	1.97	0.46
13:M:453:LEU:CD1	13:M:454:ILE:CG2	2.84	0.46
62:M:503:CDL:H342	14:N:242:THR:HA	1.98	0.46
14:N:123:PRO:HG2	14:N:126:MET:CG	2.40	0.46
15:O:247:PRO:O	15:O:248:LYS:C	2.59	0.46
16:P:276:LEU:O	16:P:280:ILE:HG13	2.14	0.46
16:P:285:HIS:CE1	16:P:364:SER:HB3	2.51	0.46
16:P:287:THR:HG23	16:P:289:ILE:HD11	1.97	0.46
20:T:87:LEU:CD2	20:T:122:MET:HE1	2.46	0.46
24:Y:74:LEU:HD23	24:Y:74:LEU:C	2.41	0.46
26:a:58:ASN:HB2	26:a:61:TYR:CE2	2.50	0.46
33:h:82:VAL:O	33:h:85:GLY:N	2.49	0.46
35:j:92:TRP:O	35:j:93:THR:C	2.59	0.46
36:k:69:PHE:CZ	36:k:73:ILE:HG13	2.51	0.46
58:m:201:3PE:O31	58:m:201:3PE:H342	2.16	0.46
39:n:61:THR:O	39:n:65:ARG:HG3	2.15	0.46
45:AA:52:ILE:HB	45:AA:58:ARG:HG2	1.98	0.46
47:AC:77:TRP:HZ2	48:AD:284:HIS:CD2	2.33	0.46
52:AH:69:LEU:O	52:AH:73:LEU:HG	2.15	0.46
45:Aa:454:PRO:O	45:Aa:468:TYR:OH	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:207:LYS:HE3	49:Ae:265:PHE:CG	2.51	0.46
1:A:52:SER:HB3	1:A:55:PHE:CD2	2.50	0.46
4:D:83:ASN:C	4:D:85:GLY:N	2.69	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.97	0.46
6:F:41:ILE:O	6:F:137:LYS:NZ	2.47	0.46
6:F:41:ILE:CD1	6:F:262:PHE:HE1	2.25	0.46
6:F:81:LYS:HE3	6:F:96:GLY:C	2.41	0.46
7:G:83:GLU:HB2	7:G:101:ASN:HB3	1.98	0.46
7:G:308:ARG:HH11	7:G:580:ALA:H	1.64	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
12:L:277:MET:HG3	12:L:318:GLY:CA	2.46	0.46
12:L:550:LEU:O	12:L:554:ASP:HB3	2.16	0.46
13:M:122:PHE:CZ	13:M:206:LYS:CD	2.94	0.46
14:N:277:ILE:HG22	14:N:278:MET:H	1.79	0.46
15:O:344:ASN:OD1	15:O:346:GLU:HG2	2.15	0.46
16:P:169:HIS:ND1	65:P:401:NDP:H5N	2.31	0.46
16:P:334:GLY:O	16:P:337:ASP:HB3	2.15	0.46
29:d:54:MET:HE2	29:d:54:MET:HB3	1.89	0.46
29:d:114:GLU:CD	29:d:114:GLU:H	2.23	0.46
34:i:85:TYR:CD2	58:i:201:3PE:H291	2.51	0.46
36:k:52:ALA:O	36:k:55:GLU:N	2.49	0.46
39:n:45:ARG:O	39:n:49:GLU:N	2.37	0.46
40:o:15:VAL:CG2	40:o:16:GLU:N	2.79	0.46
44:s:48:LEU:O	44:s:52:LEU:HG	2.15	0.46
45:AA:268:CYS:SG	45:AA:350:ASP:OD1	2.74	0.46
47:AC:37:LEU:CB	67:AC:402:HEM:HMB2	2.45	0.46
48:AD:237:PHE:CD1	48:AD:238:PRO:HD2	2.52	0.46
50:AF:92:GLU:O	50:AF:96:LYS:HG3	2.15	0.46
51:AG:73:LYS:NZ	52:AH:63:GLU:HA	2.29	0.46
45:Aa:287:VAL:HB	45:Aa:358:PHE:CE2	2.50	0.46
46:Ab:47:LEU:HD22	46:Ab:238:LEU:HD13	1.97	0.46
47:Ac:30:TRP:HZ3	47:Ac:96:LEU:HD22	1.81	0.46
49:Ae:214:ILE:HG12	49:Ae:261:PRO:HD3	1.98	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.45
6:F:86:ARG:HB2	6:F:88:ARG:HH12	1.81	0.45
6:F:213:ILE:HG23	6:F:235:VAL:CA	2.41	0.45
6:F:292:MET:HG2	6:F:293:SER:H	1.80	0.45
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	0.45
8:H:274:ARG:HH22	61:H:401:UQ9:C1	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:12:PHE:O	12:L:16:LEU:HG	2.15	0.45
12:L:145:GLU:HB3	13:M:370:PRO:CG	2.46	0.45
12:L:339:LEU:HD11	12:L:376:GLY:HA3	1.99	0.45
14:N:241:LEU:O	14:N:244:ILE:HG22	2.15	0.45
15:O:140:LEU:HD11	15:O:198:TYR:CE2	2.51	0.45
16:P:95:ARG:HG2	16:P:105:PHE:CE2	2.51	0.45
16:P:170:LEU:HD13	16:P:264:ALA:HB1	1.97	0.45
16:P:264:ALA:O	16:P:266:THR:HG23	2.17	0.45
18:R:32:THR:HA	18:R:55:VAL:CG2	2.45	0.45
23:X:168:PHE:O	23:X:169:PHE:CG	2.69	0.45
26:a:49:GLU:CD	26:a:52:ARG:HH11	2.22	0.45
37:l:166:LEU:HD12	37:l:170:ARG:HH22	1.81	0.45
38:m:124:LYS:C	38:m:126:ASN:N	2.70	0.45
39:n:168:TRP:O	39:n:172:THR:OG1	2.33	0.45
42:q:10:GLY:HA2	62:q:201:CDL:CA5	2.46	0.45
46:AB:225:VAL:HG22	46:AB:229:VAL:CG2	2.46	0.45
47:AC:30:TRP:HZ3	47:AC:96:LEU:HD22	1.81	0.45
47:AC:271:GLU:OE1	47:AC:273:TYR:OH	2.32	0.45
53:AJ:30:LEU:CD1	54:AK:34:TRP:HB2	2.45	0.45
47:Ac:149:LEU:HD11	47:Ac:291:VAL:HG22	1.97	0.45
47:Ac:219:PRO:HA	51:Ag:5:PHE:HZ	1.80	0.45
48:Ad:214:LEU:O	48:Ad:234:ASN:ND2	2.46	0.45
48:Ad:237:PHE:CD1	48:Ad:238:PRO:HD2	2.52	0.45
48:Ad:244:MET:HB2	69:Ad:401:HEC:C4D	2.46	0.45
50:Af:65:ARG:HD2	50:Af:76:LEU:HD21	1.98	0.45
53:Aj:34:ARG:NH1	53:Aj:38:GLN:HB2	2.31	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
4:D:55:SER:HB3	4:D:58:THR:CB	2.46	0.45
6:F:168:ASN:HD21	44:s:40:TYR:HE2	1.64	0.45
7:G:36:VAL:O	7:G:39:GLN:HG2	2.16	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45
8:H:34:ARG:NH2	61:H:401:UQ9:H4M	2.28	0.45
8:H:248:TYR:CD1	8:H:254:LEU:HD23	2.51	0.45
8:H:293:PHE:CE1	58:H:403:3PE:H32	2.52	0.45
10:J:91:PHE:O	10:J:94:LEU:HB3	2.16	0.45
12:L:60:GLU:HG2	12:L:83:ASP:HA	1.98	0.45
12:L:74:MET:HE3	12:L:74:MET:HB2	1.76	0.45
12:L:204:SER:HA	12:L:207:ASN:ND2	2.31	0.45
12:L:424:MET:HE2	12:L:502:LEU:HA	1.97	0.45
12:L:532:ILE:CG2	37:l:133:LEU:HD22	2.46	0.45
13:M:186:LEU:HD22	13:M:250:LEU:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:208:PRO:CD	13:M:236:LEU:HD22	2.38	0.45
13:M:309:PHE:O	13:M:312:ALA:HB3	2.16	0.45
13:M:393:ILE:O	13:M:397:GLY:N	2.49	0.45
14:N:215:MET:SD	14:N:244:ILE:HD11	2.56	0.45
15:O:204:VAL:O	15:O:205:ILE:C	2.60	0.45
15:O:306:ASN:O	15:O:309:THR:HG22	2.16	0.45
15:O:323:GLN:NE2	32:g:55:GLU:N	2.64	0.45
16:P:206:ILE:HB	65:P:401:NDP:N7N	2.30	0.45
18:R:39:ASP:H	18:R:42:ASP:CG	2.21	0.45
21:V:32:LEU:O	21:V:36:LYS:HG2	2.16	0.45
30:e:89:GLU:HB3	30:e:91:LYS:HE2	1.98	0.45
31:f:16:VAL:HB	31:f:17:PRO:HD3	1.97	0.45
37:l:35:ASP:O	37:l:54:LYS:HD3	2.15	0.45
38:m:15:PRO:HG2	38:m:18:LEU:HD12	1.97	0.45
40:o:63:LEU:O	40:o:64:ILE:C	2.59	0.45
42:q:6:VAL:HG13	62:q:201:CDL:CA2	2.47	0.45
42:q:14:VAL:HA	42:q:23:LEU:HD22	1.98	0.45
45:AA:55:ASN:HB3	45:AA:226:ALA:CB	2.46	0.45
45:AA:278:ARG:O	51:AG:13:HIS:N	2.49	0.45
46:AB:92:LYS:CE	46:AB:143:ALA:HB1	2.45	0.45
48:AD:159:ASN:N	48:AD:163:GLU:O	2.49	0.45
49:AE:214:ILE:HG12	49:AE:261:PRO:HD3	1.98	0.45
48:Ad:130:VAL:HA	48:Ad:134:HIS:CD2	2.51	0.45
52:Ah:76:ARG:O	52:Ah:80:VAL:HG23	2.17	0.45
4:D:58:THR:HG23	4:D:61:TRP:CH2	2.51	0.45
5:E:134:CYS:SG	5:E:175:CYS:HA	2.55	0.45
6:F:179:ALA:HB3	6:F:181:LEU:HG	1.98	0.45
12:L:135:ASN:O	12:L:198:LEU:HD13	2.16	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:56:PHE:CE1	13:M:108:MET:HG2	2.47	0.45
13:M:61:LEU:C	13:M:64:PRO:HD2	2.42	0.45
13:M:207:MET:O	13:M:208:PRO:C	2.59	0.45
13:M:282:LEU:HD11	13:M:410:MET:HE3	1.96	0.45
14:N:300:THR:CG2	14:N:301:SER:N	2.79	0.45
15:O:342:GLY:O	15:O:355:LYS:NZ	2.50	0.45
16:P:207:PHE:CZ	16:P:345:LEU:HA	2.51	0.45
20:T:133:ILE:HG23	20:T:134:ASP:N	2.32	0.45
34:i:11:ARG:HD2	39:n:154:LEU:O	2.15	0.45
47:AC:37:LEU:CB	67:AC:402:HEM:HMB1	2.27	0.45
49:AE:205:VAL:HG12	49:AE:211:VAL:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:AF:90:TYR:CG	50:AF:91:LEU:N	2.84	0.45
45:Aa:74:TRP:HH2	45:Aa:410:CYS:HG	1.57	0.45
45:Aa:193:GLN:NE2	45:Aa:273:SER:OG	2.49	0.45
50:Af:19:LYS:HA	50:Af:84:TYR:CD2	2.51	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
58:D:501:3PE:O31	58:D:501:3PE:H231	2.16	0.45
5:E:87:ARG:HD2	44:s:42:THR:HB	1.98	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.43	0.45
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.82	0.45
12:L:247:LEU:HD12	12:L:247:LEU:C	2.41	0.45
13:M:42:LEU:HD11	13:M:67:ILE:HD12	1.99	0.45
13:M:264:LEU:HD23	38:m:98:LEU:HD21	1.98	0.45
14:N:133:TRP:CE3	14:N:136:ILE:HD12	2.51	0.45
14:N:155:LEU:O	14:N:159:ILE:HG22	2.16	0.45
14:N:313:MET:HG3	15:O:305:LEU:CD2	2.46	0.45
15:O:265:ASP:O	15:O:266:PRO:C	2.58	0.45
16:P:55:VAL:HA	16:P:79:GLN:O	2.17	0.45
20:U:113:LEU:HD23	39:n:17:LEU:CD2	2.47	0.45
21:V:8:THR:CG2	21:V:9:THR:N	2.79	0.45
23:X:53:PRO:CD	23:X:54:ARG:H	2.29	0.45
24:Y:39:SER:HB2	24:Y:58:VAL:HA	1.98	0.45
24:Y:75:THR:HB	24:Y:95:GLY:HA2	1.98	0.45
33:h:73:PHE:HD2	33:h:74:TYR:CE1	2.33	0.45
36:k:26:ARG:O	36:k:27:GLN:C	2.57	0.45
41:p:24:THR:HG22	41:p:26:LEU:N	2.31	0.45
62:q:201:CDL:OB7	62:q:201:CDL:HB62	2.16	0.45
45:AA:306:VAL:O	45:AA:310:ILE:HG13	2.17	0.45
46:AB:180:VAL:HG21	46:AB:257:GLU:CA	2.46	0.45
46:AB:426:LYS:HA	46:AB:429:LYS:HZ3	1.80	0.45
49:AE:255:PRO:CG	47:Ac:287:LYS:HZ1	2.29	0.45
50:AF:93:PRO:HA	50:AF:96:LYS:HD2	1.99	0.45
52:AH:51:CYS:HB2	52:AH:54:ARG:NH2	2.31	0.45
45:Aa:275:ILE:HG12	45:Aa:276:ARG:N	2.30	0.45
47:Ac:100:ARG:HH12	67:Ac:403:HEM:CBD	2.29	0.45
49:Ae:114:SER:HB2	51:Ag:22:PHE:HE2	1.82	0.45
49:Ae:205:VAL:HG12	49:Ae:211:VAL:HG23	1.98	0.45
50:Af:92:GLU:N	50:Af:93:PRO:HD2	2.31	0.45
52:Ah:79:CYS:SG	52:Ah:80:VAL:N	2.90	0.45
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.99	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.45
6:F:69:LEU:HD22	6:F:147:ARG:HB2	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.82	0.45
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.45
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.30	0.45
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.45
58:H:403:3PE:H272	58:H:403:3PE:H241	1.56	0.45
12:L:47:SER:O	12:L:50:PRO:HD2	2.16	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:366:MET:SD	12:L:443:ILE:HG21	2.57	0.45
12:L:445:GLU:OE2	35:j:54:GLN:CG	2.62	0.45
13:M:65:LEU:O	13:M:66:ILE:C	2.59	0.45
14:N:26:LEU:HG	14:N:85:MET:SD	2.56	0.45
14:N:144:GLN:OE1	30:e:3:PHE:N	2.50	0.45
15:O:351:TRP:HB2	15:O:355:LYS:HE3	1.98	0.45
16:P:192:ARG:HH11	16:P:197:GLU:HA	1.81	0.45
16:P:208:GLY:N	16:P:211:ASP:OD2	2.49	0.45
20:U:125:GLU:OE2	35:j:44:TYR:HE1	2.00	0.45
29:d:11:LEU:HD12	29:d:11:LEU:HA	1.69	0.45
30:e:18:PHE:O	30:e:18:PHE:CD2	2.69	0.45
35:j:97:LEU:HB3	40:o:104:ARG:CA	2.45	0.45
41:p:107:GLN:O	41:p:111:LYS:HG3	2.16	0.45
45:AA:338:CYS:HB2	45:AA:364:SER:CB	2.41	0.45
46:AB:95:SER:O	46:AB:99:ILE:HG13	2.17	0.45
47:AC:116:GLY:O	67:AC:402:HEM:HMC1	2.15	0.45
49:AI:63:PRO:HB3	46:Ab:328:ALA:HB1	1.99	0.45
53:AJ:9:ARG:O	53:AJ:13:LEU:HD23	2.15	0.45
49:Ae:111:LYS:HE3	53:Aj:11:TYR:CZ	2.52	0.45
49:Ae:178:HIS:CD2	49:Ae:209:GLU:O	2.70	0.45
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
6:F:110:PRO:CB	6:F:152:ARG:HH22	2.30	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
8:H:250:ASN:OD1	8:H:250:ASN:N	2.49	0.45
12:L:195:SER:O	12:L:201:ILE:HD11	2.16	0.45
12:L:390:TYR:CE2	35:j:68:TRP:HH2	2.34	0.45
12:L:591:PHE:N	12:L:591:PHE:CD1	2.83	0.45
12:L:591:PHE:N	12:L:591:PHE:HD1	2.15	0.45
13:M:42:LEU:HD21	13:M:67:ILE:HD12	1.97	0.45
13:M:272:THR:O	13:M:275:ILE:HG13	2.17	0.45
15:O:112:CYS:HB3	15:O:131:LEU:HA	1.97	0.45
15:O:114:LEU:HA	15:O:131:LEU:HD21	1.98	0.45
15:O:341:PRO:HB2	28:c:34:PRO:HB3	1.99	0.45
19:S:65:LEU:HD23	19:S:65:LEU:O	2.16	0.45
21:V:7:LYS:O	21:V:8:THR:OG1	2.29	0.45
21:V:56:LEU:HD11	21:V:57:ASP:OD1	2.17	0.45
24:Y:83:ARG:O	24:Y:85:LYS:HG2	2.17	0.45
24:Y:83:ARG:NH1	24:Y:90:LEU:HD23	2.31	0.45
32:g:67:LYS:O	32:g:68:ASN:C	2.60	0.45
32:g:121:GLU:OE2	41:p:10:TYR:CZ	2.70	0.45
37:l:57:MET:HE2	37:l:57:MET:HB3	1.75	0.45
39:n:101:GLU:HG2	39:n:122:ARG:HH12	1.81	0.45
40:o:8:ARG:HB2	40:o:16:GLU:HG2	1.99	0.45
40:o:111:ARG:HA	40:o:114:ARG:HH11	1.82	0.45
41:p:110:LEU:O	41:p:111:LYS:C	2.58	0.45
49:AE:155:LYS:HB3	49:AE:158:ASP:OD2	2.17	0.45
45:Aa:168:ILE:HA	45:Aa:171:GLU:HG2	1.98	0.45
45:Aa:405:GLY:O	45:Aa:408:PRO:HD2	2.17	0.45
48:Ad:141:THR:OG1	48:Ad:144:GLU:HG3	2.17	0.45
49:Ae:195:LEU:HD13	49:Ae:248:ARG:HD2	1.99	0.45
1:A:4:TYR:CE2	58:H:402:3PE:H231	2.52	0.45
2:B:129:ASP:CG	8:H:54:LYS:HZ1	2.24	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.26	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
5:E:137:THR:HA	5:E:140:MET:HE2	1.98	0.45
5:E:180:VAL:CG2	6:F:286:CYS:HA	2.46	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	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:HD21	1.99	0.45
7:G:454:ASP:OD1	7:G:459:ARG:NH2	2.50	0.45
8:H:140:ILE:HG13	8:H:141:SER:N	2.32	0.45
8:H:240:ILE:HD11	8:H:259:PHE:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LYS:NZ	11:K:21:MET:O	2.43	0.45
10:J:62:GLY:O	10:J:63:MET:C	2.58	0.45
10:J:150:TRP:HA	10:J:153:VAL:HG12	1.98	0.45
12:L:241:THR:N	12:L:242:PRO:HD2	2.31	0.45
12:L:407:TRP:HE1	37:l:140:MET:CE	2.29	0.45
12:L:483:PRO:CG	12:L:486:LEU:HD12	2.47	0.45
13:M:283:LYS:HG3	13:M:327:PHE:HE1	1.78	0.45
58:M:501:3PE:H221	24:Y:135:TRP:CZ2	2.52	0.45
14:N:25:ASN:HB3	30:e:15:ASP:CG	2.41	0.45
14:N:307:THR:O	15:O:319:ILE:N	2.49	0.45
15:O:168:VAL:HG21	15:O:241:TYR:CE2	2.51	0.45
17:Q:65:THR:HG23	17:Q:67:VAL:HG23	1.99	0.45
20:T:83:VAL:HG21	20:T:145:VAL:HG22	1.99	0.45
22:W:83:ASP:O	22:W:87:ILE:HG12	2.17	0.45
23:X:165:THR:N	23:X:172:VAL:HG11	2.32	0.45
24:Y:19:GLN:HA	24:Y:21:HIS:CE1	2.52	0.45
25:Z:66:GLU:HA	25:Z:69:ILE:CG1	2.46	0.45
25:Z:98:MET:HE1	30:e:78:ASP:CG	2.42	0.45
34:i:108:ASP:OD2	41:p:18:PRO:CB	2.65	0.45
37:l:38:PRO:CG	38:m:71:ALA:HB2	2.43	0.45
45:AA:373:GLN:NE2	45:AA:471:ILE:O	2.49	0.45
48:AD:135:LEU:HD21	48:AD:175:PHE:HZ	1.81	0.45
49:AE:231:PHE:CE2	49:AE:250:ARG:HB3	2.51	0.45
49:AE:241:SER:OG	49:AE:254:ALA:HB2	2.17	0.45
45:Aa:74:TRP:CH2	45:Aa:410:CYS:SG	3.08	0.45
49:Ae:231:PHE:CE2	49:Ae:250:ARG:HB3	2.51	0.45
4:D:198:THR:OG1	4:D:261:MET:HE1	2.17	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.45
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.99	0.45
8:H:212:ASN:O	8:H:213:VAL:C	2.60	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
12:L:81:LYS:CA	12:L:135:ASN:HD21	2.29	0.45
12:L:246:LEU:C	12:L:246:LEU:CD1	2.90	0.45
12:L:527:GLY:O	12:L:528:PHE:HB2	2.17	0.45
13:M:42:LEU:CG	13:M:67:ILE:HD11	2.43	0.45
13:M:129:THR:CG2	13:M:235:LEU:CD1	2.95	0.45
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.46	0.45
14:N:153:ILE:O	14:N:154:ILE:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:214:PRO:HB2	14:N:247:MET:SD	2.56	0.45
14:N:293:TYR:O	14:N:297:ILE:HG12	2.17	0.45
16:P:68:TYR:CZ	16:P:242:VAL:HG11	2.51	0.45
16:P:227:PRO:HA	16:P:291:TYR:O	2.16	0.45
17:Q:166:TRP:CE3	44:s:67:PRO:HG2	2.51	0.45
19:S:74:GLU:OE1	19:S:74:GLU:N	2.49	0.45
19:S:83:SER:O	19:S:87:VAL:HG23	2.17	0.45
20:T:82:ARG:NH2	20:T:126:PHE:HD1	2.15	0.45
20:U:130:ILE:HG22	20:U:135:ALA:HB2	1.99	0.45
20:U:133:ILE:O	20:U:137:LYS:HE2	2.17	0.45
62:Y:201:CDL:H552	62:Y:201:CDL:H592	1.97	0.45
26:a:48:MET:HE3	26:a:48:MET:HB2	1.77	0.45
29:d:13:PHE:CE2	29:d:14:LEU:HD23	2.52	0.45
37:l:38:PRO:HD2	38:m:70:TYR:HD2	1.81	0.45
40:o:42:THR:O	40:o:45:GLU:N	2.49	0.45
41:p:6:ASP:HB3	41:p:9:VAL:CG2	2.39	0.45
42:q:71:LYS:HB2	42:q:73:THR:HG23	1.98	0.45
46:AB:418:SER:O	46:AB:419:VAL:C	2.59	0.45
48:AD:96:TRP:CD2	52:AH:85:PHE:HE2	2.35	0.45
49:AE:154:ILE:HG22	49:AE:155:LYS:N	2.32	0.45
49:AE:157:SER:HB2	49:AE:269:ASP:CG	2.41	0.45
49:AE:168:LYS:HZ3	49:AE:171:GLY:HA2	1.82	0.45
49:AE:178:HIS:CD2	49:AE:209:GLU:O	2.70	0.45
49:AI:12:ALA:HB3	49:AI:13:PRO:HD3	1.99	0.45
49:AI:22:VAL:O	49:AI:23:ALA:C	2.59	0.45
54:AK:3:SER:C	50:Af:110:LYS:HG2	2.41	0.45
54:AK:23:MET:O	54:AK:27:VAL:HG23	2.16	0.45
45:Aa:400:VAL:CG1	46:Ab:58:LEU:HG	2.44	0.45
48:Ad:213:SER:O	48:Ad:217:GLY:N	2.49	0.45
49:Ae:155:LYS:HB3	49:Ae:158:ASP:OD2	2.17	0.45
50:Af:22:TYR:CE1	50:Af:28:ASN:HB3	2.52	0.45
51:Ag:10:ARG:C	51:Ag:11:ILE:HD12	2.42	0.45
2:B:123:ALA:HB2	56:B:302:UQ1:O1	2.17	0.45
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.52	0.45
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.99	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.45
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:381:LEU:HD23	19:S:55:ILE:HG13	1.98	0.45
7:G:401:LEU:HD11	7:G:466:LEU:CD2	2.47	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:135:ALA:HB2	8:H:201:THR:HG22	1.98	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
10:J:102:LEU:O	10:J:105:VAL:HB	2.16	0.45
12:L:387:THR:HA	12:L:465:GLY:HA3	1.99	0.45
12:L:522:PHE:O	12:L:527:GLY:HA2	2.17	0.45
12:L:605:ASN:HA	24:Y:5:LYS:NZ	2.32	0.45
13:M:3:LYS:HA	13:M:7:PRO:HD2	1.99	0.45
13:M:209:LEU:HD11	13:M:261:PHE:HD1	1.81	0.45
58:M:501:3PE:H221	24:Y:135:TRP:CH2	2.52	0.45
14:N:109:ALA:HB3	14:N:110:PRO:CD	2.46	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
15:O:129:TYR:CD2	15:O:183:CYS:HB3	2.52	0.45
16:P:298:TYR:O	16:P:299:SER:C	2.60	0.45
16:P:315:THR:CG2	16:P:316:LYS:N	2.80	0.45
20:T:90:TYR:O	20:T:91:ASP:HB2	2.17	0.45
29:d:78:ARG:O	29:d:79:GLN:C	2.59	0.45
30:e:87:MET:HE3	30:e:92:TYR:O	2.16	0.45
31:f:38:ARG:HA	31:f:56:TRP:HE1	1.82	0.45
45:AA:274:GLU:HB3	51:AG:18:SER:HB2	1.98	0.45
47:AC:170:VAL:O	47:AC:170:VAL:HG13	2.16	0.45
49:AE:225:ILE:HD11	49:AE:237:PRO:HG3	1.99	0.45
49:AE:263:TYR:CB	49:AE:273:VAL:HA	2.47	0.45
47:Ac:10:LEU:O	47:Ac:14:ILE:HG12	2.17	0.45
47:Ac:21:LEU:HD23	47:Ac:22:PRO:O	2.17	0.45
47:Ac:149:LEU:CD1	47:Ac:291:VAL:HG22	2.47	0.45
47:Ac:218:ILE:HD11	47:Ac:224:TYR:CE2	2.52	0.45
48:Ad:159:ASN:CG	48:Ad:160:ASP:H	2.24	0.45
48:Ad:161:ASP:HB2	48:Ad:163:GLU:CD	2.41	0.45
49:Ae:93:ARG:CA	51:Ag:25:ARG:HG3	2.46	0.45
1:A:52:SER:HB2	10:J:73:MET:SD	2.56	0.45
3:C:102:HIS:CE1	21:V:44:TYR:HE1	2.35	0.45
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.47	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
6:F:268:GLU:CG	6:F:269:ARG:H	2.30	0.45
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.45
7:G:432:ILE:HG12	7:G:451:ILE:HD11	1.99	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
10:J:153:VAL:HG23	58:J:201:3PE:H3D2	1.99	0.45
12:L:485:PHE:CE1	12:L:486:LEU:HG	2.52	0.45
13:M:55:MET:HE1	62:d:201:CDL:C51	2.47	0.45
13:M:87:ASP:HB3	13:M:91:LEU:HB2	1.99	0.45
16:P:169:HIS:N	16:P:184:LYS:HE3	2.29	0.45
16:P:182:ARG:O	16:P:186:VAL:HG23	2.17	0.45
17:Q:51:GLN:HB3	22:W:26:ARG:HH22	1.82	0.45
23:X:9:THR:O	23:X:12:GLU:HB3	2.17	0.45
29:d:93:TYR:CG	33:h:160:MET:HE2	2.52	0.45
33:h:57:VAL:HG13	39:n:104:LEU:CG	2.46	0.45
33:h:73:PHE:CE2	33:h:74:TYR:HE1	2.35	0.45
40:o:22:ILE:O	40:o:105:GLU:OE2	2.35	0.45
47:AC:341:GLN:HE21	47:AC:342:PRO:HD2	1.82	0.45
67:AC:402:HEM:CBA	68:AC:403:UQ6:O4	2.65	0.45
49:AE:195:LEU:HD13	49:AE:248:ARG:HD2	1.99	0.45
50:AF:51:LEU:HD23	50:AF:94:TYR:HE2	1.80	0.45
45:Aa:286:HIS:ND1	45:Aa:359:VAL:HG22	2.31	0.45
46:Ab:233:VAL:HA	46:Ab:236:GLN:CG	2.46	0.45
46:Ab:312:SER:HA	46:Ab:315:LYS:HE3	1.99	0.45
48:Ad:259:THR:O	48:Ad:260:PRO:C	2.60	0.45
49:Ae:154:ILE:HG22	49:Ae:155:LYS:N	2.32	0.45
50:Af:22:TYR:HB2	50:Af:84:TYR:HD2	1.80	0.45
50:Af:35:ASP:HB2	50:Af:90:TYR:CZ	2.52	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
58:D:501:3PE:H272	14:N:288:LEU:HD13	1.98	0.44
5:E:128:LYS:HD3	5:E:167:LEU:HG	2.00	0.44
6:F:209:GLU:CD	6:F:230:PRO:HG2	2.42	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
58:H:403:3PE:H331	9:I:63:TRP:CZ2	2.51	0.44
12:L:71:MET:CE	13:M:376:MET:HE1	2.47	0.44
12:L:100:ILE:O	12:L:104:SER:N	2.42	0.44
12:L:264:HIS:O	12:L:267:THR:N	2.49	0.44
12:L:532:ILE:HG21	37:l:133:LEU:CD2	2.47	0.44
13:M:42:LEU:CG	13:M:67:ILE:CD1	2.95	0.44
13:M:187:ASP:H	13:M:192:ASN:ND2	2.15	0.44
13:M:249:ILE:O	13:M:250:LEU:CG	2.47	0.44
14:N:154:ILE:CD1	14:N:195:PRO:HG2	2.47	0.44
15:O:241:TYR:HD1	15:O:245:PHE:CD2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:351:TRP:O	15:O:355:LYS:HG2	2.16	0.44
19:S:37:ILE:HD12	19:S:55:ILE:HD12	1.98	0.44
20:U:116:VAL:HG12	20:U:120:MET:HE2	1.98	0.44
23:X:115:LEU:HB3	23:X:117:TRP:CE2	2.52	0.44
24:Y:110:TYR:HB3	58:m:201:3PE:H31	1.97	0.44
32:g:64:VAL:HG11	32:g:71:PHE:CE1	2.52	0.44
33:h:56:VAL:O	33:h:58:LYS:HG3	2.16	0.44
62:h:201:CDL:HA21	58:i:201:3PE:H112	1.99	0.44
39:n:35:ASP:OD1	39:n:35:ASP:N	2.51	0.44
39:n:170:ILE:O	39:n:173:ARG:NH1	2.50	0.44
45:AA:395:LEU:O	45:AA:398:ALA:HB3	2.17	0.44
46:AB:148:ARG:HG2	46:AB:202:SER:OG	2.16	0.44
47:AC:218:ILE:HD11	47:AC:224:TYR:CE2	2.52	0.44
48:AD:259:THR:O	48:AD:260:PRO:C	2.60	0.44
50:AF:83:LYS:H	50:AF:86:GLU:HB3	1.81	0.44
51:AG:12:ARG:HB3	51:AG:13:HIS:CD2	2.52	0.44
53:AJ:34:ARG:NH1	53:AJ:38:GLN:HB2	2.32	0.44
45:Aa:46:PRO:HB2	45:Aa:62:GLU:HG2	1.99	0.44
45:Aa:62:GLU:OE1	45:Aa:423:ARG:NH1	2.45	0.44
46:Ab:138:LEU:CD1	46:Ab:233:VAL:HB	2.47	0.44
47:Ac:341:GLN:HE21	47:Ac:342:PRO:HD2	1.82	0.44
48:Ad:146:LYS:HD2	48:Ad:146:LYS:HA	1.74	0.44
53:Aj:31:PHE:CD1	54:Ak:47:TYR:HD2	2.32	0.44
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.82	0.44
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
5:E:147:ILE:CG2	5:E:200:ILE:HG12	2.37	0.44
6:F:158:ILE:HD13	6:F:166:ALA:HB2	1.98	0.44
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.98	0.44
7:G:163:LYS:HE2	18:R:97:LYS:HZ3	1.82	0.44
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.44
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.44
8:H:305:ILE:O	8:H:308:PRO:HD2	2.17	0.44
10:J:126:TYR:C	25:Z:120:LEU:HD22	2.42	0.44
11:K:93:LEU:CD2	14:N:54:GLU:HG2	2.47	0.44
12:L:117:PHE:CE1	12:L:243:VAL:CG2	3.00	0.44
12:L:437:PHE:CZ	12:L:441:ILE:HG12	2.43	0.44
12:L:604:ILE:O	24:Y:5:LYS:CD	2.63	0.44
13:M:131:ILE:CD1	14:N:302:LEU:HD21	2.48	0.44
13:M:415:GLN:O	13:M:416:ARG:CG	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:220:MET:O	14:N:221:LEU:C	2.60	0.44
14:N:250:SER:O	14:N:259:GLY:HA3	2.17	0.44
14:N:258:THR:CB	14:N:333:SER:O	2.64	0.44
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.82	0.44
15:O:69:GLY:HA2	15:O:72:LYS:NZ	2.32	0.44
16:P:178:SER:O	16:P:182:ARG:HG3	2.17	0.44
20:U:114:ASP:OD1	39:n:45:ARG:NH2	2.50	0.44
23:X:45:LEU:HD23	23:X:135:ARG:HH21	1.82	0.44
23:X:54:ARG:HA	23:X:57:LEU:HG	1.99	0.44
23:X:154:ILE:HG12	33:h:167:PRO:HG2	1.98	0.44
25:Z:68:ARG:O	25:Z:69:ILE:C	2.60	0.44
25:Z:98:MET:HB2	25:Z:104:TRP:CE2	2.52	0.44
26:a:2:TRP:HZ2	62:q:201:CDL:OB7	2.00	0.44
33:h:54:LEU:HD23	34:i:27:GLU:HA	2.00	0.44
40:o:110:GLN:O	40:o:111:ARG:C	2.59	0.44
45:AA:119:HIS:CE1	46:AB:298:HIS:HA	2.49	0.44
48:AD:290:LEU:CD2	53:AJ:44:TYR:CB	2.94	0.44
49:AE:178:HIS:NE2	49:AE:209:GLU:HB2	2.33	0.44
50:AF:95:LEU:O	50:AF:96:LYS:C	2.59	0.44
45:Aa:169:LEU:HD11	45:Aa:209:ARG:HG2	1.97	0.44
46:Ab:155:ARG:HD2	46:Ab:198:GLY:H	1.83	0.44
46:Ab:418:SER:O	46:Ab:419:VAL:C	2.59	0.44
48:Ad:156:ASP:HB2	48:Ad:167:ARG:HG3	2.00	0.44
49:Ae:127:TYR:CD2	53:Aj:32:PHE:HE2	2.36	0.44
49:Ae:154:ILE:HD12	49:Ae:154:ILE:N	2.33	0.44
52:Ah:76:ARG:O	52:Ah:79:CYS:SG	2.75	0.44
1:A:62:PHE:O	1:A:63:LEU:C	2.60	0.44
1:A:109:LYS:HG2	1:A:109:LYS:O	2.17	0.44
2:B:98:ALA:N	2:B:135:GLY:HA3	2.33	0.44
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.44
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.81	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:246:ALA:O	5:E:247:GLY:C	2.60	0.44
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.99	0.44
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:288:LEU:O	8:H:293:PHE:N	2.50	0.44
12:L:231:PRO:C	12:L:234:PRO:HD2	2.41	0.44
12:L:389:PHE:HZ	35:j:79:ALA:CB	2.28	0.44
12:L:477:ILE:HG13	40:o:91:GLU:CD	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:73:LEU:HB3	13:M:103:GLN:OE1	2.16	0.44
13:M:200:MET:HE2	13:M:250:LEU:HD21	2.00	0.44
15:O:201:PRO:HG2	15:O:249:MET:HE2	1.98	0.44
15:O:202:HIS:O	15:O:253:CYS:HB2	2.17	0.44
15:O:223:ASP:O	15:O:224:PRO:C	2.60	0.44
15:O:262:GLU:HB3	15:O:268:LYS:NZ	2.33	0.44
16:P:323:HIS:O	16:P:323:HIS:CG	2.71	0.44
18:R:44:ARG:C	18:R:46:VAL:N	2.73	0.44
19:S:42:VAL:HB	19:S:46:LYS:HE3	1.98	0.44
20:T:119:ILE:CD1	20:T:138:LEU:HD11	2.43	0.44
24:Y:115:MET:O	24:Y:119:TYR:HD2	2.01	0.44
25:Z:66:GLU:HG3	27:b:50:PRO:HG3	1.98	0.44
28:c:61:THR:HG21	29:d:74:PHE:CE1	2.52	0.44
33:h:55:PHE:C	33:h:55:PHE:CD1	2.94	0.44
43:r:113:LEU:HD12	43:r:113:LEU:HA	1.77	0.44
47:AC:237:LEU:HD22	48:AD:300:LEU:HD11	1.98	0.44
52:AH:34:HIS:CD2	52:AH:83:LYS:HE2	2.52	0.44
54:AK:29:ALA:O	54:AK:33:VAL:HG23	2.18	0.44
46:Ab:180:VAL:HG21	46:Ab:257:GLU:CA	2.46	0.44
48:Ad:201:VAL:HG22	48:Ad:278:SER:OG	2.18	0.44
49:Ae:178:HIS:NE2	49:Ae:209:GLU:HB2	2.33	0.44
49:Ae:243:TYR:CD2	49:Ae:258:LEU:HG	2.52	0.44
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.47	0.44
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.00	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.53	0.44
6:F:98:LYS:HA	6:F:101:PHE:CE2	2.52	0.44
6:F:234:GLY:HA3	6:F:240:THR:HB	1.98	0.44
7:G:43:VAL:HG12	7:G:55:LYS:CD	2.46	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.99	0.44
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.99	0.44
9:I:59:ARG:HA	9:I:64:THR:HG23	1.99	0.44
11:K:61:ILE:O	11:K:62:THR:C	2.58	0.44
12:L:2:ASN:O	12:L:3:ILE:C	2.59	0.44
12:L:155:ILE:HG12	12:L:248:HIS:CE1	2.53	0.44
12:L:366:MET:SD	12:L:443:ILE:CG2	3.06	0.44
13:M:22:LYS:HG2	13:M:26:ASN:ND2	2.33	0.44
13:M:24:TRP:CE3	13:M:81:GLN:HG2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:321:LEU:HD23	13:M:321:LEU:HA	1.81	0.44
13:M:424:ILE:O	13:M:424:ILE:CG2	2.65	0.44
20:T:92:LYS:O	20:T:92:LYS:HG2	2.16	0.44
23:X:46:CYS:HA	23:X:135:ARG:CZ	2.48	0.44
23:X:57:LEU:HD21	25:Z:84:LEU:HD11	1.98	0.44
24:Y:120:MET:HE2	24:Y:120:MET:HB3	1.90	0.44
40:o:4:HIS:CD2	40:o:7:ARG:HH12	2.35	0.44
46:AB:327:ASN:ND2	49:AI:7:ARG:HD2	2.32	0.44
49:AE:127:TYR:CD2	53:AJ:32:PHE:HE2	2.35	0.44
50:Af:27:PHE:O	50:Af:31:GLY:N	2.51	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.44
5:E:131:ILE:HD11	5:E:168:PHE:CD2	2.49	0.44
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.17	0.44
6:F:168:ASN:ND2	44:s:40:TYR:CE2	2.85	0.44
6:F:226:LYS:O	6:F:227:PRO:C	2.60	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.44
7:G:607:LYS:HG2	17:Q:78:ARG:HH11	1.82	0.44
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.44
8:H:264:LEU:HD23	8:H:264:LEU:HA	1.81	0.44
12:L:249:SER:HB2	12:L:340:PHE:CD2	2.53	0.44
12:L:537:THR:N	12:L:538:PRO:HD2	2.32	0.44
13:M:123:GLU:CD	14:N:255:PRO:HG2	2.43	0.44
14:N:23:SER:HB2	30:e:15:ASP:OD2	2.17	0.44
14:N:87:GLN:O	14:N:88:GLN:C	2.59	0.44
14:N:208:TYR:O	14:N:212:THR:HG22	2.18	0.44
15:O:336:GLY:HA2	15:O:344:ASN:HB3	1.99	0.44
17:Q:62:THR:HG22	17:Q:141:ASN:O	2.18	0.44
19:S:20:ARG:HG3	19:S:54:LEU:CB	2.43	0.44
20:T:79:ILE:O	20:T:83:VAL:HG23	2.17	0.44
20:T:109:GLY:O	20:T:110:LEU:C	2.61	0.44
20:U:136:GLU:O	34:i:2:SER:OG	2.36	0.44
30:e:42:GLU:OE2	33:h:181:HIS:NE2	2.46	0.44
34:i:11:ARG:NH1	39:n:154:LEU:HD12	2.32	0.44
40:o:49:ALA:O	40:o:50:GLN:C	2.60	0.44
43:r:5:THR:HG22	43:r:5:THR:O	2.18	0.44
46:AB:233:VAL:HA	46:AB:236:GLN:CG	2.47	0.44
46:AB:312:SER:HA	46:AB:315:LYS:HE3	1.99	0.44
47:AC:206:ASN:HB3	67:AC:402:HEM:O1D	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:309:HIS:CE1	51:AG:21:PRO:HB2	2.52	0.44
48:Ad:167:ARG:HH12	48:Ad:170:LYS:H	1.65	0.44
49:Ae:178:HIS:HA	49:Ae:209:GLU:O	2.18	0.44
49:Ae:241:SER:OG	49:Ae:254:ALA:HB2	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.44
5:E:94:ILE:O	5:E:98:ASN:ND2	2.50	0.44
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.44
6:F:283:ASN:ND2	6:F:306:GLY:H	2.16	0.44
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
8:H:289:LEU:O	8:H:294:LEU:HB2	2.18	0.44
10:J:3:ASN:O	10:J:4:TYR:C	2.60	0.44
10:J:33:ILE:CD1	10:J:60:LEU:HA	2.48	0.44
10:J:59:TYR:C	10:J:61:GLY:N	2.71	0.44
10:J:61:GLY:O	10:J:65:VAL:HG23	2.18	0.44
10:J:129:ASP:O	10:J:130:ASP:C	2.61	0.44
12:L:54:PHE:CB	12:L:87:ILE:HD11	2.48	0.44
12:L:556:ILE:CG2	38:m:80:PHE:CE1	2.96	0.44
13:M:186:LEU:HD13	13:M:250:LEU:HA	2.00	0.44
14:N:31:VAL:C	14:N:35:PHE:CD2	2.91	0.44
14:N:122:ILE:HD11	14:N:127:GLY:HA2	1.98	0.44
15:O:272:ASP:O	15:O:275:TYR:HB2	2.18	0.44
18:R:32:THR:HG21	42:q:129:THR:HG23	2.00	0.44
20:T:113:LEU:O	20:T:116:VAL:HB	2.17	0.44
22:W:86:VAL:O	22:W:90:LYS:HG3	2.18	0.44
23:X:153:VAL:O	23:X:155:GLU:HG3	2.18	0.44
24:Y:7:PHE:CZ	24:Y:26:ILE:HG12	2.52	0.44
28:c:61:THR:HG22	28:c:65:ASP:OD2	2.18	0.44
28:c:73:ASN:OD1	28:c:75:LEU:N	2.50	0.44
29:d:27:ASN:O	29:d:28:ASP:C	2.61	0.44
31:f:14:ILE:O	31:f:15:LEU:C	2.61	0.44
35:j:102:ASP:O	35:j:103:ASP:HB2	2.17	0.44
48:AD:167:ARG:HH12	48:AD:170:LYS:H	1.65	0.44
52:AH:43:LYS:O	52:AH:47:ARG:HG3	2.18	0.44
54:AK:17:TRP:O	54:AK:18:ILE:C	2.60	0.44
45:Aa:78:GLY:H	45:Aa:81:TYR:HD2	1.65	0.44
45:Aa:373:GLN:NE2	45:Aa:471:ILE:O	2.49	0.44
50:Af:52:PRO:HD2	50:Af:55:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:HIS:HE1	8:H:205:SER:O	2.01	0.44
5:E:49:ASP:O	5:E:50:THR:C	2.60	0.44
5:E:81:VAL:O	5:E:82:LEU:C	2.59	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:47:GLY:C	6:F:49:HIS:H	2.24	0.44
6:F:93:PHE:O	6:F:94:PRO:C	2.59	0.44
7:G:114:GLU:HG3	7:G:148:SER:HB3	2.00	0.44
7:G:346:VAL:O	7:G:521:SER:HB3	2.17	0.44
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.44
58:H:402:3PE:H2I2	58:H:402:3PE:H2E1	2.00	0.44
10:J:5:ILE:HG13	10:J:124:LEU:CD1	2.48	0.44
11:K:29:THR:C	11:K:31:LEU:N	2.76	0.44
12:L:68:TRP:HE3	12:L:76:LEU:HD21	1.82	0.44
12:L:524:THR:HG23	12:L:525:LEU:HG	1.98	0.44
12:L:550:LEU:CD1	13:M:275:ILE:HB	2.31	0.44
13:M:18:SER:OG	13:M:26:ASN:ND2	2.51	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
14:N:120:GLN:HE22	14:N:174:GLN:HB3	1.83	0.44
14:N:146:TYR:CD1	14:N:198:PRO:HG2	2.53	0.44
15:O:200:PRO:HG3	15:O:282:PRO:CD	2.47	0.44
16:P:96:LEU:C	16:P:96:LEU:HD12	2.43	0.44
16:P:165:ILE:HG12	16:P:199:ILE:HB	1.99	0.44
17:Q:77:VAL:HG21	17:Q:99:MET:CE	2.48	0.44
17:Q:99:MET:HG2	17:Q:128:PHE:HE2	1.82	0.44
19:S:48:HIS:HE1	19:S:95:LEU:CD2	2.25	0.44
23:X:172:VAL:HG23	29:d:30:ARG:NH1	2.33	0.44
25:Z:120:LEU:HD21	30:e:32:ARG:NH2	2.33	0.44
28:c:40:ASN:O	28:c:41:TRP:C	2.60	0.44
30:e:19:MET:HE2	30:e:19:MET:HB3	1.85	0.44
31:f:7:LEU:HD13	31:f:11:TRP:HA	1.99	0.44
34:i:88:TYR:CE2	41:p:49:ARG:HB2	2.52	0.44
38:m:45:ARG:NE	39:n:140:LEU:HD11	2.33	0.44
48:AD:207:GLY:O	48:AD:208:GLU:C	2.58	0.44
49:AE:155:LYS:HE2	49:AE:157:SER:HB3	1.99	0.44
49:AE:220:LEU:HD22	47:Ac:149:LEU:CA	2.48	0.44
52:AH:44:ALA:HB1	52:AH:72:PHE:HA	2.00	0.44
48:Ad:234:ASN:O	48:Ad:235:PRO:C	2.59	0.44
48:Ad:248:ILE:HD12	48:Ad:266:VAL:HG11	2.00	0.44
49:Ae:156:LEU:HD23	49:Ae:156:LEU:HA	1.62	0.44
50:Af:51:LEU:HG	50:Af:91:LEU:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD23	10:J:58:ILE:HD12	1.99	0.44
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.48	0.44
4:D:55:SER:OG	4:D:56:LYS:N	2.50	0.44
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.48	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
5:E:196:THR:O	5:E:197:PRO:C	2.61	0.44
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.33	0.44
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.82	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:666:GLN:HE22	19:S:38:VAL:HG13	1.82	0.44
12:L:66:TRP:CZ3	12:L:68:TRP:HD1	2.34	0.44
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.99	0.44
12:L:529:PHE:O	12:L:533:ILE:HG22	2.16	0.44
14:N:227:ILE:HG13	14:N:228:ASN:N	2.32	0.44
15:O:132:GLN:HE22	64:O:401:ADP:N6	2.14	0.44
16:P:55:VAL:HG11	16:P:122:HIS:O	2.18	0.44
16:P:163:ARG:NE	16:P:253:THR:HA	2.33	0.44
16:P:246:SER:O	16:P:249:ILE:N	2.51	0.44
16:P:321:ARG:CZ	16:P:321:ARG:HB2	2.48	0.44
16:P:345:LEU:C	16:P:345:LEU:HD23	2.43	0.44
17:Q:77:VAL:CG1	17:Q:101:PHE:CD2	3.00	0.44
20:U:88:LYS:HG3	20:U:98:LEU:HD23	1.98	0.44
22:W:87:ILE:O	22:W:91:MET:HG3	2.18	0.44
26:a:37:ARG:HB2	26:a:48:MET:HE2	2.00	0.44
30:e:74:ARG:O	30:e:75:ARG:C	2.59	0.44
35:j:43:ARG:HG3	35:j:48:PRO:HA	2.00	0.44
35:j:96:GLU:O	40:o:31:PHE:HZ	2.01	0.44
45:AA:286:HIS:CG	45:AA:359:VAL:HG22	2.53	0.44
46:AB:47:LEU:HD23	46:AB:234:ALA:HB1	2.00	0.44
48:AD:143:GLU:CD	48:AD:143:GLU:C	2.86	0.44
48:AD:321:TYR:HB2	50:AF:61:PHE:CE2	2.52	0.44
49:AE:220:LEU:HD21	47:Ac:149:LEU:HA	2.00	0.44
50:AF:93:PRO:O	50:AF:96:LYS:HB2	2.17	0.44
47:Ac:170:VAL:HG13	47:Ac:170:VAL:O	2.16	0.44
47:Ac:379:LEU:HG	50:Af:34:ARG:HD2	1.98	0.44
48:Ad:157:GLY:O	48:Ad:164:MET:HA	2.18	0.44
49:Ae:146:VAL:HA	49:Ae:149:MET:SD	2.58	0.44
49:Ae:155:LYS:HE2	49:Ae:157:SER:HB3	1.99	0.44
49:Ae:161:GLU:HA	49:Ae:178:HIS:CB	2.48	0.44
49:Ae:273:VAL:O	49:Ae:274:GLY:C	2.60	0.44
1:A:81:THR:O	27:b:46:ASN:ND2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
6:F:147:ARG:HD2	6:F:191:TYR:CD1	2.53	0.44
7:G:279:GLU:HG3	17:Q:154:LYS:HG3	2.00	0.44
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.44
7:G:462:PHE:CD2	7:G:466:LEU:HG	2.52	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:16:ALA:HB2	26:a:15:CYS:HB2	1.99	0.44
8:H:39:ILE:HG13	42:q:31:ASN:ND2	2.33	0.44
8:H:116:ILE:CG1	8:H:117:LEU:N	2.74	0.44
12:L:152:PHE:HD2	12:L:153:LEU:HD12	1.83	0.44
13:M:344:MET:HE3	13:M:423:MET:CE	2.48	0.44
14:N:146:TYR:O	14:N:147:PRO:C	2.53	0.44
19:S:51:LEU:CD1	19:S:95:LEU:HD12	2.46	0.44
28:c:55:TRP:HZ2	29:d:66:THR:HG22	1.76	0.44
29:d:57:GLY:O	29:d:60:ARG:N	2.51	0.44
33:h:55:PHE:CD2	39:n:115:TYR:CD1	3.06	0.44
35:j:38:VAL:HG12	35:j:39:HIS:H	1.80	0.44
38:m:37:LEU:HA	38:m:40:ARG:CG	2.46	0.44
41:p:140:GLN:HG2	41:p:144:LEU:CD1	2.47	0.44
46:AB:97:PHE:CZ	46:AB:101:ARG:HG3	2.53	0.44
48:AD:201:VAL:HG22	48:AD:278:SER:HB2	2.00	0.44
49:AE:122:THR:O	49:AE:123:VAL:C	2.61	0.44
49:AE:154:ILE:HD12	49:AE:154:ILE:N	2.32	0.44
54:AK:33:VAL:CG1	54:AK:42:LEU:HG	2.45	0.44
45:Aa:50:VAL:HG12	45:Aa:51:SER:N	2.32	0.44
46:Ab:230:LEU:O	46:Ab:233:VAL:HG22	2.18	0.44
48:Ad:94:TYR:HE2	48:Ad:209:ASP:HA	1.83	0.44
49:Ae:261:PRO:HB2	49:Ae:273:VAL:HG11	1.99	0.44
51:Ag:19:LEU:HG	51:Ag:20:SER:N	2.33	0.44
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.48	0.43
1:A:24:LEU:HD23	1:A:24:LEU:C	2.43	0.43
1:A:49:LEU:HD12	1:A:50:PRO:CD	2.47	0.43
2:B:95:PHE:CE2	2:B:97:LEU:HD21	2.53	0.43
2:B:114:MET:SD	2:B:119:VAL:CG1	3.06	0.43
4:D:72:LEU:HD12	14:N:50:PRO:CG	2.42	0.43
5:E:235:GLU:HB2	6:F:37:ASP:HB2	2.00	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:306:MET:HA	7:G:316:TYR:HA	1.99	0.43
7:G:355:LYS:HG2	7:G:359:ASN:ND2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:651:PRO:HB3	19:S:57:GLU:O	2.18	0.43
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.43
11:K:57:MET:O	11:K:60:PRO:HD2	2.18	0.43
12:L:73:SER:HB3	41:p:100:GLN:HE21	1.82	0.43
12:L:305:SER:OG	12:L:336:LYS:HE2	2.18	0.43
12:L:588:PHE:O	12:L:589:MET:C	2.60	0.43
12:L:589:MET:O	12:L:592:LEU:HB3	2.18	0.43
13:M:123:GLU:CG	14:N:255:PRO:HG2	2.48	0.43
14:N:12:THR:CG2	14:N:39:ALA:HB2	2.48	0.43
14:N:175:MET:HE2	14:N:175:MET:HB2	1.85	0.43
14:N:309:ASN:HA	15:O:319:ILE:HG22	1.99	0.43
16:P:55:VAL:HA	16:P:79:GLN:HB3	1.99	0.43
16:P:72:HIS:HB2	16:P:250:VAL:HG21	2.00	0.43
16:P:126:VAL:HG23	16:P:161:VAL:HG11	2.00	0.43
17:Q:59:LEU:O	17:Q:140:LYS:HA	2.18	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
25:Z:87:LEU:HD21	25:Z:119:PRO:HG3	2.00	0.43
30:e:72:THR:O	30:e:73:MET:C	2.58	0.43
37:l:38:PRO:HD2	38:m:70:TYR:CD2	2.53	0.43
37:l:119:THR:CG2	38:m:13:THR:HG23	2.48	0.43
39:n:131:GLU:O	39:n:131:GLU:HG2	2.17	0.43
41:p:165:GLU:C	41:p:167:ARG:H	2.26	0.43
43:r:109:ASP:OD1	43:r:110:GLN:N	2.51	0.43
46:AB:43:LEU:HG	46:AB:49:ILE:HG12	2.00	0.43
46:AB:89:LEU:CD2	46:AB:150:GLU:HB3	2.42	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:116:GLY:O	67:AC:402:HEM:CMC	2.66	0.43
47:AC:287:LYS:CB	49:Ae:219:HIS:CD2	3.01	0.43
48:AD:262:THR:O	48:AD:263:MET:C	2.61	0.43
49:AE:111:LYS:HE3	53:AJ:11:TYR:CZ	2.52	0.43
51:AG:25:ARG:NH2	51:AG:29:SER:H	2.16	0.43
46:Ab:232:GLN:O	46:Ab:235:GLU:HG3	2.17	0.43
48:Ad:89:LEU:HD11	52:Ah:78:HIS:CE1	2.53	0.43
48:Ad:112:ARG:HB3	48:Ad:255:TYR:CE1	2.53	0.43
54:Ak:48:ILE:C	54:Ak:50:GLY:N	2.72	0.43
4:D:378:LEU:HD23	7:G:126:LEU:HB2	2.00	0.43
6:F:62:TRP:CH2	6:F:140:GLU:HA	2.53	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.18	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
12:L:446:ASN:HD21	35:j:40:ILE:HD11	1.82	0.43
13:M:8:SER:O	13:M:11:LEU:HB2	2.18	0.43
13:M:423:MET:C	13:M:424:ILE:O	2.56	0.43
58:M:502:3PE:H2A1	58:M:502:3PE:H3A2	2.00	0.43
15:O:211:VAL:HB	15:O:212:PRO:HD3	2.00	0.43
15:O:316:GLU:HG3	32:g:51:MET:CE	2.48	0.43
17:Q:91:VAL:HG22	17:Q:91:VAL:O	2.18	0.43
17:Q:101:PHE:CE1	17:Q:124:MET:HE3	2.53	0.43
19:S:23:LEU:HB3	19:S:33:VAL:HG12	2.01	0.43
29:d:72:GLY:O	29:d:73:TYR:C	2.60	0.43
30:e:102:GLU:HG2	30:e:103:GLU:N	2.33	0.43
37:l:142:PHE:O	37:l:145:TRP:N	2.51	0.43
42:q:74:PHE:HD2	42:q:75:TRP:CD1	2.33	0.43
45:AA:78:GLY:H	45:AA:81:TYR:HD2	1.65	0.43
48:AD:112:ARG:HB3	48:AD:255:TYR:CE1	2.53	0.43
48:AD:155:GLN:HB2	48:AD:166:MET:CG	2.42	0.43
49:AE:265:PHE:HA	49:AE:271:VAL:HG22	2.00	0.43
46:Ab:38:LEU:C	46:Ab:38:LEU:CD1	2.79	0.43
46:Ab:63:LEU:HD12	46:Ab:220:LEU:HD13	2.00	0.43
46:Ab:142:THR:HB	46:Ab:240:MET:CG	2.48	0.43
48:Ad:137:GLY:N	48:Ad:140:TYR:O	2.51	0.43
52:Ah:80:VAL:O	52:Ah:84:LEU:HB2	2.18	0.43
1:A:63:LEU:HD11	10:J:66:VAL:HG11	1.99	0.43
1:A:105:GLU:HG2	1:A:111:LEU:HB3	1.99	0.43
4:D:67:ASN:HB3	4:D:69:VAL:CG1	2.44	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.87	0.43
5:E:179:CYS:SG	6:F:123:GLY:HA2	2.58	0.43
7:G:306:MET:HG2	7:G:316:TYR:CA	2.46	0.43
7:G:336:ASN:HB3	7:G:540:ASN:ND2	2.33	0.43
7:G:338:VAL:HA	7:G:544:MET:O	2.17	0.43
8:H:116:ILE:HD12	8:H:135:ALA:HB3	1.99	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
10:J:162:GLY:O	10:J:166:ILE:HD12	2.19	0.43
12:L:226:GLN:O	12:L:230:HIS:HB3	2.17	0.43
12:L:291:CYS:O	12:L:295:GLN:HG2	2.18	0.43
12:L:309:GLN:HB2	12:L:336:LYS:HZ1	1.83	0.43
12:L:598:ILE:CD1	14:N:153:ILE:HG12	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:L:703:CDL:H321	33:h:71:MET:HE1	1.99	0.43
14:N:324:LEU:HD13	29:d:45:ASP:OD2	2.19	0.43
16:P:211:ASP:CG	16:P:214:LEU:HB3	2.43	0.43
19:S:24:CYS:SG	19:S:61:VAL:HG12	2.58	0.43
19:S:62:GLN:HB2	19:S:80:ASN:CG	2.42	0.43
21:V:56:LEU:CD1	21:V:57:ASP:OD1	2.67	0.43
25:Z:53:TRP:CE2	25:Z:57:ARG:HD2	2.52	0.43
27:b:82:LYS:HB3	27:b:82:LYS:HE2	1.81	0.43
45:AA:342:GLN:NE2	45:AA:344:PHE:HD2	2.15	0.43
46:AB:63:LEU:HD12	46:AB:220:LEU:HD13	2.00	0.43
46:AB:180:VAL:HG21	46:AB:257:GLU:N	2.34	0.43
47:AC:181:PHE:HA	47:AC:184:ILE:HG22	2.00	0.43
48:AD:240:GLN:HG2	52:AH:70:PHE:HZ	1.82	0.43
50:AF:90:TYR:O	50:AF:93:PRO:HD2	2.18	0.43
50:AF:97:GLU:HA	50:AF:100:ARG:NH1	2.32	0.43
52:AH:35:CYS:HA	52:AH:38:LEU:HD13	2.00	0.43
46:Ab:180:VAL:HG21	46:Ab:257:GLU:N	2.34	0.43
48:Ad:89:LEU:CD2	52:Ah:74:HIS:HA	2.49	0.43
49:Ae:217:CYS:C	49:Ae:219:HIS:N	2.72	0.43
51:Ag:38:VAL:HA	51:Ag:41:ARG:HD3	1.99	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
2:B:81:LEU:HD23	57:B:303:PC1:H251	2.00	0.43
3:C:85:ILE:HD12	3:C:140:ILE:CD1	2.48	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.43
4:D:299:GLN:HB3	43:r:104:TRP:CE3	2.53	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:355:LYS:HG3	7:G:366:LEU:HD12	2.00	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
13:M:348:LEU:O	13:M:349:GLN:C	2.60	0.43
14:N:202:LEU:HD11	30:e:3:PHE:CE1	2.53	0.43
14:N:240:MET:O	14:N:240:MET:HG2	2.18	0.43
14:N:323:ASN:N	14:N:323:ASN:OD1	2.49	0.43
15:O:210:PRO:O	15:O:213:GLU:N	2.51	0.43
16:P:156:SER:HB2	16:P:161:VAL:CG2	2.47	0.43
16:P:172:ALA:N	16:P:202:ARG:HH21	2.13	0.43
19:S:85:ASP:O	19:S:89:ARG:N	2.41	0.43
21:V:19:THR:N	21:V:20:PRO:CD	2.82	0.43
22:W:20:VAL:HG21	22:W:80:ARG:CZ	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:28:ARG:O	25:Z:28:ARG:CG	2.64	0.43
29:d:78:ARG:HG2	29:d:82:LEU:HD23	2.00	0.43
30:e:38:LYS:HG2	33:h:179:ILE:CG2	2.48	0.43
32:g:58:GLU:CD	32:g:59:PRO:HD2	2.44	0.43
35:j:38:VAL:CG1	35:j:39:HIS:H	2.31	0.43
37:l:41:TYR:HD2	37:l:43:ARG:HD3	1.82	0.43
37:l:97:LEU:O	37:l:98:ARG:C	2.60	0.43
38:m:17:THR:O	38:m:18:LEU:CB	2.66	0.43
38:m:28:GLU:HA	38:m:31:ARG:NH2	2.33	0.43
38:m:34:VAL:O	38:m:34:VAL:HG12	2.17	0.43
40:o:39:MET:HE1	40:o:57:ASP:O	2.18	0.43
41:p:75:THR:HG22	41:p:156:LEU:HD13	2.00	0.43
46:AB:155:ARG:HD2	46:AB:198:GLY:H	1.83	0.43
47:AC:21:LEU:CD1	68:AC:403:UQ6:O2	2.66	0.43
47:AC:105:GLY:HA3	47:AC:313:ARG:O	2.18	0.43
47:AC:171:ASP:CG	47:AC:172:LYS:N	2.76	0.43
48:AD:312:SER:O	48:AD:313:VAL:C	2.59	0.43
49:AE:156:LEU:H	49:AE:269:ASP:C	2.27	0.43
49:AE:173:PRO:HG2	49:AE:223:VAL:CG2	2.45	0.43
49:AE:222:CYS:HB2	49:AE:236:CYS:SG	2.59	0.43
47:Ac:105:GLY:HA3	47:Ac:313:ARG:O	2.18	0.43
47:Ac:313:ARG:N	50:Af:39:HIS:HB2	2.33	0.43
49:Ae:235:TYR:CE1	49:Ae:240:GLY:HA2	2.53	0.43
50:Af:75:ILE:HD13	51:Ag:40:ARG:HH11	1.84	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.43
2:B:163:SER:HB2	9:I:150:THR:O	2.18	0.43
2:B:192:PRO:HD3	9:I:176:SER:HA	1.99	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.43
7:G:169:VAL:HG11	7:G:231:LEU:HD13	2.00	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:662:THR:HB	19:S:25:GLN:HE21	1.84	0.43
8:H:186:PHE:CE2	58:H:403:3PE:H2B1	2.54	0.43
12:L:203:PHE:CZ	41:p:110:LEU:HD11	2.54	0.43
12:L:553:LEU:CD1	38:m:93:ALA:CB	2.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:564:LYS:HG2	38:m:77:TYR:OH	2.19	0.43
13:M:304:GLN:HA	13:M:309:PHE:HE1	1.83	0.43
14:N:186:HIS:O	14:N:190:MET:HG3	2.18	0.43
16:P:310:PHE:O	16:P:311:GLU:C	2.60	0.43
16:P:376:ASN:O	16:P:377:TYR:C	2.61	0.43
21:V:36:LYS:HA	21:V:36:LYS:HD3	1.89	0.43
24:Y:26:ILE:O	24:Y:30:LEU:HG	2.17	0.43
25:Z:10:MET:HE2	25:Z:10:MET:HB3	1.72	0.43
30:e:22:SER:HA	30:e:34:HIS:HD2	1.84	0.43
30:e:38:LYS:HB3	30:e:38:LYS:HE2	1.74	0.43
38:m:45:ARG:O	38:m:45:ARG:CG	2.61	0.43
41:p:103:MET:HE1	41:p:135:VAL:HG12	1.98	0.43
45:AA:190:THR:HG21	45:AA:275:ILE:HG22	2.01	0.43
45:AA:278:ARG:NH1	51:AG:11:ILE:HD13	2.33	0.43
46:AB:81:HIS:O	46:AB:85:LEU:HG	2.18	0.43
46:AB:378:LEU:HD23	46:AB:416:ILE:CG2	2.49	0.43
47:AC:244:LEU:HA	48:AD:285:ARG:HD2	2.00	0.43
48:AD:201:VAL:HG22	48:AD:278:SER:OG	2.18	0.43
49:AE:166:ALA:HB2	49:AE:175:PHE:HD1	1.84	0.43
49:AE:243:TYR:CD2	49:AE:258:LEU:HG	2.52	0.43
54:AK:7:GLY:H	54:AK:10:TYR:HD1	1.58	0.43
45:Aa:175:ASN:C	45:Aa:177:ALA:N	2.76	0.43
45:Aa:338:CYS:SG	45:Aa:358:PHE:HB2	2.58	0.43
46:Ab:130:ILE:HA	46:Ab:133:LEU:HB2	2.01	0.43
48:Ad:321:TYR:HD1	51:Ag:14:VAL:HG12	1.84	0.43
49:Ae:201:ASP:OD1	49:Ae:202:LEU:N	2.50	0.43
50:Af:59:ARG:O	50:Af:63:ILE:HG13	2.18	0.43
1:A:78:ALA:HA	1:A:81:THR:HG23	2.01	0.43
1:A:105:GLU:O	1:A:110:GLY:N	2.52	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.33	0.43
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.43
5:E:157:ILE:HG13	5:E:161:GLU:HB3	2.01	0.43
5:E:170:LEU:HD12	5:E:171:ILE:H	1.83	0.43
6:F:88:ARG:HH21	6:F:262:PHE:HZ	1.66	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:126:LEU:HD13	18:R:89:PRO:HB3	2.01	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
8:H:89:LEU:HG	8:H:90:PRO:HD2	1.99	0.43
10:J:54:MET:HE2	10:J:54:MET:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:97:ILE:HB	10:J:101:PHE:CZ	2.54	0.43
10:J:101:PHE:O	10:J:105:VAL:HG23	2.18	0.43
12:L:22:SER:HA	12:L:27:ILE:HG21	2.00	0.43
12:L:92:VAL:HG21	12:L:330:CYS:HB3	2.00	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:HG13	12:L:428:TYR:N	2.33	0.43
12:L:563:PRO:HG3	13:M:152:TYR:OH	2.18	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.19	0.43
13:M:119:TYR:HD1	13:M:160:LEU:HD22	1.80	0.43
13:M:159:PRO:HG2	58:M:501:3PE:H391	1.99	0.43
14:N:223:ASN:HB3	15:O:306:ASN:HD21	1.83	0.43
14:N:254:LEU:HA	14:N:255:PRO:HD3	1.61	0.43
14:N:279:ALA:HA	14:N:282:MET:HE2	2.00	0.43
15:O:72:LYS:O	15:O:76:GLU:HG2	2.18	0.43
18:R:47:ARG:HG3	18:R:48:PHE:N	2.32	0.43
26:a:4:GLU:C	26:a:7:PRO:HD2	2.44	0.43
33:h:127:ASP:OD1	33:h:127:ASP:C	2.60	0.43
39:n:37:TYR:O	39:n:38:ARG:C	2.61	0.43
42:q:129:THR:O	42:q:129:THR:CG2	2.67	0.43
45:AA:341:PHE:CD2	45:AA:368:MET:HE3	2.40	0.43
46:AB:195:TYR:OH	46:Ab:261:GLN:HG3	2.18	0.43
47:AC:128:PHE:CZ	47:AC:146:ILE:HB	2.54	0.43
46:Ab:277:ALA:H	46:Ab:280:ASN:ND2	2.16	0.43
46:Ab:378:LEU:HD23	46:Ab:416:ILE:CG2	2.49	0.43
48:Ad:133:ARG:HB3	48:Ad:171:LEU:O	2.18	0.43
48:Ad:287:ARG:HA	53:Aj:44:TYR:CD1	2.53	0.43
49:Ae:222:CYS:HB2	49:Ae:236:CYS:SG	2.59	0.43
51:Ag:25:ARG:NH2	51:Ag:29:SER:H	2.16	0.43
52:Ah:46:GLU:O	52:Ah:50:LEU:HG	2.18	0.43
52:Ah:70:PHE:HA	52:Ah:73:LEU:HD12	2.00	0.43
1:A:81:THR:O	1:A:82:ILE:C	2.62	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:263:THR:HG23	4:D:264:ASN:OD1	2.18	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:126:VAL:HG21	5:E:130:HIS:CG	2.53	0.43
5:E:233:LEU:CD2	6:F:40:ARG:HD3	2.48	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.43
7:G:347:ASP:O	7:G:351:LEU:HG	2.18	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:GLY:HA2	10:J:42:MET:CE	2.49	0.43
12:L:53:MET:HE2	12:L:53:MET:HB3	1.78	0.43
12:L:70:THR:O	12:L:75:GLU:HA	2.18	0.43
12:L:81:LYS:HD3	12:L:262:ARG:NH1	2.34	0.43
12:L:172:ILE:HD13	12:L:172:ILE:HA	1.88	0.43
12:L:442:SER:OG	20:U:71:ALA:HB2	2.18	0.43
12:L:574:THR:O	12:L:578:THR:N	2.46	0.43
13:M:1:MET:HB3	13:M:1:MET:HE3	1.73	0.43
13:M:63:THR:N	13:M:64:PRO:CD	2.81	0.43
13:M:207:MET:SD	13:M:240:SER:CA	3.06	0.43
14:N:11:PHE:O	14:N:15:LEU:N	2.49	0.43
14:N:154:ILE:HD12	14:N:155:LEU:N	2.33	0.43
15:O:86:TYR:HE1	15:O:157:VAL:HG12	1.82	0.43
16:P:203:PRO:HG2	65:P:401:NDP:C5N	2.48	0.43
16:P:280:ILE:HG23	16:P:353:LEU:HD22	2.01	0.43
19:S:30:SER:O	19:S:33:VAL:N	2.51	0.43
22:W:120:ASP:HB3	22:W:123:SER:OG	2.18	0.43
23:X:49:GLU:CG	23:X:138:PRO:HG2	2.39	0.43
25:Z:107:GLY:HA2	30:e:75:ARG:HH22	1.82	0.43
26:a:2:TRP:NE1	62:q:201:CDL:OB4	2.51	0.43
29:d:87:ASP:O	29:d:88:HIS:C	2.59	0.43
33:h:57:VAL:HG12	39:n:99:VAL:CG2	2.49	0.43
40:o:22:ILE:CA	40:o:105:GLU:OE2	2.65	0.43
43:r:109:ASP:O	43:r:110:GLN:CG	2.64	0.43
45:AA:175:ASN:C	45:AA:177:ALA:N	2.76	0.43
45:AA:364:SER:O	45:AA:365:ILE:C	2.62	0.43
47:AC:100:ARG:HH12	67:AC:402:HEM:CBD	2.31	0.43
47:AC:257:MET:HG3	48:AD:203:ALA:HB1	2.00	0.43
49:AE:249:ILE:HG12	49:AE:254:ALA:HB3	2.01	0.43
45:Aa:49:GLN:CG	45:Aa:239:HIS:CG	3.01	0.43
46:Ab:411:THR:O	46:Ab:414:GLN:HG2	2.19	0.43
47:Ac:19:ILE:HG22	47:Ac:20:ASP:OD1	2.18	0.43
2:B:126:ARG:HG3	8:H:213:VAL:O	2.18	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:339:GLN:HE22	9:I:37:LYS:HZ1	1.64	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.34	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:77:LEU:O	8:H:81:LEU:HG	2.19	0.43
8:H:140:ILE:O	8:H:143:GLU:HB3	2.19	0.43
10:J:67:PHE:CE1	11:K:75:LEU:HD21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:169:ILE:CD1	11:K:77:LEU:CD2	2.86	0.43
12:L:38:THR:O	12:L:41:LYS:HB3	2.19	0.43
12:L:60:GLU:C	12:L:61:TYR:CD1	2.97	0.43
12:L:68:TRP:CD2	62:h:201:CDL:H242	2.54	0.43
12:L:217:LEU:CD1	12:L:273:ILE:HG23	2.49	0.43
12:L:446:ASN:O	12:L:447:ASP:C	2.58	0.43
12:L:496:LEU:CD1	12:L:497:GLY:N	2.73	0.43
62:L:703:CDL:H142	62:L:703:CDL:OA9	2.18	0.43
58:L:705:3PE:H2A1	58:L:705:3PE:H232	2.01	0.43
58:L:705:3PE:H3B2	13:M:71:TRP:CD2	2.54	0.43
13:M:73:LEU:HD23	13:M:103:GLN:HE22	1.84	0.43
13:M:127:ILE:HD11	14:N:256:PRO:CD	2.49	0.43
13:M:154:LEU:HA	13:M:154:LEU:HD23	1.84	0.43
13:M:231:LEU:CD1	13:M:235:LEU:CD1	2.85	0.43
14:N:12:THR:HG22	14:N:39:ALA:HB2	2.00	0.43
14:N:219:LEU:CD2	14:N:230:ILE:HD12	2.49	0.43
15:O:76:GLU:CB	15:O:266:PRO:HB3	2.49	0.43
16:P:169:HIS:H	16:P:184:LYS:CE	2.30	0.43
16:P:269:ASN:ND2	16:P:271:TYR:OH	2.51	0.43
17:Q:59:LEU:HD23	17:Q:59:LEU:HA	1.84	0.43
20:U:100:VAL:HA	20:U:141:PRO:HG2	2.00	0.43
23:X:36:CYS:SG	23:X:66:CYS:CB	3.05	0.43
24:Y:22:ARG:O	24:Y:26:ILE:HG13	2.19	0.43
25:Z:129:THR:HG22	25:Z:131:GLU:N	2.33	0.43
39:n:45:ARG:O	39:n:46:ALA:C	2.61	0.43
41:p:118:GLY:O	41:p:119:GLU:HB2	2.19	0.43
48:AD:156:ASP:HB3	48:AD:165:PHE:CZ	2.53	0.43
49:AE:161:GLU:HA	49:AE:178:HIS:HB3	2.00	0.43
49:AE:178:HIS:HA	49:AE:209:GLU:O	2.18	0.43
49:AI:72:VAL:HG22	46:Ab:109:LYS:HD2	2.00	0.43
45:Aa:61:SER:HB3	45:Aa:242:LEU:HD22	2.01	0.43
47:Ac:208:PRO:HB2	47:Ac:316:MET:HE3	2.01	0.43
49:Ae:166:ALA:HB2	49:Ae:175:PHE:HD1	1.84	0.43
50:Af:23:ASN:HA	50:Af:28:ASN:HD21	1.84	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43
4:D:52:MET:O	4:D:54:PRO:HD3	2.19	0.43
4:D:92:HIS:HD2	4:D:456:ILE:O	2.02	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
6:F:64:LYS:O	6:F:68:ILE:HG13	2.19	0.43
6:F:226:LYS:N	6:F:227:PRO:CD	2.82	0.43
7:G:381:LEU:HD23	19:S:55:ILE:CG1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:54:LYS:CG	8:H:55:LEU:N	2.78	0.43
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.43
8:H:224:PHE:HD2	61:H:401:UQ9:H20B	1.79	0.43
12:L:441:ILE:HG21	35:j:48:PRO:CD	2.42	0.43
12:L:493:ILE:O	12:L:496:LEU:HG	2.19	0.43
13:M:208:PRO:HG2	13:M:216:LEU:CD1	2.44	0.43
14:N:39:ALA:O	14:N:42:PRO:HD2	2.19	0.43
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.89	0.43
16:P:235:THR:O	16:P:273:LEU:N	2.52	0.43
16:P:283:MET:HE3	16:P:357:ARG:HH11	1.83	0.43
16:P:298:TYR:C	16:P:300:TRP:N	2.71	0.43
18:R:72:VAL:HG11	18:R:77:ILE:CG2	2.49	0.43
20:U:137:LYS:O	20:U:139:MET:N	2.50	0.43
25:Z:108:GLU:O	25:Z:109:SER:C	2.61	0.43
25:Z:110:VAL:CG1	30:e:72:THR:HA	2.49	0.43
27:b:15:LYS:O	27:b:15:LYS:HG3	2.18	0.43
27:b:45:ILE:HG23	27:b:46:ASN:N	2.34	0.43
38:m:49:LEU:HA	39:n:133:TRP:HH2	1.83	0.43
40:o:120:ALA:O	40:o:121:ARG:C	2.61	0.43
45:AA:273:SER:HB3	51:AG:18:SER:O	2.19	0.43
45:AA:276:ARG:HG2	45:AA:462:ILE:HD11	2.01	0.43
46:AB:230:LEU:O	46:AB:233:VAL:HG22	2.19	0.43
67:AC:402:HEM:CAA	68:AC:403:UQ6:C4	2.92	0.43
48:AD:214:LEU:O	48:AD:234:ASN:ND2	2.46	0.43
48:AD:234:ASN:O	48:AD:235:PRO:C	2.59	0.43
49:AE:161:GLU:HA	49:AE:178:HIS:CB	2.48	0.43
49:Ae:122:THR:CG2	53:Aj:25:ILE:HG21	2.49	0.43
50:Af:48:ILE:O	50:Af:51:LEU:HB2	2.19	0.43
54:Ak:15:ARG:NH1	54:Ak:15:ARG:HB2	2.34	0.43
1:A:61:THR:O	1:A:62:PHE:C	2.62	0.43
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.43
2:B:131:MET:HE1	2:B:149:TYR:HB2	2.00	0.43
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.43
4:D:104:GLU:CG	8:H:130:PHE:HZ	2.32	0.43
5:E:180:VAL:HG22	5:E:221:ARG:NH1	2.33	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:388:ASN:O	7:G:511:LYS:HE2	2.19	0.43
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.43
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
10:J:125:MET:HE3	10:J:128:VAL:CG2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:121:PRO:HB3	15:O:178:TYR:HE1	1.83	0.43
15:O:303:GLU:O	15:O:304:VAL:C	2.59	0.43
16:P:279:TYR:O	16:P:280:ILE:C	2.62	0.43
19:S:30:SER:HB3	19:S:63:PRO:HG3	2.00	0.43
20:T:87:LEU:HD11	20:T:141:PRO:HB3	2.01	0.43
20:U:91:ASP:OD2	36:k:48:ARG:NH2	2.51	0.43
28:c:72:ARG:HH11	29:d:19:ARG:HD3	1.83	0.43
31:f:25:TYR:CZ	31:f:29:LYS:HD3	2.54	0.43
33:h:129:PRO:HD2	33:h:130:GLU:OE1	2.18	0.43
45:AA:167:VAL:O	45:AA:170:ARG:HG2	2.19	0.43
46:AB:326:PHE:CD1	49:AI:11:PHE:CG	3.02	0.43
49:AE:235:TYR:CE1	49:AE:240:GLY:HA2	2.53	0.43
50:AF:35:ASP:OD2	50:AF:89:PHE:HA	2.19	0.43
45:Aa:470:ARG:HH12	47:Ac:20:ASP:CG	2.26	0.43
52:Ah:34:HIS:HB3	52:Ah:83:LYS:HZ3	1.84	0.43
52:Ah:81:ALA:O	52:Ah:82:HIS:C	2.60	0.43
4:D:318:VAL:HG21	43:r:104:TRP:CZ3	2.54	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
6:F:128:ARG:HD2	6:F:162:PHE:CE1	2.54	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
10:J:134:MET:O	10:J:139:ILE:HD13	2.19	0.42
11:K:22:PHE:HB2	12:L:585:LYS:HG2	2.00	0.42
11:K:50:ASN:C	11:K:50:ASN:OD1	2.62	0.42
12:L:601:LEU:HD13	14:N:156:MET:SD	2.59	0.42
13:M:100:ILE:O	13:M:103:GLN:HG2	2.19	0.42
13:M:214:LEU:C	13:M:217:PRO:HD2	2.44	0.42
13:M:367:LEU:C	13:M:367:LEU:HD12	2.44	0.42
14:N:193:ILE:HD11	14:N:269:GLU:CB	2.49	0.42
14:N:193:ILE:HD12	14:N:266:ILE:HA	2.01	0.42
14:N:219:LEU:HD23	14:N:230:ILE:HD12	2.01	0.42
14:N:316:HIS:HA	15:O:331:PHE:HZ	1.83	0.42
16:P:134:TRP:CD1	16:P:134:TRP:O	2.72	0.42
17:Q:99:MET:O	17:Q:99:MET:HG3	2.18	0.42
20:T:130:ILE:CG2	20:T:131:PRO:CD	2.95	0.42
20:U:142:GLN:O	20:U:143:GLU:C	2.60	0.42
21:V:37:HIS:O	21:V:38:PHE:C	2.62	0.42
23:X:10:LEU:H	23:X:10:LEU:HD12	1.84	0.42
62:Y:201:CDL:H151	62:Y:201:CDL:H381	2.00	0.42
27:b:42:ALA:HA	27:b:45:ILE:HG22	2.01	0.42
27:b:67:PRO:O	27:b:68:SER:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:38:ARG:HD3	31:f:56:TRP:CE2	2.54	0.42
33:h:59:PRO:O	33:h:61:LEU:HG	2.19	0.42
36:k:28:TRP:CE3	36:k:60:MET:HG2	2.54	0.42
39:n:81:ILE:HD12	39:n:87:GLY:C	2.44	0.42
40:o:46:MET:HE2	40:o:60:ALA:HB3	2.00	0.42
41:p:49:ARG:O	41:p:50:GLU:C	2.59	0.42
45:AA:49:GLN:O	45:AA:60:ALA:HA	2.18	0.42
45:AA:74:TRP:CE2	45:AA:414:GLY:HA3	2.54	0.42
46:AB:43:LEU:N	46:AB:47:LEU:O	2.52	0.42
49:AE:221:GLY:HA3	47:Ac:148:ASN:ND2	2.33	0.42
48:Ad:312:SER:O	48:Ad:313:VAL:C	2.59	0.42
49:Ae:161:GLU:HA	49:Ae:178:HIS:HB3	2.00	0.42
49:Ae:249:ILE:HG12	49:Ae:254:ALA:HB3	2.01	0.42
1:A:68:GLU:O	1:A:71:LEU:N	2.50	0.42
1:A:83:LYS:HE2	10:J:146:SER:HB3	1.92	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
6:F:272:GLY:O	6:F:292:MET:HB2	2.19	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
9:I:153:ILE:CD1	9:I:155:CYS:HB3	2.38	0.42
9:I:188:GLU:OE2	18:R:56:ASN:HB2	2.19	0.42
10:J:66:VAL:O	10:J:70:THR:N	2.42	0.42
12:L:5:THR:O	12:L:6:THR:C	2.62	0.42
12:L:141:PHE:CB	12:L:182:PHE:CE2	2.81	0.42
12:L:253:VAL:HG21	12:L:310:LEU:HD11	2.00	0.42
13:M:369:LEU:CD2	13:M:371:PRO:CD	2.84	0.42
15:O:73:LEU:HD22	15:O:207:ILE:HD11	2.02	0.42
15:O:114:LEU:O	15:O:117:PHE:HB3	2.19	0.42
15:O:117:PHE:HD1	15:O:128:SER:CA	2.31	0.42
15:O:146:ALA:CB	15:O:159:LEU:HD21	2.49	0.42
15:O:209:VAL:HG23	15:O:214:VAL:CG1	2.49	0.42
15:O:297:LEU:C	15:O:297:LEU:HD23	2.43	0.42
16:P:313:TRP:CE3	16:P:314:THR:HB	2.54	0.42
16:P:354:ARG:HG3	16:P:362:LEU:CD2	2.48	0.42
18:R:72:VAL:HG11	18:R:77:ILE:HG22	2.01	0.42
19:S:16:LEU:HD13	19:S:19:ILE:HD11	2.02	0.42
21:V:8:THR:HG22	21:V:9:THR:N	2.34	0.42
22:W:65:LYS:O	22:W:69:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:8:PRO:CG	23:X:54:ARG:HG2	2.49	0.42
23:X:47:ARG:NH1	23:X:51:LYS:O	2.52	0.42
24:Y:68:ILE:HG22	24:Y:102:THR:OG1	2.19	0.42
25:Z:74:LEU:O	25:Z:78:GLU:HG3	2.20	0.42
25:Z:93:GLU:OE1	30:e:95:PRO:HG3	2.19	0.42
26:a:28:LYS:HE3	26:a:35:GLU:HG2	2.01	0.42
28:c:40:ASN:HB3	28:c:43:ALA:HB3	2.00	0.42
30:e:49:GLY:O	30:e:50:THR:C	2.61	0.42
32:g:117:ARG:NH2	41:p:10:TYR:OH	2.52	0.42
32:g:148:PRO:O	41:p:167:ARG:NH2	2.52	0.42
33:h:89:VAL:HG11	33:h:117:ILE:HG12	2.01	0.42
35:j:98:GLY:HA3	40:o:104:ARG:NH1	2.33	0.42
40:o:57:ASP:OD2	40:o:59:CYS:HB2	2.19	0.42
41:p:43:TRP:NE1	41:p:47:LEU:HD11	2.33	0.42
42:q:85:GLU:CG	42:q:98:PRO:HB3	2.39	0.42
45:AA:49:GLN:HB2	45:AA:239:HIS:CG	2.54	0.42
46:AB:49:ILE:HD11	46:AB:234:ALA:HB2	2.01	0.42
46:AB:286:PHE:CD1	46:AB:427:ALA:HB1	2.54	0.42
47:AC:37:LEU:HD13	67:AC:402:HEM:C2B	2.54	0.42
47:AC:148:ASN:OD1	49:Ae:221:GLY:HA3	2.18	0.42
48:AD:248:ILE:HD12	48:AD:266:VAL:HG11	2.00	0.42
48:AD:252:VAL:HG13	48:AD:253:LEU:N	2.34	0.42
49:AI:72:VAL:CG2	46:Ab:109:LYS:HD2	2.49	0.42
47:Ac:169:SER:O	47:Ac:170:VAL:C	2.62	0.42
47:Ac:219:PRO:HA	51:Ag:5:PHE:CZ	2.54	0.42
48:Ad:240:GLN:CD	52:Ah:70:PHE:HZ	2.27	0.42
54:Ak:48:ILE:C	54:Ak:50:GLY:H	2.27	0.42
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.33	0.42
3:C:236:SER:OG	7:G:145:MET:HE1	2.19	0.42
5:E:109:MET:HE1	7:G:198:THR:CG2	2.50	0.42
6:F:120:GLY:O	6:F:121:GLU:C	2.61	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.49	0.42
8:H:293:PHE:O	8:H:296:LEU:N	2.52	0.42
11:K:3:SER:O	11:K:4:THR:C	2.61	0.42
12:L:13:ILE:HD11	58:i:201:3PE:C2B	2.49	0.42
12:L:60:GLU:N	12:L:60:GLU:OE2	2.53	0.42
12:L:246:LEU:CD1	12:L:247:LEU:N	2.68	0.42
12:L:264:HIS:HA	12:L:267:THR:HG23	2.02	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	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:526:LEU:HD12	12:L:526:LEU:N	2.34	0.42
12:L:591:PHE:O	12:L:595:ILE:HG13	2.19	0.42
13:M:68:LEU:HD23	13:M:234:ILE:CD1	2.49	0.42
14:N:80:GLN:O	14:N:81:LEU:HG	2.19	0.42
14:N:170:LEU:HD12	14:N:292:PHE:CD2	2.54	0.42
15:O:211:VAL:O	15:O:214:VAL:HG22	2.19	0.42
16:P:241:TYR:HD2	16:P:243:ALA:HB3	1.84	0.42
18:R:31:ILE:HG22	18:R:55:VAL:HG21	2.02	0.42
19:S:75:LYS:HE2	19:S:75:LYS:HA	2.01	0.42
20:T:87:LEU:CD2	20:T:104:PHE:HZ	2.12	0.42
23:X:75:LYS:O	23:X:79:ALA:HB2	2.19	0.42
24:Y:8:PHE:CD1	24:Y:30:LEU:HD21	2.53	0.42
24:Y:87:ASP:HA	24:Y:128:LYS:NZ	2.34	0.42
26:a:55:SER:O	26:a:56:GLY:C	2.61	0.42
30:e:44:ALA:HA	30:e:47:ILE:CG1	2.49	0.42
30:e:69:ARG:O	30:e:73:MET:HG3	2.19	0.42
34:i:22:TRP:O	34:i:26:GLN:HG2	2.19	0.42
46:AB:130:ILE:HA	46:AB:133:LEU:HB2	2.01	0.42
46:AB:162:LYS:HG3	46:AB:191:TYR:HB3	2.00	0.42
47:AC:153:ILE:HB	47:AC:157:GLY:N	2.34	0.42
68:AC:403:UQ6:H72	68:AC:403:UQ6:H111	1.68	0.42
52:AH:31:VAL:HG12	52:AH:80:VAL:HG22	2.01	0.42
45:Aa:79:SER:O	45:Aa:199:GLN:NE2	2.53	0.42
46:Ab:47:LEU:HD12	46:Ab:218:MET:O	2.19	0.42
46:Ab:396:ILE:HG12	46:Ab:406:TYR:HE1	1.85	0.42
68:Ac:406:UQ6:H72	68:Ac:406:UQ6:H112	1.72	0.42
48:Ad:154:VAL:O	48:Ad:167:ARG:HG3	2.19	0.42
48:Ad:252:VAL:HG13	48:Ad:253:LEU:N	2.34	0.42
49:Ae:112:GLY:O	49:Ae:116:LEU:HB2	2.19	0.42
50:Af:15:ASP:O	50:Af:19:LYS:HG3	2.19	0.42
50:Af:29:LYS:HA	50:Af:81:TRP:CD2	2.53	0.42
1:A:106:TRP:N	1:A:106:TRP:CD1	2.85	0.42
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.43	0.42
2:B:154:GLU:CB	8:H:59:GLU:HB2	2.49	0.42
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.83	0.42
4:D:379:ILE:HG23	7:G:140:GLN:HB2	2.01	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.20	0.42
6:F:65:THR:HA	6:F:68:ILE:HD12	2.01	0.42
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:MET:O	9:I:54:THR:HG23	2.19	0.42
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
11:K:32:CYS:O	11:K:33:LEU:C	2.60	0.42
12:L:220:ALA:HB2	12:L:260:LEU:CD1	2.49	0.42
12:L:357:ARG:NH2	39:n:78:GLN:O	2.53	0.42
12:L:489:THR:HG23	12:L:490:ALA:N	2.34	0.42
13:M:14:LEU:HD21	13:M:26:ASN:CB	2.50	0.42
13:M:72:LEU:HD12	13:M:234:ILE:HG12	2.01	0.42
13:M:200:MET:CE	13:M:247:SER:HB2	2.46	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	2.01	0.42
14:N:80:GLN:O	14:N:80:GLN:HG2	2.19	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	2.19	0.42
14:N:342:GLN:H	14:N:342:GLN:CD	2.27	0.42
15:O:170:LEU:HD21	15:O:184:VAL:HG13	2.00	0.42
16:P:223:PHE:O	16:P:224:LEU:C	2.62	0.42
16:P:300:TRP:NE1	16:P:304:LEU:HD21	2.35	0.42
21:V:35:LEU:HA	21:V:38:PHE:CE1	2.54	0.42
22:W:61:GLN:O	22:W:64:ASP:HB2	2.19	0.42
24:Y:143:VAL:HG21	33:h:169:TYR:CZ	2.54	0.42
33:h:87:THR:HG22	62:h:201:CDL:C51	2.49	0.42
34:i:81:PHE:O	34:i:82:VAL:C	2.60	0.42
58:i:201:3PE:H2B2	58:i:201:3PE:H281	1.88	0.42
37:l:57:MET:HG2	37:l:104:PRO:CG	2.49	0.42
41:p:6:ASP:C	41:p:8:ASP:H	2.27	0.42
41:p:73:ASP:O	41:p:74:ILE:C	2.59	0.42
45:AA:118:ALA:O	46:AB:298:HIS:HB3	2.19	0.42
46:AB:171:THR:HA	49:AI:14:VAL:CG1	2.48	0.42
47:AC:208:PRO:HB2	47:AC:316:MET:HE3	2.01	0.42
47:AC:278:TYR:CE2	47:AC:282:ARG:HD2	2.54	0.42
48:AD:142:GLU:O	48:AD:145:ALA:HB3	2.19	0.42
49:AE:122:THR:CG2	53:AJ:25:ILE:HG21	2.49	0.42
51:AG:19:LEU:HG	51:AG:20:SER:N	2.33	0.42
52:AH:36:GLU:HG2	52:AH:72:PHE:HZ	1.83	0.42
52:AH:67:GLU:HG3	52:AH:68:GLU:CD	2.43	0.42
45:Aa:269:ARG:HD2	49:Ae:92:ARG:HH22	1.84	0.42
46:Ab:215:SER:N	46:Ab:241:ARG:O	2.52	0.42
46:Ab:225:VAL:HG22	46:Ab:229:VAL:HG21	2.01	0.42
46:Ab:332:ASP:OD1	46:Ab:332:ASP:N	2.52	0.42
47:Ac:181:PHE:HA	47:Ac:184:ILE:HG22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ae:173:PRO:HG2	49:Ae:223:VAL:CG2	2.45	0.42
49:Ae:225:ILE:HD11	49:Ae:237:PRO:HG3	2.00	0.42
52:Ah:35:CYS:O	52:Ah:38:LEU:HB2	2.19	0.42
52:Ah:51:CYS:O	52:Ah:55:VAL:N	2.40	0.42
4:D:36:GLN:HG3	4:D:38:GLN:HE21	1.83	0.42
4:D:90:ALA:O	4:D:91:ALA:C	2.61	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
5:E:84:LEU:HD12	44:s:46:LEU:CD1	2.49	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:233:LEU:HB2	6:F:48:ARG:HH12	1.84	0.42
6:F:226:LYS:HA	6:F:226:LYS:HD3	1.86	0.42
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
9:I:93:LEU:O	42:q:93:MET:CG	2.65	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
11:K:36:MET:O	11:K:39:SER:N	2.52	0.42
12:L:224:SER:HB3	12:L:226:GLN:HE21	1.84	0.42
12:L:277:MET:CG	12:L:318:GLY:CA	2.97	0.42
12:L:519:TYR:O	12:L:520:SER:C	2.60	0.42
13:M:77:LEU:O	13:M:81:GLN:HG3	2.19	0.42
13:M:293:HIS:O	13:M:294:MET:HE2	2.20	0.42
13:M:446:LEU:CD1	32:g:97:LEU:HD12	2.50	0.42
14:N:241:LEU:HG	14:N:301:SER:OG	2.19	0.42
15:O:310:ILE:HG23	15:O:312:VAL:HG23	2.02	0.42
16:P:247:LYS:NZ	16:P:340:VAL:HG23	2.35	0.42
18:R:45:ARG:HA	18:R:48:PHE:HE1	1.83	0.42
20:T:80:LYS:O	20:T:84:LEU:HG	2.20	0.42
23:X:20:VAL:O	26:a:54:ILE:CD1	2.67	0.42
24:Y:83:ARG:NH1	24:Y:90:LEU:HB3	2.34	0.42
35:j:44:TYR:CE2	35:j:45:ARG:HG3	2.54	0.42
37:l:62:TYR:CE2	37:l:64:PRO:HG3	2.55	0.42
45:AA:402:HIS:CG	45:AA:426:LEU:HD21	2.54	0.42
46:AB:39:GLU:HB2	46:AB:227:HIS:ND1	2.35	0.42
46:AB:177:LEU:HD21	46:AB:272:VAL:CG1	2.49	0.42
47:AC:33:PHE:O	47:AC:36:LEU:HB2	2.19	0.42
48:AD:107:HIS:ND1	48:AD:138:VAL:HB	2.35	0.42
52:AH:35:CYS:SG	52:AH:83:LYS:HD2	2.60	0.42
62:Aa:501:CDL:H321	47:Ac:19:ILE:HG12	2.01	0.42
47:Ac:133:LEU:HD23	47:Ac:133:LEU:HA	1.85	0.42
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:258:VAL:O	4:D:259:GLU:C	2.61	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
5:E:180:VAL:HG11	5:E:224:CYS:HB2	2.02	0.42
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.54	0.42
6:F:295:PRO:O	6:F:296:LEU:C	2.60	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.42
12:L:70:THR:HG21	41:p:101:GLU:OE2	2.20	0.42
12:L:309:GLN:CG	12:L:336:LYS:HZ1	2.32	0.42
12:L:335:PHE:O	12:L:339:LEU:HD13	2.19	0.42
12:L:365:ILE:CD1	12:L:366:MET:HG3	2.24	0.42
12:L:405:ASN:HB2	12:L:408:ALA:HB3	2.01	0.42
12:L:594:ASN:CG	14:N:110:PRO:CG	2.92	0.42
13:M:206:LYS:HA	13:M:215:TRP:CZ2	2.54	0.42
13:M:347:GLY:O	13:M:348:LEU:C	2.63	0.42
15:O:229:VAL:HG21	15:O:234:LEU:HD21	2.02	0.42
17:Q:58:LYS:O	17:Q:58:LYS:HG3	2.20	0.42
19:S:19:ILE:O	19:S:53:ILE:HD12	2.20	0.42
22:W:58:THR:O	22:W:61:GLN:HB3	2.20	0.42
23:X:50:GLU:OE2	23:X:135:ARG:NH1	2.53	0.42
24:Y:45:LEU:O	24:Y:46:ASN:C	2.62	0.42
24:Y:76:THR:CG2	24:Y:92:TYR:HA	2.48	0.42
26:a:49:GLU:OE2	26:a:49:GLU:HA	2.20	0.42
28:c:69:TYR:O	28:c:73:ASN:ND2	2.52	0.42
31:f:10:HIS:HB3	31:f:13:HIS:CD2	2.54	0.42
39:n:18:ARG:O	39:n:22:ARG:HD3	2.19	0.42
41:p:36:ALA:O	41:p:37:TYR:C	2.60	0.42
45:AA:278:ARG:CZ	45:AA:463:GLU:HB2	2.50	0.42
46:AB:51:SER:CB	46:AB:227:HIS:HA	2.49	0.42
48:AD:152:VAL:O	48:AD:168:PRO:HA	2.20	0.42
49:AE:205:VAL:CG1	49:AE:211:VAL:HG23	2.49	0.42
45:Aa:167:VAL:O	45:Aa:170:ARG:HG2	2.19	0.42
45:Aa:204:PRO:HB3	49:Ae:84:LYS:NZ	2.35	0.42
45:Aa:463:GLU:OE1	51:Ag:8:LEU:HB2	2.20	0.42
46:Ab:177:LEU:HD21	46:Ab:272:VAL:CG1	2.49	0.42
48:Ad:262:THR:O	48:Ad:263:MET:C	2.61	0.42
53:Aj:21:PHE:O	53:Aj:24:THR:HG22	2.20	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.67	0.42
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.42
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:128:LYS:HB3	5:E:167:LEU:CA	2.45	0.42
6:F:81:LYS:HE2	6:F:97:LEU:CD2	2.47	0.42
6:F:110:PRO:O	6:F:238:CYS:HB3	2.20	0.42
6:F:153:ALA:HB1	6:F:194:ASP:O	2.19	0.42
6:F:166:ALA:O	6:F:167:SER:C	2.63	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:287:HIS:O	8:H:291:LYS:N	2.51	0.42
10:J:18:GLY:O	10:J:23:PRO:HD3	2.19	0.42
10:J:168:GLU:OE1	14:N:5:THR:HG21	2.20	0.42
11:K:59:ILE:HB	11:K:60:PRO:HD3	2.01	0.42
12:L:81:LYS:HD3	12:L:262:ARG:HH11	1.83	0.42
12:L:136:ASN:ND2	62:h:201:CDL:H273	2.29	0.42
12:L:396:ILE:HD13	12:L:396:ILE:HA	1.89	0.42
12:L:466:PHE:HZ	35:j:72:ARG:HH22	1.62	0.42
13:M:17:LEU:CD2	62:M:503:CDL:H522	2.46	0.42
13:M:118:PHE:HE2	13:M:203:PHE:CE1	2.37	0.42
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.02	0.42
13:M:344:MET:CE	38:m:59:HIS:NE2	2.83	0.42
13:M:430:HIS:HB3	32:g:73:GLY:HA3	2.02	0.42
14:N:154:ILE:HD11	14:N:155:LEU:HG	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
15:O:323:GLN:HE21	32:g:55:GLU:CA	2.33	0.42
16:P:216:HIS:CD2	16:P:318:LYS:HE3	2.54	0.42
17:Q:75:ARG:NH1	17:Q:104:ARG:HG2	2.34	0.42
17:Q:111:LEU:HD11	42:q:126:PRO:HG2	2.01	0.42
19:S:64:LYS:HE2	19:S:66:TRP:CZ2	2.55	0.42
20:T:90:TYR:CD2	20:T:92:LYS:HB3	2.54	0.42
20:U:91:ASP:OD2	36:k:48:ARG:NH1	2.53	0.42
22:W:120:ASP:OD1	22:W:120:ASP:C	2.61	0.42
33:h:178:PHE:O	33:h:179:ILE:C	2.63	0.42
37:l:167:TYR:CG	37:l:178:PRO:HG3	2.55	0.42
41:p:6:ASP:O	41:p:7:LYS:C	2.63	0.42
45:AA:80:ARG:NH2	45:AA:268:CYS:HB3	2.34	0.42
45:AA:337:LEU:HB3	45:AA:368:MET:SD	2.59	0.42
47:AC:116:GLY:HA3	67:AC:402:HEM:C2C	2.54	0.42
47:AC:285:PRO:O	49:Ae:253:PRO:CB	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:112:GLY:O	49:AE:116:LEU:HB2	2.19	0.42
49:AE:115:TYR:HB3	53:AJ:21:PHE:HE1	1.84	0.42
53:AJ:19:SER:HA	54:AK:24:TRP:CH2	2.55	0.42
45:Aa:74:TRP:HH2	45:Aa:410:CYS:SG	2.42	0.42
48:Ad:102:LEU:O	53:AJ:48:ASN:ND2	2.45	0.42
48:Ad:104:SER:HB3	53:AJ:48:ASN:ND2	2.35	0.42
48:Ad:156:ASP:HB3	48:Ad:165:PHE:CZ	2.53	0.42
48:Ad:201:VAL:HG22	48:Ad:278:SER:HB2	2.00	0.42
49:Ae:93:ARG:O	49:Ae:94:ALA:C	2.62	0.42
49:Ae:178:HIS:CD2	49:Ae:179:ARG:N	2.88	0.42
49:Ae:195:LEU:CD1	49:Ae:248:ARG:HD2	2.50	0.42
1:A:55:PHE:CZ	8:H:282:TYR:CE2	2.85	0.42
1:A:56:PHE:HA	10:J:69:TYR:HE2	1.82	0.42
1:A:98:LEU:HD13	1:A:98:LEU:HA	1.90	0.42
1:A:104:TYR:HA	1:A:107:THR:OG1	2.20	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
5:E:179:CYS:SG	6:F:123:GLY:CA	3.08	0.42
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.42
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.42
10:J:124:LEU:CD2	10:J:125:MET:H	2.26	0.42
12:L:21:ILE:HG23	12:L:27:ILE:CG2	2.50	0.42
12:L:49:LEU:HD12	41:p:33:LEU:HD23	2.02	0.42
12:L:51:LEU:HA	12:L:87:ILE:HD12	2.02	0.42
12:L:189:PHE:CZ	12:L:212:PRO:HB2	2.55	0.42
12:L:346:ILE:HG21	12:L:362:ILE:HD11	2.02	0.42
58:L:702:3PE:H3A1	58:L:702:3PE:H372	1.87	0.42
13:M:123:GLU:OE2	13:M:154:LEU:HD21	2.20	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:315:THR:O	14:N:316:HIS:C	2.61	0.42
14:N:340:ALA:N	14:N:341:PRO:CD	2.83	0.42
15:O:48:LYS:O	15:O:52:LYS:HE3	2.20	0.42
15:O:272:ASP:HA	15:O:275:TYR:HD2	1.85	0.42
16:P:207:PHE:HB3	16:P:213:PHE:HD2	1.85	0.42
18:R:54:GLU:HB2	42:q:124:TYR:HD1	1.84	0.42
28:c:70:LYS:HB3	28:c:75:LEU:HD12	2.01	0.42
31:f:22:PHE:CE2	31:f:26:LEU:HD11	2.55	0.42
31:f:25:TYR:HA	31:f:28:ARG:HH11	1.84	0.42
33:h:159:LEU:CB	33:h:163:ARG:HH12	2.25	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:109:LEU:HG	37:l:109:LEU:O	2.20	0.42
39:n:85:SER:O	39:n:86:PRO:C	2.61	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
46:AB:407:MET:HE1	46:AB:415:GLN:CD	2.45	0.42
48:AD:199:TYR:HA	48:AD:278:SER:OG	2.20	0.42
49:AE:196:ARG:HD2	49:AE:249:ILE:HG23	2.01	0.42
53:AJ:19:SER:HA	54:AK:24:TRP:CZ2	2.55	0.42
49:Ae:205:VAL:CG1	49:Ae:211:VAL:HG23	2.49	0.42
50:Af:83:LYS:HB3	50:Af:85:GLU:OE2	2.20	0.42
54:Ak:38:TRP:O	54:Ak:42:LEU:HG	2.19	0.42
54:Ak:45:VAL:O	54:Ak:49:ASN:N	2.49	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.42
2:B:124:SER:HB2	2:B:127:GLN:OE1	2.20	0.42
4:D:37:TRP:O	4:D:37:TRP:CE3	2.73	0.42
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:53:LEU:O	6:F:57:LEU:HG	2.20	0.42
6:F:113:LEU:HB3	6:F:154:ALA:CB	2.49	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
8:H:19:PHE:CB	26:a:12:MET:HG3	2.49	0.42
8:H:25:ARG:NH1	61:H:401:UQ9:H15	2.34	0.42
8:H:203:GLY:O	8:H:205:SER:N	2.49	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
9:I:80:GLU:CG	26:a:1:MET:SD	2.98	0.42
12:L:141:PHE:CD2	13:M:375:LEU:HD21	2.48	0.42
12:L:385:PHE:HE2	35:j:73:PHE:CD1	2.32	0.42
12:L:477:ILE:HG22	40:o:54:GLN:NE2	2.34	0.42
12:L:571:THR:O	12:L:574:THR:HG22	2.19	0.42
13:M:191:SER:O	13:M:194:LEU:HB2	2.20	0.42
14:N:108:LEU:HD22	14:N:191:LEU:HD22	2.02	0.42
17:Q:167:ASN:C	17:Q:168:LYS:CG	2.93	0.42
19:S:16:LEU:CB	19:S:69:TYR:CD1	2.97	0.42
22:W:117:ARG:HA	22:W:118:PRO:HD3	1.95	0.42
23:X:26:LYS:HD3	23:X:95:GLN:OE1	2.19	0.42
24:Y:41:TYR:CZ	62:Y:201:CDL:H772	2.55	0.42
27:b:31:ILE:HG23	27:b:32:MET:N	2.34	0.42
27:b:41:TYR:CD1	27:b:80:TRP:CZ3	3.08	0.42
29:d:87:ASP:HB3	29:d:91:PHE:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:42:MET:HB2	41:p:87:GLU:OE1	2.19	0.42
35:j:51:THR:O	35:j:52:ARG:C	2.61	0.42
35:j:96:GLU:HG2	35:j:97:LEU:HD23	2.01	0.42
37:l:48:ARG:NE	37:l:64:PRO:HD2	2.35	0.42
37:l:59:VAL:O	37:l:59:VAL:HG12	2.19	0.42
39:n:100:PRO:HB2	39:n:102:TRP:NE1	2.35	0.42
40:o:5:LEU:H	40:o:5:LEU:HD12	1.84	0.42
43:r:18:GLN:OE1	43:r:18:GLN:N	2.53	0.42
45:AA:136:LEU:HD21	46:AB:380:ALA:HA	2.01	0.42
46:AB:293:LEU:HD23	46:AB:308:LEU:HD12	2.02	0.42
46:AB:299:ILE:O	46:AB:300:LYS:C	2.61	0.42
48:AD:210:TYR:O	48:AD:211:VAL:C	2.63	0.42
45:Aa:46:PRO:HB3	45:Aa:63:GLN:O	2.20	0.42
45:Aa:178:SER:OG	45:Aa:181:ASN:ND2	2.53	0.42
45:Aa:278:ARG:CZ	51:Ag:11:ILE:HB	2.50	0.42
46:Ab:162:LYS:HG3	46:Ab:191:TYR:HB3	2.00	0.42
46:Ab:304:ASN:C	46:Ab:306:THR:H	2.27	0.42
48:Ad:210:TYR:O	48:Ad:211:VAL:C	2.62	0.42
49:Ae:122:THR:O	49:Ae:123:VAL:C	2.61	0.42
49:Ae:156:LEU:H	49:Ae:270:VAL:HA	1.84	0.42
49:Ae:160:PRO:C	49:Ae:178:HIS:HB3	2.45	0.42
52:Ah:31:VAL:HG22	52:Ah:87:ASN:ND2	2.35	0.42
52:Ah:83:LYS:HE3	52:Ah:83:LYS:HB2	1.73	0.42
3:C:121:ARG:NH2	21:V:114:TRP:HA	2.35	0.42
5:E:230:LEU:HD13	5:E:232:SER:O	2.19	0.42
6:F:38:GLU:HG3	6:F:39:ASP:OD1	2.20	0.42
6:F:315:LEU:HD23	6:F:315:LEU:O	2.20	0.42
7:G:365:ASN:HB3	7:G:537:ILE:HD11	2.02	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.42
10:J:3:ASN:O	10:J:7:VAL:HG23	2.19	0.42
10:J:28:GLY:C	11:K:31:LEU:HD21	2.44	0.42
10:J:51:LEU:HD12	10:J:51:LEU:N	2.31	0.42
12:L:117:PHE:HZ	12:L:242:PRO:HG2	1.85	0.42
58:L:702:3PE:H222	58:L:702:3PE:H2	1.94	0.42
13:M:127:ILE:CD1	14:N:256:PRO:HG2	2.44	0.42
20:T:87:LEU:CD2	20:T:122:MET:CE	2.98	0.42
20:U:89:LEU:HA	36:k:53:ARG:HH22	1.85	0.42
20:U:93:ILE:CD1	20:U:110:LEU:HD11	2.49	0.42
27:b:32:MET:N	27:b:33:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:87:ASP:HB3	29:d:91:PHE:CD2	2.55	0.42
31:f:38:ARG:NH1	31:f:54:VAL:HB	2.35	0.42
40:o:59:CYS:SG	40:o:91:GLU:HG2	2.60	0.42
49:AE:160:PRO:C	49:AE:178:HIS:HB3	2.45	0.42
45:Aa:204:PRO:O	45:Aa:205:SER:C	2.63	0.42
45:Aa:340:SER:O	45:Aa:358:PHE:HA	2.20	0.42
46:Ab:346:ALA:O	46:Ab:347:ALA:C	2.62	0.42
47:Ac:278:TYR:CE2	47:Ac:282:ARG:HD2	2.54	0.42
48:Ad:324:PRO:O	48:Ad:325:LYS:C	2.63	0.42
49:Ae:123:VAL:HG13	53:Aj:29:ALA:CA	2.41	0.42
52:Ah:51:CYS:O	52:Ah:54:ARG:HB3	2.20	0.42
1:A:49:LEU:HA	1:A:50:PRO:HD3	1.92	0.41
1:A:94:LEU:O	1:A:97:ILE:HG12	2.19	0.41
2:B:84:TRP:HA	2:B:87:ARG:HG2	2.02	0.41
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.48	0.41
3:C:75:VAL:HG13	3:C:83:LEU:HD11	2.02	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:345:GLU:HB2	25:Z:19:ILE:HD12	2.02	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.34	0.41
5:E:47:ASN:CG	5:E:49:ASP:HB3	2.45	0.41
6:F:115:VAL:HG22	6:F:248:VAL:HG21	2.02	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.41
11:K:90:VAL:O	11:K:91:GLN:C	2.62	0.41
11:K:93:LEU:HA	14:N:54:GLU:OE2	2.20	0.41
12:L:224:SER:CB	12:L:226:GLN:HE21	2.33	0.41
12:L:293:LEU:O	12:L:425:ARG:HD2	2.20	0.41
12:L:407:TRP:CE3	12:L:410:LEU:HD21	2.54	0.41
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.02	0.41
13:M:177:MET:HE2	33:h:140:LEU:HD21	2.02	0.41
14:N:108:LEU:CD2	14:N:191:LEU:HD22	2.50	0.41
14:N:180:ALA:O	14:N:184:ILE:HG13	2.20	0.41
14:N:285:MET:HE1	14:N:288:LEU:HD22	2.02	0.41
15:O:261:TRP:H	15:O:261:TRP:HE3	1.68	0.41
16:P:284:THR:HG22	16:P:286:ARG:HG3	2.02	0.41
18:R:60:ALA:O	18:R:61:ILE:C	2.63	0.41
20:T:93:ILE:HD11	20:T:118:ILE:HD11	2.00	0.41
20:T:134:ASP:HA	20:T:137:LYS:NZ	2.35	0.41
20:U:131:PRO:O	20:U:135:ALA:N	2.52	0.41
22:W:101:LYS:HB3	22:W:101:LYS:NZ	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:31:ILE:O	27:b:32:MET:C	2.63	0.41
32:g:106:TYR:CE2	33:h:86:ILE:CD1	3.00	0.41
33:h:55:PHE:HE1	33:h:57:VAL:HA	1.85	0.41
37:l:101:TRP:HE1	38:m:62:ASP:CA	2.32	0.41
38:m:8:PRO:HD3	38:m:14:LEU:HD13	2.02	0.41
38:m:15:PRO:HG2	38:m:18:LEU:HB2	2.01	0.41
40:o:42:THR:O	40:o:43:GLN:C	2.61	0.41
40:o:104:ARG:O	40:o:108:LEU:HG	2.20	0.41
42:q:74:PHE:HE2	42:q:75:TRP:HE1	1.68	0.41
49:AE:159:ILE:HG23	49:AE:163:LYS:HB3	2.02	0.41
52:AH:58:ARG:HD3	52:AH:61:THR:HB	2.02	0.41
49:AI:61:ALA:O	46:Ab:326:PHE:HA	2.20	0.41
45:Aa:338:CYS:SG	45:Aa:359:VAL:O	2.79	0.41
47:Ac:33:PHE:O	47:Ac:36:LEU:HB2	2.19	0.41
47:Ac:284:ILE:HG21	47:Ac:289:GLY:HA3	2.02	0.41
48:Ad:138:VAL:C	48:Ad:140:TYR:N	2.78	0.41
54:Ak:38:TRP:CD1	54:Ak:41:ILE:HD12	2.55	0.41
2:B:194:CYS:O	55:B:301:SF4:S2	2.78	0.41
5:E:213:PRO:O	5:E:215:PRO:HD3	2.20	0.41
6:F:170:GLN:HG2	44:s:52:LEU:HD11	2.02	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.41
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.41
8:H:110:SER:O	8:H:113:VAL:HG12	2.19	0.41
9:I:54:THR:HA	27:b:13:TRP:NE1	2.35	0.41
10:J:19:LEU:HD21	11:K:32:CYS:HA	2.03	0.41
12:L:534:HIS:O	12:L:538:PRO:CG	2.60	0.41
12:L:546:LEU:HD23	37:l:108:ASP:OD1	2.19	0.41
14:N:215:MET:SD	14:N:244:ILE:CD1	3.08	0.41
14:N:218:ALA:CB	14:N:240:MET:SD	3.08	0.41
15:O:143:TYR:HD1	15:O:159:LEU:HD22	1.84	0.41
15:O:179:ILE:CD1	15:O:184:VAL:HG22	2.50	0.41
15:O:195:LEU:N	15:O:196:PRO:HD2	2.35	0.41
15:O:231:SER:O	15:O:232:ALA:C	2.62	0.41
15:O:267:THR:O	15:O:271:GLU:HG3	2.19	0.41
16:P:208:GLY:O	16:P:211:ASP:N	2.53	0.41
18:R:55:VAL:HG22	18:R:56:ASN:N	2.35	0.41
20:T:115:GLN:O	20:T:116:VAL:C	2.63	0.41
22:W:53:MET:SD	22:W:106:VAL:HG21	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:148:PRO:HG3	30:e:47:ILE:HD13	2.02	0.41
24:Y:10:SER:O	24:Y:11:TYR:C	2.62	0.41
25:Z:102:PRO:O	25:Z:103:ASN:C	2.62	0.41
26:a:17:VAL:O	26:a:18:ILE:C	2.62	0.41
27:b:35:ILE:O	27:b:35:ILE:CG1	2.67	0.41
29:d:24:PRO:HD2	29:d:73:TYR:CE2	2.55	0.41
29:d:119:VAL:O	29:d:120:ARG:C	2.62	0.41
35:j:100:PRO:HD3	40:o:108:LEU:CD2	2.50	0.41
39:n:114:MET:HG3	39:n:115:TYR:CD2	2.55	0.41
39:n:133:TRP:C	39:n:136:GLU:HG2	2.45	0.41
40:o:28:ASP:OD1	40:o:28:ASP:N	2.53	0.41
40:o:53:LEU:HD23	40:o:56:ARG:NE	2.34	0.41
45:AA:148:ALA:O	45:AA:152:GLN:HG2	2.20	0.41
46:AB:272:VAL:HA	46:AB:337:GLY:HA3	2.02	0.41
47:AC:21:LEU:CD2	68:AC:403:UQ6:C3M	2.78	0.41
48:AD:323:PRO:HB2	48:AD:325:LYS:HG3	2.02	0.41
49:AE:152:ILE:HG21	49:AE:273:VAL:O	2.19	0.41
49:AE:152:ILE:CG2	49:AE:272:VAL:HG13	2.50	0.41
49:AE:225:ILE:CD1	49:AE:237:PRO:HG3	2.50	0.41
50:AF:52:PRO:HD3	46:Ab:148:ARG:NH2	2.36	0.41
51:AG:29:SER:CB	51:AG:32:SER:HB2	2.38	0.41
58:Ac:404:3PE:H2F1	58:Ac:404:3PE:H2C2	1.66	0.41
48:Ad:317:ARG:HD2	48:Ad:319:LEU:HD21	2.02	0.41
49:Ae:115:TYR:HB3	53:Aj:21:PHE:HE1	1.85	0.41
50:Af:78:LYS:HA	50:Af:81:TRP:CG	2.56	0.41
2:B:93:MET:HG2	4:D:87:GLN:NE2	2.35	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
6:F:76:ILE:O	6:F:79:GLU:HB2	2.20	0.41
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:253:VAL:O	7:G:253:VAL:CG1	2.68	0.41
8:H:96:ILE:HG23	25:Z:143:TYR:CE1	2.54	0.41
8:H:123:SER:O	8:H:124:ASN:HB2	2.21	0.41
10:J:36:GLY:C	10:J:60:LEU:HD11	2.45	0.41
10:J:136:GLU:H	10:J:139:ILE:HD12	1.85	0.41
12:L:25:ASN:HB2	33:h:72:LYS:HZ1	1.85	0.41
12:L:355:ASP:O	12:L:359:MET:HG3	2.21	0.41
12:L:489:THR:O	12:L:492:ILE:HG13	2.20	0.41
58:L:702:3PE:H362	58:L:702:3PE:H331	1.74	0.41
13:M:85:LYS:O	13:M:85:LYS:HG2	2.21	0.41
13:M:255:LYS:NZ	29:d:117:HIS:HB3	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:258:ALA:O	13:M:259:TYR:C	2.62	0.41
14:N:233:LEU:CD2	14:N:241:LEU:HD12	2.26	0.41
15:O:117:PHE:CE1	15:O:128:SER:CB	2.96	0.41
20:U:119:ILE:HD13	20:U:119:ILE:HA	1.81	0.41
20:U:128:PHE:HZ	20:U:148:ILE:CD1	2.33	0.41
23:X:44:MET:HG3	27:b:53:TYR:OH	2.20	0.41
23:X:70:PHE:CE1	23:X:117:TRP:CZ3	3.08	0.41
27:b:11:ASN:O	27:b:15:LYS:HG2	2.20	0.41
27:b:78:LEU:O	27:b:81:LEU:N	2.53	0.41
28:c:74:GLY:O	28:c:75:LEU:HB2	2.20	0.41
30:e:22:SER:HB2	30:e:34:HIS:CD2	2.55	0.41
32:g:106:TYR:HE2	33:h:86:ILE:CD1	2.32	0.41
34:i:14:GLN:HE22	39:n:157:ALA:HB3	1.85	0.41
34:i:20:ARG:HH11	34:i:20:ARG:HG3	1.84	0.41
35:j:40:ILE:HD11	35:j:51:THR:HG23	2.02	0.41
35:j:44:TYR:CD2	36:k:22:LEU:HD22	2.56	0.41
37:l:159:LYS:HE3	37:l:161:TYR:HE1	1.86	0.41
38:m:129:TYR:HE2	41:p:146:LEU:O	2.03	0.41
39:n:56:ASP:O	39:n:59:ARG:N	2.54	0.41
41:p:9:VAL:O	41:p:109:ARG:NH2	2.51	0.41
42:q:87:HIS:O	42:q:91:HIS:HD2	2.04	0.41
45:AA:403:LEU:CG	45:AA:404:ASP:N	2.55	0.41
45:AA:454:PRO:O	45:AA:468:TYR:OH	2.35	0.41
48:AD:317:ARG:HD2	48:AD:319:LEU:HD21	2.02	0.41
49:AE:177:ARG:HB3	49:AE:211:VAL:CG1	2.49	0.41
50:AF:102:ARG:HA	50:AF:105:ARG:CZ	2.49	0.41
49:AI:8:SER:HB2	49:AI:12:ALA:HA	2.02	0.41
45:Aa:358:PHE:CD2	45:Aa:368:MET:HG2	2.54	0.41
46:Ab:237:PHE:C	46:Ab:239:ASN:H	2.27	0.41
47:Ac:8:HIS:ND1	47:Ac:11:PHE:HD1	2.18	0.41
47:Ac:138:MET:HE1	47:Ac:268:ILE:HA	2.01	0.41
48:Ad:199:TYR:HA	48:Ad:278:SER:OG	2.20	0.41
49:Ae:196:ARG:HD2	49:Ae:249:ILE:HG23	2.01	0.41
4:D:50:ALA:C	4:D:51:VAL:HG13	2.45	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
6:F:62:TRP:CE2	6:F:181:LEU:HD13	2.56	0.41
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.41
6:F:270:ASN:CG	6:F:338:ASP:HB2	2.46	0.41
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.41
7:G:41:VAL:HG21	7:G:56:VAL:CA	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.41
8:H:25:ARG:HH11	61:H:401:UQ9:C15	2.34	0.41
8:H:42:PRO:HG3	42:q:28:PHE:HE1	1.85	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
12:L:202:MET:HE3	12:L:265:PRO:CB	2.50	0.41
13:M:142:ARG:HG3	13:M:143:LEU:N	2.36	0.41
14:N:83:THR:HG22	14:N:84:TRP:N	2.35	0.41
15:O:64:GLY:O	15:O:161:ARG:NH1	2.53	0.41
15:O:117:PHE:CZ	15:O:173:MET:HE3	2.54	0.41
15:O:179:ILE:HD12	15:O:184:VAL:HG22	2.02	0.41
23:X:37:ASP:OD1	23:X:37:ASP:C	2.62	0.41
23:X:47:ARG:HH12	33:h:188:ASP:CB	2.32	0.41
23:X:137:LEU:HD13	27:b:58:ARG:NE	2.34	0.41
24:Y:14:VAL:HG21	24:Y:19:GLN:OE1	2.21	0.41
26:a:64:LYS:CE	26:a:66:LEU:HD12	2.31	0.41
27:b:15:LYS:O	27:b:16:GLU:HB2	2.20	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
36:k:58:ARG:CD	39:n:34:ARG:HG3	2.48	0.41
37:l:88:PRO:HB2	39:n:86:PRO:CB	2.51	0.41
37:l:152:SER:HA	40:o:5:LEU:CD2	2.46	0.41
38:m:124:LYS:O	38:m:126:ASN:N	2.54	0.41
42:q:50:GLU:HA	42:q:59:HIS:O	2.20	0.41
43:r:12:ARG:HH21	43:r:20:LEU:CD1	2.33	0.41
46:AB:225:VAL:HG22	46:AB:229:VAL:HG21	2.01	0.41
46:AB:396:ILE:HG12	46:AB:406:TYR:HE1	1.85	0.41
47:AC:141:TRP:CZ3	49:Ae:223:VAL:HG23	2.55	0.41
48:AD:202:ARG:HG3	48:AD:278:SER:HB3	2.02	0.41
49:AE:162:GLY:N	49:AE:178:HIS:O	2.54	0.41
49:AE:263:TYR:CA	49:AE:273:VAL:HA	2.50	0.41
52:AH:51:CYS:CA	52:AH:54:ARG:HB3	2.47	0.41
45:Aa:80:ARG:NH1	45:Aa:197:LEU:HD22	2.34	0.41
45:Aa:278:ARG:CZ	45:Aa:463:GLU:HB2	2.50	0.41
48:Ad:323:PRO:HB2	48:Ad:325:LYS:HG3	2.03	0.41
49:Ae:159:ILE:HG23	49:Ae:163:LYS:HB3	2.03	0.41
49:Ae:225:ILE:CD1	49:Ae:237:PRO:HG3	2.51	0.41
1:A:111:LEU:HD23	1:A:112:GLU:H	1.86	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LYS:O	21:V:103:LEU:HA	2.21	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:71:ILE:HG13	4:D:72:LEU:N	2.34	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.41
7:G:102:ILE:HD12	7:G:102:ILE:N	2.34	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:87:VAL:O	8:H:95:LEU:HB3	2.21	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
9:I:78:PHE:HD1	26:a:2:TRP:CD1	2.37	0.41
10:J:165:ILE:HG23	14:N:42:PRO:CG	2.37	0.41
12:L:231:PRO:O	12:L:234:PRO:HD2	2.20	0.41
12:L:286:LEU:HG	12:L:290:ILE:HD11	2.01	0.41
12:L:546:LEU:HD22	38:m:72:ARG:NH2	2.35	0.41
13:M:247:SER:OG	13:M:304:GLN:NE2	2.53	0.41
13:M:319:HIS:HA	13:M:322:THR:CG2	2.44	0.41
13:M:350:MET:HE3	13:M:350:MET:HB2	1.80	0.41
62:M:503:CDL:H632	62:M:503:CDL:H602	1.94	0.41
16:P:355:ARG:HH11	16:P:356:HIS:HE1	1.66	0.41
23:X:38:LYS:HD2	23:X:38:LYS:HA	1.75	0.41
30:e:34:HIS:HB3	33:h:189:ASN:ND2	2.35	0.41
30:e:41:ILE:CG2	33:h:179:ILE:CD1	2.92	0.41
32:g:140:PHE:HB3	41:p:75:THR:CG2	2.50	0.41
32:g:145:ILE:CG2	41:p:160:LYS:HE2	2.39	0.41
33:h:175:GLU:HB2	33:h:178:PHE:CE2	2.55	0.41
37:l:48:ARG:NH2	37:l:64:PRO:HD2	2.36	0.41
37:l:122:THR:HG22	37:l:124:VAL:H	1.85	0.41
42:q:39:VAL:HG21	42:q:89:TRP:CZ2	2.55	0.41
46:AB:346:ALA:O	46:AB:347:ALA:C	2.62	0.41
47:AC:312:GLN:HE21	50:AF:37:THR:CB	2.34	0.41
49:AE:220:LEU:HD22	47:Ac:149:LEU:HA	2.03	0.41
46:Ab:286:PHE:CD1	46:Ab:427:ALA:HB1	2.54	0.41
47:Ac:221:HIS:HE1	58:Ac:401:3PE:O32	2.03	0.41
50:Af:51:LEU:CG	50:Af:91:LEU:HD13	2.50	0.41
2:B:114:MET:SD	2:B:121:PHE:HD2	2.42	0.41
3:C:72:VAL:O	3:C:72:VAL:HG23	2.20	0.41
3:C:195:HIS:HE1	22:W:88:LYS:NZ	2.19	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
8:H:306:SER:O	8:H:307:LEU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:258:PHE:O	12:L:261:VAL:HG22	2.20	0.41
12:L:477:ILE:HG13	40:o:91:GLU:OE1	2.21	0.41
12:L:533:ILE:HG12	58:L:702:3PE:H3A2	2.02	0.41
13:M:4:ILE:CD1	13:M:41:LEU:HD21	2.51	0.41
13:M:177:MET:HE3	13:M:177:MET:HB3	1.70	0.41
13:M:270:ILE:HD12	13:M:395:LEU:HD22	2.02	0.41
14:N:168:GLY:HA3	14:N:181:TYR:CE1	2.56	0.41
14:N:191:LEU:HG	14:N:191:LEU:O	2.20	0.41
14:N:338:PRO:HB3	62:d:201:CDL:H732	2.02	0.41
15:O:354:LEU:HD12	15:O:354:LEU:HA	1.95	0.41
16:P:214:LEU:HD23	16:P:352:VAL:HG12	2.01	0.41
19:S:20:ARG:HD2	19:S:22:HIS:NE2	2.35	0.41
23:X:70:PHE:O	23:X:74:ILE:HG13	2.21	0.41
27:b:16:GLU:N	27:b:17:PRO:HD3	2.35	0.41
30:e:32:ARG:NH1	30:e:67:LEU:HA	2.35	0.41
30:e:41:ILE:CG1	33:h:174:PRO:HB2	2.51	0.41
31:f:16:VAL:O	31:f:17:PRO:C	2.63	0.41
41:p:132:PHE:O	41:p:136:THR:OG1	2.17	0.41
45:AA:388:VAL:HG21	45:AA:438:ALA:HA	2.02	0.41
46:AB:138:LEU:HD22	46:AB:238:LEU:HG	2.01	0.41
47:AC:133:LEU:HD23	47:AC:133:LEU:HA	1.85	0.41
47:AC:149:LEU:CD1	47:AC:291:VAL:HG22	2.50	0.41
47:AC:157:GLY:O	47:AC:161:VAL:HG23	2.19	0.41
47:AC:287:LYS:HG3	49:Ae:219:HIS:NE2	2.31	0.41
67:AC:402:HEM:HMA2	67:AC:402:HEM:HBA2	2.01	0.41
48:AD:115:GLN:HE22	48:AD:256:ASP:CG	2.29	0.41
49:AE:195:LEU:CD1	49:AE:248:ARG:HD2	2.50	0.41
51:AG:26:ALA:C	51:AG:28:PRO:HD3	2.46	0.41
45:Aa:478:LEU:HA	53:Aj:18:THR:HG21	2.01	0.41
46:Ab:47:LEU:CD2	46:Ab:238:LEU:HD13	2.50	0.41
49:Ae:177:ARG:HB3	49:Ae:211:VAL:CG1	2.49	0.41
50:Af:37:THR:O	50:Af:38:LEU:C	2.63	0.41
52:Ah:66:THR:O	52:Ah:67:GLU:C	2.63	0.41
1:A:20:VAL:O	1:A:21:ALA:C	2.62	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
4:D:301:ASP:N	43:r:104:TRP:HH2	2.18	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
6:F:274:LYS:HB3	6:F:276:PHE:CZ	2.56	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:309:ASN:CG	7:G:310:GLU:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.51	0.41
8:H:283:ASP:OD1	8:H:284:GLN:N	2.54	0.41
8:H:288:LEU:HD23	8:H:288:LEU:C	2.45	0.41
12:L:13:ILE:HD11	58:i:201:3PE:H2B1	2.02	0.41
12:L:149:ILE:HG21	13:M:364:LEU:HD21	2.02	0.41
12:L:389:PHE:CE1	35:j:79:ALA:HB1	2.56	0.41
12:L:482:MET:CE	12:L:486:LEU:HB3	2.51	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.02	0.41
13:M:270:ILE:HD11	13:M:395:LEU:HA	2.03	0.41
13:M:301:ILE:HG22	13:M:301:ILE:O	2.19	0.41
13:M:329:LEU:HD23	13:M:437:MET:CE	2.49	0.41
14:N:159:ILE:HB	14:N:278:MET:HE1	2.01	0.41
15:O:52:LYS:HD3	15:O:152:SER:O	2.20	0.41
15:O:90:GLY:H	15:O:93:TYR:HB2	1.85	0.41
15:O:105:ASP:OD1	15:O:106:ILE:N	2.54	0.41
15:O:262:GLU:O	15:O:265:ASP:HB3	2.21	0.41
15:O:287:ASP:HB3	15:O:290:THR:HG23	2.02	0.41
16:P:212:ARG:O	16:P:213:PHE:C	2.61	0.41
16:P:263:PHE:CD1	16:P:333:PRO:HB2	2.49	0.41
19:S:41:TYR:HE1	19:S:53:ILE:HG23	1.85	0.41
21:V:98:LYS:HG2	21:V:100:TRP:CZ2	2.55	0.41
22:W:78:ASP:HB3	22:W:81:VAL:HG23	2.03	0.41
27:b:53:TYR:CE2	27:b:55:VAL:HA	2.56	0.41
41:p:71:VAL:HB	41:p:72:PRO:CD	2.50	0.41
41:p:73:ASP:OD1	41:p:73:ASP:N	2.54	0.41
41:p:91:GLN:O	41:p:91:GLN:HG2	2.21	0.41
42:q:132:LYS:HE2	42:q:135:HIS:HA	2.01	0.41
45:AA:310:ILE:HD11	45:AA:388:VAL:HA	2.02	0.41
45:AA:463:GLU:OE2	51:AG:8:LEU:N	2.52	0.41
47:AC:71:ARG:NH1	48:AD:130:VAL:HG22	2.36	0.41
47:AC:284:ILE:HG21	47:AC:289:GLY:HA3	2.02	0.41
48:AD:153:GLU:HA	48:AD:168:PRO:HA	2.01	0.41
48:AD:235:PRO:HA	48:AD:240:GLN:CG	2.50	0.41
51:AG:28:PRO:O	51:AG:29:SER:C	2.63	0.41
51:AG:35:ILE:O	51:AG:36:PRO:C	2.63	0.41
46:Ab:297:PRO:HB3	46:Ab:302:GLY:CA	2.49	0.41
46:Ab:303:ASN:O	46:Ab:304:ASN:C	2.63	0.41
47:Ac:171:ASP:CG	47:Ac:172:LYS:N	2.76	0.41
48:Ad:141:THR:N	48:Ad:144:GLU:HB2	2.35	0.41
48:Ad:321:TYR:HB2	50:Af:61:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Ag:26:ALA:C	51:Ag:28:PRO:HD3	2.46	0.41
54:Ak:10:TYR:HA	54:Ak:13:LEU:HD12	2.03	0.41
5:E:71:GLU:HB3	44:s:60:PRO:O	2.21	0.41
6:F:225:LEU:HD13	17:Q:160:TYR:CZ	2.56	0.41
6:F:265:PHE:HB3	6:F:291:GLU:CG	2.51	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:277:MET:HE1	17:Q:153:PRO:HD3	2.03	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
7:G:649:VAL:HA	19:S:20:ARG:NH1	2.36	0.41
7:G:651:PRO:HG3	19:S:57:GLU:N	2.29	0.41
11:K:30:LEU:HD22	11:K:78:LEU:HD13	2.03	0.41
12:L:253:VAL:HB	12:L:310:LEU:CD1	2.50	0.41
12:L:364:LYS:O	35:j:47:PHE:HZ	2.03	0.41
12:L:368:PHE:HB3	12:L:445:GLU:OE1	2.20	0.41
62:L:703:CDL:H512	62:L:703:CDL:H711	2.02	0.41
13:M:22:LYS:HE3	13:M:26:ASN:HD21	1.86	0.41
13:M:49:TYR:CD1	13:M:60:PRO:HD2	2.55	0.41
13:M:164:LEU:HB3	13:M:174:LEU:HD11	2.03	0.41
13:M:178:ILE:O	13:M:179:LEU:C	2.60	0.41
13:M:216:LEU:CG	13:M:220:HIS:CE1	2.88	0.41
13:M:250:LEU:HD12	13:M:250:LEU:C	2.39	0.41
62:M:503:CDL:H1	62:M:503:CDL:OA7	2.20	0.41
14:N:324:LEU:HD11	29:d:64:PHE:CZ	2.56	0.41
15:O:229:VAL:HG13	15:O:229:VAL:O	2.21	0.41
15:O:263:ALA:C	15:O:265:ASP:N	2.77	0.41
16:P:170:LEU:O	16:P:171:ASN:C	2.62	0.41
16:P:293:LEU:HD12	16:P:294:PRO:HD2	2.01	0.41
18:R:72:VAL:HG12	18:R:73:GLU:H	1.85	0.41
23:X:23:ALA:HB2	23:X:95:GLN:HE22	1.82	0.41
23:X:167:PHE:HD2	23:X:170:TRP:HE1	1.65	0.41
27:b:11:ASN:CG	27:b:15:LYS:HE3	2.46	0.41
30:e:49:GLY:O	30:e:52:ALA:N	2.54	0.41
36:k:49:ASP:OD2	39:n:38:ARG:HG3	2.21	0.41
36:k:81:PHE:O	36:k:85:VAL:HG23	2.21	0.41
37:l:63:GLU:O	37:l:64:PRO:C	2.63	0.41
39:n:70:GLU:OE1	66:n:201:EHZ:O1	2.38	0.41
62:q:201:CDL:H112	62:q:201:CDL:H312	2.02	0.41
45:AA:56:GLY:HA3	45:AA:227:PRO:HA	2.02	0.41
45:AA:61:SER:HA	45:AA:233:ALA:O	2.20	0.41
45:AA:178:SER:OG	45:AA:181:ASN:ND2	2.53	0.41
67:AC:402:HEM:CMA	68:AC:403:UQ6:O5	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AG:57:TYR:O	51:AG:61:THR:HG23	2.21	0.41
46:Ab:272:VAL:HA	46:Ab:337:GLY:HA3	2.02	0.41
46:Ab:407:MET:HE1	46:Ab:415:GLN:CD	2.45	0.41
48:Ad:93:SER:HA	48:Ad:209:ASP:OD2	2.20	0.41
49:Ae:231:PHE:CD2	49:Ae:250:ARG:NH1	2.89	0.41
1:A:16:THR:O	1:A:20:VAL:HG23	2.21	0.41
2:B:224:ARG:HG3	16:P:85:ARG:HH22	1.85	0.41
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.56	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.41
6:F:102:MET:O	6:F:102:MET:HG3	2.21	0.41
6:F:210:THR:HG23	6:F:226:LYS:HE3	2.01	0.41
6:F:280:GLY:O	6:F:281:HIS:C	2.63	0.41
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:48:THR:O	7:G:49:VAL:C	2.63	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:388:ASN:N	7:G:514:ASN:CB	2.83	0.41
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.41
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.41
8:H:136:VAL:HG13	8:H:137:ALA:N	2.35	0.41
58:H:403:3PE:H122	9:I:60:ILE:HG21	2.03	0.41
9:I:36:TYR:CZ	43:r:106:LEU:HD23	2.56	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.55	0.41
9:I:162:CYS:SG	55:I:303:SF4:S3	3.18	0.41
10:J:124:LEU:CD2	10:J:125:MET:HG2	2.50	0.41
10:J:135:LEU:O	10:J:136:GLU:HB3	2.21	0.41
12:L:58:ASN:HA	12:L:58:ASN:HD22	1.65	0.41
12:L:68:TRP:CE3	12:L:76:LEU:CD2	3.04	0.41
12:L:321:GLN:NE2	12:L:324:LEU:HD13	2.36	0.41
12:L:598:ILE:HD11	14:N:153:ILE:CD1	2.51	0.41
13:M:160:LEU:O	13:M:164:LEU:HD13	2.21	0.41
13:M:248:ILE:HG13	13:M:249:ILE:H	1.85	0.41
13:M:307:TRP:HB2	38:m:129:TYR:O	2.21	0.41
58:M:501:3PE:H241	24:Y:135:TRP:CZ3	2.55	0.41
14:N:109:ALA:O	14:N:112:HIS:ND1	2.52	0.41
14:N:125:HIS:CE1	14:N:129:ILE:HD11	2.56	0.41
14:N:307:THR:CG2	14:N:308:ASN:N	2.79	0.41
14:N:331:ILE:HD12	14:N:335:MET:HE3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:256:LEU:HD21	15:O:276:LEU:HD23	2.03	0.41
16:P:61:ALA:HA	16:P:66:GLY:HA3	2.02	0.41
16:P:93:HIS:O	16:P:96:LEU:HG	2.21	0.41
16:P:146:VAL:HG13	16:P:147:ASN:OD1	2.21	0.41
16:P:201:ILE:HD13	16:P:265:PHE:CZ	2.55	0.41
17:Q:85:ASN:C	17:Q:87:MET:N	2.76	0.41
17:Q:166:TRP:O	17:Q:167:ASN:C	2.64	0.41
20:T:100:VAL:O	20:T:141:PRO:HD2	2.20	0.41
20:T:123:GLU:HG2	20:T:130:ILE:HD12	2.02	0.41
20:T:140:CYS:HB2	20:T:143:GLU:HB2	2.02	0.41
20:U:128:PHE:CZ	20:U:148:ILE:CD1	3.04	0.41
24:Y:51:THR:HG23	24:Y:52:LEU:N	2.35	0.41
25:Z:19:ILE:HG22	25:Z:20:ASP:N	2.36	0.41
29:d:25:LYS:HE3	29:d:27:ASN:OD1	2.21	0.41
29:d:45:ASP:O	29:d:46:ASN:C	2.62	0.41
30:e:49:GLY:HA2	30:e:52:ALA:HB3	2.02	0.41
30:e:65:GLU:CD	30:e:71:LYS:HB2	2.46	0.41
32:g:121:GLU:OE2	41:p:10:TYR:CE2	2.74	0.41
34:i:29:SER:O	34:i:32:GLU:HB2	2.21	0.41
34:i:106:PRO:HD2	40:o:64:ILE:HG21	2.03	0.41
37:l:44:THR:HG23	37:l:46:GLU:HG2	2.03	0.41
38:m:50:GLN:O	38:m:50:GLN:HG2	2.21	0.41
38:m:82:PRO:HB2	58:m:201:3PE:H12	2.02	0.41
40:o:71:ARG:NH1	40:o:72:ASP:OD1	2.54	0.41
41:p:40:VAL:O	41:p:44:PRO:HG2	2.21	0.41
42:q:5:GLU:HG2	42:q:9:ARG:HE	1.85	0.41
45:AA:74:TRP:HB3	45:AA:418:LEU:CD1	2.50	0.41
45:AA:398:ALA:C	45:AA:400:VAL:N	2.75	0.41
46:AB:195:TYR:OH	46:Ab:261:GLN:CG	2.68	0.41
46:AB:326:PHE:HD1	49:AI:11:PHE:CD2	2.38	0.41
47:AC:294:LEU:HD23	47:AC:294:LEU:C	2.46	0.41
47:AC:295:ILE:HG22	47:AC:299:LEU:HD12	2.02	0.41
48:AD:132:TYR:HD1	48:AD:173:ASP:O	2.04	0.41
49:AE:205:VAL:HA	49:AE:263:TYR:OH	2.21	0.41
54:AK:18:ILE:N	54:AK:19:PRO:HD2	2.35	0.41
45:Aa:170:ARG:HG3	45:Aa:171:GLU:N	2.36	0.41
46:Ab:47:LEU:HA	46:Ab:218:MET:O	2.21	0.41
46:Ab:216:ALA:HB3	46:Ab:244:LEU:HA	2.03	0.41
46:Ab:304:ASN:C	46:Ab:306:THR:N	2.78	0.41
46:Ab:426:LYS:HA	46:Ab:429:LYS:NZ	2.36	0.41
47:Ac:146:ILE:HG13	70:Ac:405:U10:C4M	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ac:146:ILE:O	47:Ac:149:LEU:HB3	2.21	0.41
47:Ac:295:ILE:HG22	47:Ac:299:LEU:HD12	2.02	0.41
48:Ad:127:MET:HE1	48:Ad:198:SER:HA	2.03	0.41
48:Ad:202:ARG:HG3	48:Ad:278:SER:HB3	2.02	0.41
48:Ad:250:THR:HG23	48:Ad:262:THR:HA	2.03	0.41
49:Ae:162:GLY:N	49:Ae:178:HIS:O	2.53	0.41
50:Af:33:MET:O	50:Af:36:ASP:HB2	2.21	0.41
51:Ag:28:PRO:O	51:Ag:29:SER:C	2.63	0.41
51:Ag:57:TYR:O	51:Ag:61:THR:HG23	2.21	0.41
1:A:1:MET:O	1:A:2:ASN:C	2.64	0.41
1:A:65:PHE:O	1:A:69:ILE:HG13	2.20	0.41
4:D:90:ALA:HB2	8:H:205:SER:O	2.21	0.41
4:D:235:ASP:OD2	25:Z:8:GLN:HG3	2.21	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.41
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.56	0.41
6:F:297:LYS:HG3	6:F:301:GLU:CG	2.51	0.41
7:G:47:THR:HG23	7:G:51:GLN:HB2	2.03	0.41
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.86	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
12:L:3:ILE:HG22	12:L:49:LEU:CD2	2.51	0.41
13:M:6:LEU:O	13:M:7:PRO:C	2.60	0.41
13:M:303:ILE:HG13	13:M:385:LEU:HD23	2.03	0.41
14:N:146:TYR:CG	14:N:147:PRO:N	2.88	0.41
14:N:175:MET:O	14:N:176:ARG:C	2.63	0.41
14:N:224:SER:HB2	14:N:229:SER:HB2	2.01	0.41
15:O:104:LEU:HD23	15:O:104:LEU:HA	1.90	0.41
15:O:263:ALA:C	15:O:265:ASP:H	2.29	0.41
15:O:332:ARG:O	15:O:338:LYS:HA	2.21	0.41
16:P:198:ALA:O	16:P:199:ILE:C	2.61	0.41
23:X:137:LEU:HD12	23:X:138:PRO:HD2	2.03	0.41
25:Z:90:ASN:O	25:Z:94:GLU:HB2	2.21	0.41
32:g:112:MET:HE3	32:g:115:TRP:CE3	2.56	0.41
62:h:201:CDL:HB61	34:i:84:TYR:CE2	2.56	0.41
34:i:26:GLN:HA	39:n:118:TYR:HE1	1.86	0.41
34:i:93:LYS:HB3	34:i:94:PRO:HD2	2.03	0.41
35:j:47:PHE:O	35:j:48:PRO:C	2.62	0.41
36:k:57:TRP:HA	36:k:60:MET:HB3	2.02	0.41
39:n:139:GLN:O	39:n:140:LEU:C	2.64	0.41
44:s:66:SER:O	44:s:67:PRO:C	2.63	0.41
47:AC:22:PRO:HG3	51:AG:5:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AD:89:LEU:HB2	52:AH:70:PHE:CE2	2.56	0.41
49:AE:201:ASP:OD1	49:AE:202:LEU:N	2.50	0.41
49:AE:236:CYS:HA	49:AE:237:PRO:HD2	1.91	0.41
45:Aa:388:VAL:HG21	45:Aa:438:ALA:HA	2.02	0.41
45:Aa:403:LEU:HD22	45:Aa:426:LEU:HG	2.03	0.41
47:Ac:21:LEU:HD13	68:Ac:406:UQ6:O2	2.21	0.41
47:Ac:244:LEU:O	48:Ad:285:ARG:NH1	2.48	0.41
70:Ac:405:U10:H72	70:Ac:405:U10:H1M1	1.79	0.41
48:Ad:89:LEU:HD21	52:Ah:77:ASP:HB2	2.03	0.41
48:Ad:146:LYS:HD3	48:Ad:171:LEU:HG	2.02	0.41
49:Ae:172:LYS:HA	49:Ae:172:LYS:HE2	2.02	0.41
50:Af:108:TRP:HA	50:Af:111:LYS:HZ2	1.86	0.41
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.54	0.40
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.40
4:D:47:PHE:CG	14:N:227:ILE:HD11	2.57	0.40
4:D:106:VAL:N	4:D:442:HIS:O	2.41	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
4:D:375:MET:HG2	7:G:121:LEU:HD22	2.02	0.40
58:D:501:3PE:H322	58:D:501:3PE:H351	1.72	0.40
6:F:76:ILE:O	6:F:80:MET:HG2	2.21	0.40
6:F:127:ASP:O	6:F:128:ARG:C	2.65	0.40
6:F:171:VAL:HG13	6:F:174:ARG:HH22	1.86	0.40
6:F:225:LEU:HB2	17:Q:160:TYR:HE2	1.75	0.40
6:F:294:VAL:HA	6:F:295:PRO:HD3	1.84	0.40
6:F:296:LEU:HB2	6:F:337:MET:HE3	2.03	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.40
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.49	0.40
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.40
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.40
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.40
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.40
58:H:403:3PE:N	27:b:18:VAL:HG23	2.36	0.40
10:J:159:LEU:CD2	11:K:69:CYS:SG	3.09	0.40
10:J:164:PHE:CE2	14:N:8:ILE:CG1	2.90	0.40
12:L:67:HIS:C	58:L:705:3PE:HN1	2.29	0.40
12:L:358:LYS:CG	39:n:80:TYR:CE1	2.86	0.40
12:L:424:MET:HE2	12:L:502:LEU:CA	2.51	0.40
12:L:427:ILE:CD1	36:k:69:PHE:HE1	2.34	0.40
58:L:702:3PE:H232	37:l:116:ARG:HA	2.03	0.40
13:M:173:THR:HB	33:h:143:GLU:OE2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:M:502:3PE:H321	58:M:502:3PE:H352	1.92	0.40
14:N:22:SER:HB2	30:e:6:ILE:HG22	2.03	0.40
19:S:22:HIS:CD2	19:S:66:TRP:HD1	2.39	0.40
23:X:130:LYS:NZ	27:b:63:MET:O	2.53	0.40
28:c:35:VAL:HG23	28:c:36:ASN:N	2.36	0.40
32:g:63:ASN:OD1	39:n:106:TYR:HE1	2.04	0.40
37:l:159:LYS:HE3	37:l:161:TYR:CE1	2.56	0.40
38:m:59:HIS:O	38:m:60:ILE:C	2.64	0.40
39:n:157:ALA:O	39:n:158:ARG:HB2	2.21	0.40
39:n:167:TRP:CD1	39:n:167:TRP:H	2.38	0.40
40:o:52:THR:O	40:o:53:LEU:C	2.62	0.40
45:AA:170:ARG:HG3	45:AA:171:GLU:N	2.36	0.40
47:AC:116:GLY:HA3	67:AC:402:HEM:C3C	2.56	0.40
47:AC:156:ILE:O	47:AC:157:GLY:C	2.62	0.40
68:AC:403:UQ6:H151	68:AC:403:UQ6:H171	1.71	0.40
49:AE:168:LYS:NZ	49:AE:171:GLY:HA2	2.36	0.40
53:AJ:21:PHE:O	53:AJ:24:THR:HG22	2.20	0.40
48:Ad:91:PRO:HA	48:Ad:236:TYR:CE1	2.56	0.40
48:Ad:161:ASP:O	48:Ad:162:GLY:C	2.64	0.40
51:Ag:19:LEU:HD12	51:Ag:20:SER:H	1.86	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.64	0.40
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.40
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.40
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.04	0.40
7:G:36:VAL:O	7:G:37:ASP:HB2	2.22	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.40
57:I:301:PC1:H112	25:Z:29:GLY:HA3	2.02	0.40
10:J:10:SER:O	10:J:14:VAL:HG23	2.21	0.40
12:L:52:LEU:O	12:L:53:MET:C	2.63	0.40
12:L:210:LEU:O	12:L:211:ILE:C	2.62	0.40
62:L:703:CDL:H352	33:h:72:LYS:HA	2.03	0.40
13:M:158:ILE:HG21	14:N:283:ALA:HB1	2.03	0.40
13:M:428:PRO:HD3	39:n:106:TYR:CG	2.56	0.40
14:N:215:MET:HE3	14:N:215:MET:HB3	1.96	0.40
15:O:219:GLN:NE2	15:O:219:GLN:HA	2.35	0.40
15:O:221:LYS:HG3	15:O:221:LYS:O	2.21	0.40
16:P:163:ARG:NH1	16:P:199:ILE:HD11	2.36	0.40
17:Q:57:GLU:O	17:Q:58:LYS:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:48:PHE:CD2	18:R:53:LYS:HB2	2.56	0.40
20:U:93:ILE:CG1	20:U:110:LEU:HD11	2.51	0.40
22:W:124:LYS:HE3	22:W:124:LYS:HB2	1.86	0.40
24:Y:5:LYS:C	24:Y:7:PHE:N	2.77	0.40
27:b:69:HIS:CD2	27:b:71:GLN:H	2.39	0.40
37:l:122:THR:CG2	37:l:129:MET:HE1	2.45	0.40
37:l:129:MET:HE3	37:l:129:MET:HB2	1.90	0.40
39:n:41:ALA:C	39:n:43:LEU:N	2.78	0.40
40:o:39:MET:CE	40:o:58:TYR:HA	2.48	0.40
45:AA:45:VAL:HG21	45:AA:426:LEU:HB2	2.02	0.40
47:AC:30:TRP:CB	47:AC:100:ARG:HD3	2.52	0.40
47:AC:77:TRP:HZ2	48:AD:284:HIS:HD2	1.69	0.40
49:AE:231:PHE:CD2	49:AE:250:ARG:NH1	2.88	0.40
49:AE:263:TYR:HE1	49:AE:265:PHE:CE2	2.39	0.40
47:Ac:296:LEU:O	47:Ac:297:SER:C	2.64	0.40
49:Ae:156:LEU:N	49:Ae:269:ASP:O	2.54	0.40
50:Af:65:ARG:O	50:Af:69:LEU:HG	2.21	0.40
1:A:88:MET:HG3	1:A:92:PHE:CE2	2.56	0.40
3:C:55:LYS:HB3	3:C:55:LYS:HE2	1.83	0.40
4:D:61:TRP:CD1	4:D:61:TRP:N	2.89	0.40
5:E:68:ASN:OD1	44:s:56:ARG:NH1	2.54	0.40
5:E:139:CYS:HB3	5:E:144:SER:HB3	2.03	0.40
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.52	0.40
7:G:64:CYS:SG	7:G:75:CYS:SG	3.14	0.40
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:283:GLU:O	7:G:283:GLU:CG	2.50	0.40
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.50	0.40
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.80	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:J:136:GLU:O	10:J:137:GLY:C	2.58	0.40
12:L:324:LEU:HB3	12:L:395:ILE:CD1	2.51	0.40
12:L:399:ILE:HG22	12:L:409:LEU:CD1	2.51	0.40
12:L:400:ASN:HD22	12:L:409:LEU:HD11	1.85	0.40
12:L:466:PHE:HB3	35:j:68:TRP:CZ2	2.45	0.40
13:M:53:SER:O	13:M:54:ASN:C	2.63	0.40
13:M:197:LEU:O	13:M:201:MET:HB2	2.21	0.40
13:M:259:TYR:HB2	13:M:260:PRO:HD3	2.03	0.40
13:M:394:ILE:O	13:M:398:ILE:HG13	2.22	0.40
13:M:398:ILE:HD11	58:M:502:3PE:H2I3	2.02	0.40
14:N:106:LEU:HD21	14:N:138:PRO:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:170:LEU:CD2	15:O:184:VAL:HG13	2.51	0.40
15:O:268:LYS:HA	15:O:271:GLU:OE1	2.21	0.40
15:O:276:LEU:HD12	15:O:276:LEU:C	2.46	0.40
16:P:143:ASP:OD1	16:P:147:ASN:ND2	2.54	0.40
19:S:36:PHE:HZ	19:S:44:LEU:CD1	2.26	0.40
19:S:59:SER:O	19:S:60:GLU:C	2.63	0.40
20:T:87:LEU:HD11	20:T:141:PRO:HG3	2.03	0.40
26:a:12:MET:HE2	26:a:12:MET:HB3	1.90	0.40
33:h:148:GLU:O	33:h:152:LYS:HG3	2.21	0.40
34:i:11:ARG:NE	39:n:154:LEU:HB2	2.37	0.40
43:r:20:LEU:C	43:r:20:LEU:CD1	2.89	0.40
43:r:24:LEU:HD23	43:r:24:LEU:HA	1.85	0.40
44:s:44:THR:O	44:s:48:LEU:HG	2.21	0.40
45:AA:367:ASP:O	45:AA:370:PHE:N	2.53	0.40
46:AB:326:PHE:CZ	49:AI:15:LEU:HD11	2.57	0.40
47:AC:150:LEU:O	47:AC:151:SER:C	2.64	0.40
47:AC:275:LEU:O	47:AC:276:PHE:C	2.64	0.40
48:AD:127:MET:HE1	48:AD:198:SER:HA	2.03	0.40
49:AE:244:ASP:OD2	49:AE:248:ARG:NE	2.54	0.40
52:AH:27:PRO:HB3	52:AH:87:ASN:ND2	2.36	0.40
52:AH:67:GLU:HG3	52:AH:68:GLU:N	2.36	0.40
49:Ae:168:LYS:NZ	49:Ae:171:GLY:HA2	2.36	0.40
49:Ae:180:THR:O	49:Ae:181:LYS:C	2.64	0.40
51:Ag:35:ILE:O	51:Ag:36:PRO:C	2.63	0.40
1:A:55:PHE:HZ	8:H:282:TYR:HE2	1.56	0.40
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
2:B:114:MET:HG3	2:B:115:ASP:N	2.36	0.40
2:B:116:ARG:HG3	8:H:38:ASN:H	1.85	0.40
6:F:185:ASN:HA	6:F:189:SER:O	2.21	0.40
6:F:225:LEU:N	17:Q:160:TYR:HE2	2.16	0.40
6:F:335:VAL:HG12	6:F:336:LEU:N	2.36	0.40
8:H:130:PHE:CZ	8:H:134:ARG:HD3	2.56	0.40
8:H:293:PHE:O	8:H:294:LEU:C	2.63	0.40
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.40
10:J:22:LYS:NZ	11:K:21:MET:C	2.79	0.40
12:L:22:SER:HA	12:L:27:ILE:CG2	2.52	0.40
12:L:210:LEU:HD12	12:L:270:ASN:HD21	1.86	0.40
12:L:364:LYS:HE2	36:k:67:ILE:HD12	1.90	0.40
12:L:371:SER:O	12:L:374:VAL:HG12	2.21	0.40
13:M:3:LYS:HD3	31:f:20:PHE:HE1	1.86	0.40
13:M:17:LEU:HD13	31:f:11:TRP:HH2	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:435:THR:HG23	13:M:436:LEU:N	2.36	0.40
14:N:59:TYR:O	14:N:63:GLN:HG2	2.21	0.40
14:N:139:LEU:HD23	14:N:139:LEU:HA	1.86	0.40
15:O:153:THR:OG1	15:O:154:GLY:N	2.55	0.40
16:P:54:VAL:O	16:P:78:SER:HB3	2.21	0.40
16:P:120:VAL:O	16:P:121:GLN:C	2.64	0.40
16:P:164:PHE:CE2	16:P:166:HIS:HB2	2.50	0.40
21:V:96:LYS:HE2	21:V:96:LYS:HB2	1.95	0.40
22:W:86:VAL:O	22:W:87:ILE:C	2.62	0.40
23:X:117:TRP:CD1	23:X:117:TRP:N	2.87	0.40
24:Y:64:THR:O	24:Y:68:ILE:HG23	2.20	0.40
25:Z:110:VAL:HG13	30:e:72:THR:HG22	2.03	0.40
26:a:9:LEU:O	26:a:10:ALA:C	2.64	0.40
26:a:49:GLU:O	26:a:50:ARG:C	2.62	0.40
30:e:81:LYS:HB3	30:e:81:LYS:HE2	1.77	0.40
33:h:87:THR:O	33:h:91:ILE:HG13	2.22	0.40
34:i:32:GLU:OE2	39:n:117:ASP:N	2.55	0.40
34:i:99:SER:O	34:i:100:SER:C	2.64	0.40
35:j:71:TRP:HZ3	35:j:72:ARG:NH2	2.19	0.40
38:m:28:GLU:HG2	38:m:31:ARG:NH2	2.37	0.40
38:m:124:LYS:HG2	38:m:125:PHE:CD2	2.57	0.40
41:p:43:TRP:HB3	41:p:44:PRO:HD3	2.03	0.40
45:AA:73:VAL:HG11	45:AA:151:VAL:HG11	2.03	0.40
45:AA:204:PRO:HB3	49:AE:82:ASP:HA	2.02	0.40
45:AA:204:PRO:O	45:AA:205:SER:C	2.63	0.40
46:AB:65:VAL:HG22	46:AB:218:MET:HG2	2.03	0.40
46:AB:426:LYS:HA	46:AB:429:LYS:NZ	2.36	0.40
46:AB:453:LEU:O	46:AB:453:LEU:HD23	2.21	0.40
48:AD:324:PRO:O	48:AD:325:LYS:C	2.63	0.40
49:AE:86:PRO:HD2	51:AG:17:TYR:CG	2.57	0.40
49:AE:88:PHE:O	49:AE:89:SER:C	2.65	0.40
49:AE:123:VAL:HG13	53:AJ:29:ALA:CA	2.41	0.40
49:AE:178:HIS:CD2	49:AE:179:ARG:N	2.88	0.40
49:AE:196:ARG:HD2	49:AE:249:ILE:HG21	2.03	0.40
51:AG:78:TYR:CB	52:AH:63:GLU:HG3	2.50	0.40
45:Aa:86:ASN:OD1	45:Aa:86:ASN:N	2.54	0.40
45:Aa:148:ALA:O	45:Aa:152:GLN:HG2	2.21	0.40
45:Aa:148:ALA:HB2	45:Aa:250:LEU:HG	2.04	0.40
46:Ab:312:SER:OG	46:Ab:357:GLN:NE2	2.40	0.40
51:Ag:73:LYS:HZ2	52:Ah:63:GLU:HG2	1.86	0.40
3:C:49:ARG:NH2	3:C:79:CYS:HA	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:LEU:O	4:D:387:GLU:HG3	2.22	0.40
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.40
4:D:116:LEU:O	4:D:118:ARG:HG3	2.22	0.40
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:272:ARG:NH2	17:Q:87:MET:HE3	2.36	0.40
7:G:462:PHE:HD2	7:G:466:LEU:HG	1.86	0.40
8:H:187:ILE:CD1	58:H:403:3PE:H242	2.42	0.40
8:H:204:GLU:HA	8:H:204:GLU:OE1	2.22	0.40
58:H:403:3PE:O21	9:I:63:TRP:NE1	2.54	0.40
9:I:92:PRO:HB3	42:q:92:CYS:HB2	2.04	0.40
12:L:67:HIS:HD2	12:L:76:LEU:O	2.05	0.40
12:L:277:MET:HG3	12:L:318:GLY:HA3	2.04	0.40
12:L:381:THR:HG22	12:L:420:ALA:HA	2.04	0.40
13:M:218:LYS:HE3	13:M:218:LYS:HB3	1.58	0.40
13:M:437:MET:O	13:M:438:ALA:C	2.62	0.40
14:N:122:ILE:CD1	14:N:127:GLY:HA2	2.52	0.40
14:N:132:THR:HB	14:N:209:ILE:HG12	2.03	0.40
14:N:211:LEU:CD2	14:N:333:SER:HB2	2.45	0.40
14:N:223:ASN:OD1	14:N:223:ASN:O	2.39	0.40
14:N:297:ILE:O	14:N:298:TYR:C	2.63	0.40
16:P:105:PHE:C	16:P:106:LEU:HD12	2.47	0.40
16:P:300:TRP:CE2	16:P:304:LEU:HD21	2.57	0.40
19:S:45:LYS:O	19:S:46:LYS:C	2.64	0.40
23:X:16:GLU:CD	23:X:68:LEU:HD13	2.46	0.40
23:X:38:LYS:O	23:X:42:GLU:HG3	2.22	0.40
23:X:60:GLY:O	23:X:63:VAL:HB	2.22	0.40
29:d:93:TYR:HD2	33:h:156:VAL:HG13	1.86	0.40
29:d:100:ASP:OD2	33:h:163:ARG:NH2	2.55	0.40
31:f:10:HIS:HB3	31:f:13:HIS:HD2	1.85	0.40
34:i:4:TYR:HB2	34:i:9:LYS:HE2	2.04	0.40
34:i:18:LEU:CD2	39:n:125:TRP:HH2	2.34	0.40
36:k:56:ALA:O	36:k:60:MET:N	2.53	0.40
38:m:37:LEU:CA	38:m:40:ARG:HG2	2.50	0.40
41:p:45:VAL:O	41:p:46:THR:C	2.64	0.40
41:p:128:GLU:OE2	41:p:128:GLU:N	2.51	0.40
41:p:167:ARG:O	41:p:171:ARG:NE	2.53	0.40
42:q:3:LEU:HD13	62:q:201:CDL:C51	2.51	0.40
48:AD:110:ILE:HG23	48:AD:273:PHE:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AE:114:SER:CB	51:AG:22:PHE:CE2	3.04	0.40
51:AG:62:TRP:O	51:AG:65:GLN:HG3	2.22	0.40
49:AI:8:SER:HB2	49:AI:12:ALA:CA	2.52	0.40
49:AI:69:GLY:CA	46:Ab:111:SER:HA	2.50	0.40
54:AK:10:TYR:HE1	50:Af:110:LYS:HA	1.86	0.40
46:Ab:138:LEU:HD22	46:Ab:237:PHE:CB	2.51	0.40
46:Ab:142:THR:HB	46:Ab:240:MET:HG3	2.03	0.40
47:Ac:283:SER:OG	47:Ac:284:ILE:HD12	2.22	0.40
50:Af:75:ILE:HD13	51:Ag:40:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	11 (7%)	1 (1%)	21	59
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	423/463 (91%)	392 (93%)	31 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100
6	F	422/464 (91%)	403 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	632 (92%)	53 (8%)	0	100	100
8	H	313/318 (98%)	295 (94%)	18 (6%)	0	100	100
9	I	169/212 (80%)	169 (100%)	0	0	100	100
10	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
11	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
12	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
13	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	72
15	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
16	P	337/377 (89%)	314 (93%)	23 (7%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	111 (99%)	1 (1%)	0	100	100
23	X	167/172 (97%)	153 (92%)	14 (8%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
35	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
36	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	59
40	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
41	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
42	q	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	s	27/104 (26%)	27 (100%)	0	0	100	100
45	AA	397/480 (83%)	385 (97%)	12 (3%)	0	100	100
45	Aa	394/480 (82%)	385 (98%)	9 (2%)	0	100	100
46	AB	409/453 (90%)	397 (97%)	12 (3%)	0	100	100
46	Ab	415/453 (92%)	406 (98%)	9 (2%)	0	100	100
47	AC	371/381 (97%)	365 (98%)	6 (2%)	0	100	100
47	Ac	365/381 (96%)	361 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	238/325 (73%)	229 (96%)	9 (4%)	0	100	100
49	AE	175/274 (64%)	164 (94%)	11 (6%)	0	100	100
49	AI	40/274 (15%)	38 (95%)	2 (5%)	0	100	100
49	Ae	180/274 (66%)	167 (93%)	13 (7%)	0	100	100
50	AF	95/111 (86%)	95 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	73/82 (89%)	73 (100%)	0	0	100	100
51	Ag	74/82 (90%)	74 (100%)	0	0	100	100
52	AH	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
52	Ah	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	39/64 (61%)	39 (100%)	0	0	100	100
54	AK	41/56 (73%)	39 (95%)	2 (5%)	0	100	100
54	Ak	43/56 (77%)	40 (93%)	3 (7%)	0	100	100
All	All	11734/14118 (83%)	11218 (96%)	513 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
2	B	195	PRO
39	n	156	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	83/104 (80%)	83 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	73	80
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	369/395 (93%)	369 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	340/370 (92%)	340 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	87
8	H	279/280 (100%)	278 (100%)	1 (0%)	84	84
9	I	147/178 (83%)	147 (100%)	0	100	100
10	J	124/138 (90%)	123 (99%)	1 (1%)	73	80
11	K	86/88 (98%)	86 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	84
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	87
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	85
15	O	282/309 (91%)	282 (100%)	0	100	100
16	P	296/325 (91%)	296 (100%)	0	100	100
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	78
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	72
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	72
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	72
20	U	80/135 (59%)	80 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
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	120/123 (98%)	119 (99%)	1 (1%)	73	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	70/73 (96%)	70 (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	91/94 (97%)	91 (100%)	0	100	100
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	90/129 (70%)	90 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	86/120 (72%)	86 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	140/161 (87%)	140 (100%)	0	100	100
38	m	112/114 (98%)	111 (99%)	1 (1%)	70	79
39	n	162/164 (99%)	161 (99%)	1 (1%)	78	83
40	o	111/121 (92%)	111 (100%)	0	100	100
41	p	152/158 (96%)	152 (100%)	0	100	100
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	28/95 (30%)	28 (100%)	0	100	100
45	AA	341/398 (86%)	340 (100%)	1 (0%)	86	85
45	Aa	339/398 (85%)	337 (99%)	2 (1%)	78	83
46	AB	324/356 (91%)	324 (100%)	0	100	100
46	Ab	327/356 (92%)	327 (100%)	0	100	100
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	85
47	Ac	322/333 (97%)	321 (100%)	1 (0%)	86	85
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	152/224 (68%)	151 (99%)	1 (1%)	76	81
49	AI	33/224 (15%)	33 (100%)	0	100	100
49	Ae	156/224 (70%)	154 (99%)	2 (1%)	61	74
50	AF	89/99 (90%)	89 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	68/74 (92%)	68 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	61/83 (74%)	61 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	33/55 (60%)	33 (100%)	0	100	100
54	AK	34/46 (74%)	34 (100%)	0	100	100
54	Ak	35/46 (76%)	35 (100%)	0	100	100
All	All	10319/12037 (86%)	10296 (100%)	23 (0%)	85	87

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	120	VAL
7	G	271	MET
8	H	250	ASN
10	J	136	GLU
12	L	3	ILE
12	L	69	VAL
13	M	218	LYS
14	N	159	ILE
17	Q	96	LYS
18	R	64	ILE
19	S	68	ARG
20	T	103	HIS
25	Z	7	LYS
38	m	49	LEU
39	n	98	LYS
45	AA	249	HIS
47	AC	294	LEU
49	AE	135	GLN
45	Aa	249	HIS
45	Aa	275	ILE
47	Ac	294	LEU
49	Ae	90	ASP
49	Ae	135	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (233)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	106	HIS
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	60	HIS
4	D	88	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	245	GLN
6	F	168	ASN
6	F	270	ASN
6	F	283	ASN
6	F	303	HIS
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	164	ASN
7	G	205	GLN
7	G	359	ASN
7	G	388	ASN
7	G	495	ASN
7	G	498	GLN
7	G	540	ASN
7	G	569	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	124	ASN
8	H	138	GLN
8	H	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	292	ASN
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	226	GLN
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	579	ASN
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN
13	M	170	HIS
13	M	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	213	HIS
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
14	N	317	GLN
15	O	80	GLN
15	O	132	GLN
15	O	175	ASN
15	O	219	GLN
15	O	286	GLN
15	O	292	HIS
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	71	ASN
16	P	79	GLN
16	P	154	GLN
16	P	166	HIS
16	P	219	ASN
16	P	238	GLN
16	P	269	ASN
16	P	275	HIS
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	88	GLN
18	R	52	GLN
18	R	56	ASN
21	V	41	HIS
21	V	50	GLN
22	W	54	GLN
22	W	94	GLN
23	X	30	HIS
23	X	77	HIS
24	Y	21	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Y	91	ASN
25	Z	76	GLN
26	a	31	ASN
27	b	69	HIS
27	b	71	GLN
27	b	83	ASN
29	d	59	HIS
29	d	79	GLN
29	d	88	HIS
30	e	98	HIS
31	f	10	HIS
31	f	13	HIS
32	g	113	GLN
33	h	109	HIS
33	h	170	GLN
34	i	74	HIS
34	i	83	HIS
35	j	41	GLN
36	k	39	GLN
36	k	66	ASN
37	l	83	GLN
37	l	91	GLN
37	l	106	HIS
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	13	GLN
39	n	14	GLN
39	n	53	ASN
39	n	62	GLN
39	n	74	ASN
39	n	76	HIS
39	n	139	GLN
40	o	4	HIS
40	o	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	124	ASN
42	q	13	GLN
42	q	31	ASN
42	q	52	ASN
42	q	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	q	87	HIS
42	q	91	HIS
43	r	21	GLN
43	r	110	GLN
45	AA	55	ASN
45	AA	87	ASN
45	AA	160	GLN
45	AA	173	GLN
45	AA	181	ASN
45	AA	207	ASN
45	AA	240	GLN
45	AA	342	GLN
45	AA	397	ASN
45	AA	469	ASN
46	AB	167	GLN
46	AB	284	ASN
46	AB	327	ASN
46	AB	357	GLN
46	AB	365	ASN
46	AB	415	GLN
47	AC	32	ASN
47	AC	148	ASN
47	AC	260	ASN
47	AC	312	GLN
48	AD	115	GLN
48	AD	155	GLN
49	AE	219	HIS
49	AE	242	HIS
50	AF	80	GLN
51	AG	7	ASN
52	AH	37	GLN
52	AH	60	GLN
52	AH	87	ASN
45	Aa	160	GLN
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	193	GLN
45	Aa	207	ASN
45	Aa	240	GLN
45	Aa	342	GLN
45	Aa	397	ASN
45	Aa	402	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	Ab	284	ASN
46	Ab	298	HIS
46	Ab	357	GLN
46	Ab	415	GLN
47	Ac	32	ASN
47	Ac	148	ASN
47	Ac	221	HIS
47	Ac	260	ASN
47	Ac	312	GLN
48	Ad	115	GLN
48	Ad	134	HIS
48	Ad	155	GLN
48	Ad	181	ASN
48	Ad	189	ASN
49	Ae	219	HIS
49	Ae	227	ASN
49	Ae	242	HIS
50	Af	73	HIS
50	Af	80	GLN
51	Ag	13	HIS
52	Ah	37	GLN
52	Ah	78	HIS
52	Ah	82	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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$
55	SF4	B	301	2	0,12,12	-	-	-		
58	3PE	H	402	-	45,45,50	0.97	2 (4%)	48,50,55	0.98	2 (4%)
68	UQ6	Ac	406	-	23,23,43	2.82	6 (26%)	30,31,55	1.91	5 (16%)
55	SF4	G	801	7	0,12,12	-	-	-		
58	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.15	4 (7%)
61	UQ9	H	401	-	35,35,58	0.79	2 (5%)	43,45,73	0.59	1 (2%)
65	NDP	P	401	-	51,52,52	1.19	5 (9%)	71,80,80	1.57	10 (14%)
67	HEM	Ac	402	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
55	SF4	F	502	6	0,12,12	-	-	-		
58	3PE	Ac	404	-	34,34,50	0.33	0	37,39,55	0.41	0
58	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.07	2 (4%)
60	FMN	F	501	-	33,33,33	1.42	4 (12%)	48,50,50	1.23	7 (14%)
62	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.22	6 (9%)
70	U10	Ac	405	-	23,23,63	1.28	3 (13%)	30,31,79	2.05	6 (20%)
62	CDL	Ag	101	-	41,41,99	0.45	0	47,53,111	0.36	0
58	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.06	3 (7%)
62	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.16	6 (8%)
58	3PE	D	501	-	37,37,50	1.07	2 (5%)	40,42,55	1.09	3 (7%)
68	UQ6	AC	403	-	28,28,43	2.46	6 (21%)	36,37,55	2.02	10 (27%)
62	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.17	7 (9%)
62	CDL	Aa	501	-	45,45,99	0.43	0	51,57,111	0.36	0
58	3PE	L	702	-	48,48,50	0.93	2 (4%)	51,53,55	1.11	3 (5%)
59	FES	E	301	5	0,4,4	-	-	-		
67	HEM	AC	402	47	50,50,50	1.54	8 (16%)	67,82,82	1.80	15 (22%)
69	HEC	AD	401	48	46,50,50	1.83	6 (13%)	58,82,82	1.92	5 (8%)
58	3PE	J	201	-	45,45,50	0.98	2 (4%)	48,50,55	1.07	3 (6%)
67	HEM	AC	401	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
62	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.15	6 (7%)
56	UQ1	B	302	-	18,18,18	2.06	2 (11%)	24,25,25	1.29	4 (16%)
66	EHZ	n	201	-	29,31,37	1.82	7 (24%)	37,41,47	1.65	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	FES	G	803	7	0,4,4	-	-	-		
66	EHZ	W	201	-	29,31,37	1.79	7 (24%)	37,41,47	1.94	12 (32%)
57	PC1	B	303	-	34,34,53	1.16	2 (5%)	40,42,61	1.17	4 (10%)
62	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.15	7 (8%)
58	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.09	3 (6%)
62	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.22	7 (10%)
62	CDL	Ag	102	-	55,55,99	0.38	0	61,67,111	0.33	0
58	3PE	Ac	401	-	22,22,50	0.47	0	25,27,55	0.76	1 (4%)
69	HEC	Ad	401	48	46,50,50	1.83	4 (8%)	58,82,82	1.93	5 (8%)
58	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.15	3 (7%)
57	PC1	I	301	-	42,42,53	1.05	2 (4%)	48,50,61	1.06	3 (6%)
64	ADP	O	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
67	HEM	Ac	403	47	50,50,50	1.33	5 (10%)	67,82,82	1.57	15 (22%)
58	3PE	H	403	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
58	3PE	m	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.16	3 (6%)
58	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.30	0
55	SF4	G	802	7	0,12,12	-	-	-		
55	SF4	I	302	9	0,12,12	-	-	-		
55	SF4	I	303	9	0,12,12	-	-	-		

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	3PE	H	402	-	-	13/49/49/54	-
68	UQ6	Ac	406	-	-	2/15/15/39	0/1/1/1
55	SF4	B	301	2	-	-	0/6/5/5
65	NDP	P	401	-	-	6/34/77/77	0/5/5/5
58	3PE	M	502	-	-	14/52/52/54	-
61	UQ9	H	401	-	-	17/30/54/81	0/1/1/1
55	SF4	G	801	7	-	-	0/6/5/5
67	HEM	Ac	402	47	-	9/14/54/54	-
55	SF4	F	502	6	-	-	0/6/5/5
58	3PE	Ac	404	-	-	12/38/38/54	-
60	FMN	F	501	-	-	1/18/18/18	0/3/3/3
58	3PE	L	701	-	-	10/43/43/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	CDL	q	201	-	-	19/67/67/110	-
70	U10	Ac	405	-	-	6/15/39/87	0/1/1/1
62	CDL	Ag	101	-	-	14/52/52/110	-
58	3PE	M	501	-	-	10/40/40/54	-
62	CDL	h	201	-	-	19/78/78/110	-
58	3PE	D	501	-	-	8/41/41/54	-
68	UQ6	AC	403	-	-	4/21/21/39	0/1/1/1
62	CDL	Y	201	-	-	15/81/81/110	-
62	CDL	Aa	501	-	-	15/56/56/110	-
58	3PE	L	702	-	-	13/52/52/54	-
69	HEC	AD	401	48	-	4/14/54/54	-
67	HEM	AC	402	47	-	8/14/54/54	-
59	FES	E	301	5	-	-	0/1/1/1
58	3PE	J	201	-	-	13/49/49/54	-
67	HEM	AC	401	47	-	9/14/54/54	-
62	CDL	L	703	-	-	20/83/83/110	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
66	EHZ	n	201	-	-	22/39/39/45	-
59	FES	G	803	7	-	-	0/1/1/1
66	EHZ	W	201	-	-	21/39/39/45	-
57	PC1	B	303	-	-	11/38/38/57	-
62	CDL	M	503	-	-	24/92/92/110	-
58	3PE	L	705	-	-	13/47/47/54	-
62	CDL	d	201	-	-	27/75/75/110	-
62	CDL	Ag	102	-	-	12/66/66/110	-
58	3PE	Ac	401	-	-	5/26/26/54	-
69	HEC	Ad	401	48	-	4/14/54/54	-
58	3PE	i	201	-	-	9/43/43/54	-
57	PC1	I	301	-	-	8/46/46/57	-
64	ADP	O	401	-	-	2/16/32/32	0/3/3/3
67	HEM	Ac	403	47	-	8/14/54/54	-
58	3PE	H	403	-	-	12/54/54/54	-
58	3PE	m	201	-	-	10/44/44/54	-
58	3PE	Ag	103	-	-	10/54/54/54	-
55	SF4	G	802	7	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SF4	I	302	9	-	-	0/6/5/5
55	SF4	I	303	9	-	-	0/6/5/5

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	403	UQ6	C5-C4	8.03	1.52	1.39
56	B	302	UQ1	C6-C5	7.73	1.49	1.35
69	Ad	401	HEC	CAC-C3C	6.11	1.54	1.35
69	AD	401	HEC	CAB-C3B	6.11	1.54	1.35
68	Ac	406	UQ6	C5-C6	6.08	1.49	1.40
69	Ad	401	HEC	CAB-C3B	6.04	1.54	1.35
69	AD	401	HEC	CAC-C3C	6.04	1.54	1.35
68	Ac	406	UQ6	C2-C3	5.96	1.49	1.39
68	Ac	406	UQ6	C5-C4	5.93	1.49	1.39
69	Ad	401	HEC	C3D-C2D	5.75	1.53	1.38
69	AD	401	HEC	C3D-C2D	5.68	1.53	1.38
68	AC	403	UQ6	C5-C6	5.48	1.48	1.40
66	n	201	EHZ	C12-N1	5.28	1.45	1.33
68	AC	403	UQ6	C6-C1	5.28	1.49	1.40
67	AC	402	HEM	FE-NB	5.24	2.11	1.94
60	F	501	FMN	C9A-C5A	5.13	1.49	1.41
66	W	201	EHZ	C15-N2	5.01	1.45	1.33
66	W	201	EHZ	C12-N1	4.97	1.45	1.33
68	Ac	406	UQ6	C6-C1	4.95	1.48	1.40
66	n	201	EHZ	C15-N2	4.93	1.45	1.33
68	Ac	406	UQ6	C4-C3	4.81	1.49	1.39
68	Ac	406	UQ6	C2-C1	4.66	1.49	1.40
68	AC	403	UQ6	C2-C1	4.50	1.48	1.40
64	O	401	ADP	C5-C4	4.50	1.47	1.39
65	P	401	NDP	C5A-C4A	4.48	1.47	1.39
62	Y	201	CDL	OA8-CA7	4.31	1.45	1.33
58	M	501	3PE	O31-C31	4.31	1.45	1.33
58	J	201	3PE	O31-C31	4.30	1.45	1.33
62	q	201	CDL	OA8-CA7	4.28	1.45	1.33
58	D	501	3PE	O31-C31	4.27	1.45	1.33
62	L	703	CDL	OB8-CB7	4.27	1.45	1.33
58	L	705	3PE	O31-C31	4.27	1.45	1.33
62	q	201	CDL	OB8-CB7	4.27	1.45	1.33
58	M	502	3PE	O31-C31	4.26	1.45	1.33
57	I	301	PC1	O31-C31	4.26	1.45	1.33
58	i	201	3PE	O31-C31	4.26	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	d	201	CDL	OB8-CB7	4.25	1.45	1.33
57	B	303	PC1	O31-C31	4.24	1.45	1.33
62	M	503	CDL	OA8-CA7	4.24	1.45	1.33
58	m	201	3PE	O31-C31	4.21	1.45	1.33
58	H	403	3PE	O31-C31	4.21	1.45	1.33
62	M	503	CDL	OB8-CB7	4.20	1.45	1.33
58	H	402	3PE	O31-C31	4.20	1.45	1.33
62	d	201	CDL	OA8-CA7	4.20	1.45	1.33
62	h	201	CDL	OB8-CB7	4.18	1.45	1.33
62	h	201	CDL	OA8-CA7	4.17	1.45	1.33
58	L	701	3PE	O21-C21	4.15	1.46	1.34
58	L	702	3PE	O31-C31	4.14	1.45	1.33
62	M	503	CDL	OB6-CB5	4.12	1.45	1.34
58	L	701	3PE	O31-C31	4.11	1.45	1.33
62	L	703	CDL	OA8-CA7	4.10	1.45	1.33
62	h	201	CDL	OB6-CB5	4.10	1.45	1.34
62	Y	201	CDL	OB8-CB7	4.09	1.45	1.33
58	H	402	3PE	O21-C21	4.09	1.45	1.34
62	d	201	CDL	OB6-CB5	4.08	1.45	1.34
62	h	201	CDL	OA6-CA5	4.08	1.45	1.34
62	q	201	CDL	OB6-CB5	4.08	1.45	1.34
58	M	501	3PE	O21-C21	4.07	1.45	1.34
58	H	403	3PE	O21-C21	4.06	1.45	1.34
58	i	201	3PE	O21-C21	4.06	1.45	1.34
62	M	503	CDL	OA6-CA5	4.06	1.45	1.34
62	L	703	CDL	OB6-CB5	4.05	1.45	1.34
57	I	301	PC1	O21-C21	4.04	1.45	1.34
62	Y	201	CDL	OB6-CB5	4.04	1.45	1.34
57	B	303	PC1	O21-C21	4.04	1.45	1.34
62	Y	201	CDL	OA6-CA5	4.04	1.45	1.34
62	q	201	CDL	OA6-CA5	4.03	1.45	1.34
58	J	201	3PE	O21-C21	4.02	1.45	1.34
58	m	201	3PE	O21-C21	4.01	1.45	1.34
58	D	501	3PE	O21-C21	4.00	1.45	1.34
58	L	705	3PE	O21-C21	4.00	1.45	1.34
58	M	502	3PE	O21-C21	3.99	1.45	1.34
58	L	702	3PE	O21-C21	3.98	1.45	1.34
62	d	201	CDL	OA6-CA5	3.94	1.45	1.34
62	L	703	CDL	OA6-CA5	3.89	1.45	1.34
67	Ac	403	HEM	C4D-ND	-3.70	1.33	1.40
67	AC	402	HEM	FE-NC	3.64	2.07	1.95
67	AC	401	HEM	C4D-ND	-3.60	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Ac	402	HEM	C4D-ND	-3.55	1.34	1.40
68	AC	403	UQ6	C2-C3	3.55	1.45	1.39
56	B	302	UQ1	C3-C2	3.44	1.48	1.36
67	AC	402	HEM	C1B-NB	-3.42	1.34	1.40
67	AC	402	HEM	C4D-ND	-3.41	1.34	1.40
68	AC	403	UQ6	C4-C3	3.34	1.46	1.39
70	Ac	405	U10	C4-C3	3.25	1.48	1.36
60	F	501	FMN	C8-C7	3.24	1.48	1.40
67	Ac	403	HEM	C1B-NB	-3.20	1.34	1.40
67	AC	401	HEM	C1B-NB	-3.02	1.35	1.40
67	Ac	402	HEM	C1B-NB	-2.98	1.35	1.40
67	Ac	403	HEM	C1C-C2C	-2.95	1.39	1.45
70	Ac	405	U10	C6-C5	-2.84	1.38	1.46
67	Ac	403	HEM	C1D-ND	-2.84	1.33	1.38
66	n	201	EHZ	P1-O7	2.78	1.65	1.54
67	Ac	402	HEM	C1C-C2C	-2.74	1.39	1.45
67	AC	401	HEM	C1C-C2C	-2.73	1.39	1.45
65	P	401	NDP	C5A-C6A	2.70	1.48	1.41
67	AC	401	HEM	C1D-ND	-2.69	1.33	1.38
61	H	401	UQ9	C3-C2	-2.68	1.41	1.48
66	W	201	EHZ	P1-O7	2.67	1.64	1.54
64	O	401	ADP	C5-C6	2.62	1.48	1.41
67	Ac	402	HEM	C1D-ND	-2.61	1.33	1.38
66	n	201	EHZ	C9-S1	2.59	1.82	1.76
66	W	201	EHZ	O4-C15	-2.54	1.18	1.23
70	Ac	405	U10	C3-C2	-2.53	1.41	1.48
67	AC	402	HEM	FE-ND	-2.51	1.87	1.94
60	F	501	FMN	C4-N3	-2.50	1.34	1.38
66	n	201	EHZ	O4-C15	-2.48	1.18	1.23
66	W	201	EHZ	O3-C12	-2.48	1.18	1.23
61	H	401	UQ9	C4-C5	-2.47	1.41	1.48
66	W	201	EHZ	C9-S1	2.39	1.81	1.76
65	P	401	NDP	C8A-N7A	2.37	1.36	1.31
65	P	401	NDP	C5A-N7A	-2.35	1.34	1.39
66	n	201	EHZ	O3-C12	-2.32	1.18	1.23
67	AC	402	HEM	C1C-C2C	-2.31	1.40	1.45
67	Ac	402	HEM	FE-NB	2.31	2.02	1.94
66	W	201	EHZ	P1-OP3	-2.31	1.46	1.54
64	O	401	ADP	C5-N7	-2.30	1.34	1.39
60	F	501	FMN	C5A-N5	-2.29	1.35	1.39
67	AC	401	HEM	FE-ND	2.29	2.01	1.94
67	AC	401	HEM	FE-NB	2.28	2.01	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	O	401	ADP	C8-N7	2.26	1.36	1.31
67	Ac	403	HEM	FE-NB	2.26	2.01	1.94
67	Ac	402	HEM	FE-ND	2.26	2.01	1.94
66	n	201	EHZ	P1-OP3	-2.24	1.46	1.54
67	Ac	402	HEM	C3C-C4C	-2.21	1.42	1.46
67	Ac	402	HEM	C4B-NB	-2.11	1.34	1.38
67	AC	401	HEM	C3C-C4C	-2.11	1.42	1.46
69	Ad	401	HEC	C3C-C2C	-2.11	1.34	1.41
69	AD	401	HEC	C3C-C2C	-2.10	1.34	1.41
65	P	401	NDP	C4A-N9A	-2.08	1.33	1.37
67	AC	401	HEM	C4B-NB	-2.07	1.34	1.38
67	AC	402	HEM	C4B-NB	-2.05	1.34	1.38
64	O	401	ADP	C4-N9	-2.03	1.33	1.37
69	AD	401	HEC	C3B-C2B	-2.02	1.34	1.41
67	AC	402	HEM	C1D-ND	-2.02	1.34	1.38
69	AD	401	HEC	CMC-C2C	2.01	1.54	1.50

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	Ad	401	HEC	CBC-CAC-C3C	-8.59	110.27	127.43
69	AD	401	HEC	CBC-CAC-C3C	-8.58	110.29	127.43
69	Ad	401	HEC	CBB-CAB-C3B	-8.33	110.79	127.43
69	AD	401	HEC	CBB-CAB-C3B	-8.33	110.79	127.43
70	Ac	405	U10	C6-C1-C2	7.75	125.28	119.17
68	AC	403	UQ6	C7-C8-C9	-6.39	118.27	127.42
66	W	201	EHZ	C8-C9-S1	6.28	121.48	113.56
68	Ac	406	UQ6	C4M-O4-C4	5.99	131.00	114.74
65	P	401	NDP	C5A-C4A-N3A	-5.73	118.82	126.72
64	O	401	ADP	C5-C4-N3	-5.66	118.92	126.72
66	n	201	EHZ	C8-C9-S1	5.50	120.50	113.56
67	AC	402	HEM	CHC-C4B-NB	5.44	130.28	124.42
68	Ac	406	UQ6	C7-C8-C9	-5.10	120.11	127.42
67	AC	402	HEM	CHD-C1D-ND	4.90	129.70	124.42
67	Ac	402	HEM	CHC-C4B-NB	4.80	129.59	124.42
67	AC	401	HEM	CHC-C4B-NB	4.78	129.56	124.42
68	AC	403	UQ6	O4-C4-C3	-4.66	109.72	120.35
62	M	503	CDL	OA6-CA5-C11	4.62	121.47	111.48
64	O	401	ADP	N3-C4-N9	4.57	134.94	127.17
65	P	401	NDP	N3A-C4A-N9A	4.52	134.85	127.17
67	AC	401	HEM	CHD-C4C-NC	4.38	129.22	124.45
67	Ac	402	HEM	CHD-C4C-NC	4.34	129.18	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	403	HEM	CHC-C4B-NB	4.24	128.99	124.42
57	B	303	PC1	O21-C21-C22	4.24	120.65	111.48
62	L	703	CDL	OB6-CB5-C51	4.22	120.61	111.48
62	h	201	CDL	OB6-CB5-C51	4.20	120.57	111.48
68	AC	403	UQ6	O4-C4-C5	4.14	127.91	119.00
58	M	502	3PE	O21-C21-C22	4.13	120.42	111.48
62	d	201	CDL	OA6-CA5-C11	4.11	120.37	111.48
62	Y	201	CDL	OA6-CA5-C11	4.07	120.28	111.48
58	L	701	3PE	O21-C21-C22	4.02	120.17	111.48
68	Ac	406	UQ6	C10-C9-C11	3.99	122.16	115.23
70	Ac	405	U10	C1-C6-C5	-3.99	115.74	119.62
58	J	201	3PE	O21-C21-C22	3.97	120.06	111.48
62	d	201	CDL	OB6-CB5-C51	3.96	120.05	111.48
67	Ac	402	HEM	CHB-C1B-NB	3.96	129.26	124.37
62	M	503	CDL	OB6-CB5-C51	3.96	120.05	111.48
58	L	702	3PE	O21-C21-C22	3.92	119.96	111.48
57	I	301	PC1	O21-C21-C22	3.91	119.95	111.48
67	Ac	403	HEM	CHB-C1B-NB	3.90	129.19	124.37
62	Y	201	CDL	OB6-CB5-C51	3.90	119.91	111.48
58	m	201	3PE	O21-C21-C22	3.90	119.91	111.48
67	Ac	403	HEM	CHD-C4C-NC	3.86	128.66	124.45
58	L	705	3PE	O21-C21-C22	3.86	119.83	111.48
62	q	201	CDL	OB6-CB5-C51	3.85	119.82	111.48
67	AC	401	HEM	CHB-C1B-NB	3.85	129.12	124.37
62	q	201	CDL	OA6-CA5-C11	3.84	119.80	111.48
58	i	201	3PE	O21-C21-C22	3.81	119.72	111.48
67	AC	402	HEM	CBD-CAD-C3D	-3.81	102.00	112.53
67	AC	402	HEM	CHA-C4D-ND	3.75	129.01	124.37
64	O	401	ADP	C2-N3-C4	3.69	120.86	111.83
65	P	401	NDP	C2A-N3A-C4A	3.69	120.83	111.83
62	h	201	CDL	OA6-CA5-C11	3.64	119.35	111.48
62	L	703	CDL	OA6-CA5-C11	3.62	119.32	111.48
58	H	402	3PE	O21-C21-C22	3.62	119.31	111.48
67	Ac	403	HEM	C4D-ND-C1D	3.62	109.49	105.21
69	Ad	401	HEC	C4D-ND-C1D	3.60	111.69	105.82
58	D	501	3PE	O21-C21-C22	3.60	119.27	111.48
58	M	501	3PE	O21-C21-C22	3.59	119.25	111.48
65	P	401	NDP	C4A-C5A-N7A	-3.58	106.49	110.58
69	AD	401	HEC	C4D-ND-C1D	3.55	111.60	105.82
70	Ac	405	U10	C4-C3-C2	-3.52	114.23	120.69
67	AC	402	HEM	CHB-C1B-NB	3.49	128.68	124.37
67	AC	402	HEM	C1B-NB-C4B	3.41	109.25	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	H	403	3PE	O21-C21-C22	3.35	118.74	111.48
64	O	401	ADP	N3-C2-N1	-3.30	123.59	128.58
64	O	401	ADP	C4-C5-N7	-3.29	106.82	110.58
65	P	401	NDP	N3A-C2A-N1A	-3.23	123.70	128.58
66	W	201	EHZ	O2-C9-C8	-3.22	118.67	123.74
67	Ac	403	HEM	CHD-C1D-ND	3.15	127.81	124.42
67	AC	402	HEM	CHD-C1D-C2D	-3.13	120.08	125.03
68	AC	403	UQ6	C10-C9-C11	3.12	120.64	115.23
66	W	201	EHZ	C14-C13-C12	-3.06	107.29	112.39
58	M	502	3PE	O31-C31-C32	3.05	121.12	111.83
58	M	502	3PE	C2-O21-C21	-3.01	110.58	117.80
65	P	401	NDP	C4A-N9A-C8A	2.99	108.88	105.74
67	AC	402	HEM	CHD-C4C-NC	2.98	127.69	124.45
62	d	201	CDL	CA4-OA6-CA5	-2.96	110.72	117.80
66	W	201	EHZ	OP3-P1-O9	-2.96	99.31	110.83
58	L	702	3PE	C2-O21-C21	-2.94	110.75	117.80
58	L	705	3PE	O31-C31-C32	2.92	120.74	111.83
66	W	201	EHZ	C7-C8-C9	-2.91	107.36	113.86
64	O	401	ADP	C4-N9-C8	2.90	108.78	105.74
66	W	201	EHZ	C13-C12-N1	2.90	121.62	116.34
67	AC	401	HEM	CHD-C1D-ND	2.89	127.54	124.42
58	i	201	3PE	C2-O21-C21	-2.89	110.88	117.80
62	M	503	CDL	OA8-CA7-C31	2.88	120.61	111.83
62	d	201	CDL	OA8-CA7-C31	2.87	120.60	111.83
58	m	201	3PE	O31-C31-C32	2.86	120.55	111.83
62	q	201	CDL	OB8-CB7-C71	2.83	120.46	111.83
58	J	201	3PE	C2-O21-C21	-2.83	111.03	117.80
58	m	201	3PE	C2-O21-C21	-2.83	111.03	117.80
66	n	201	EHZ	O2-C9-C8	-2.81	119.31	123.74
67	Ac	402	HEM	CHD-C1D-ND	2.81	127.45	124.42
58	H	403	3PE	O31-C31-C32	2.78	120.32	111.83
62	Y	201	CDL	OA8-CA7-C31	2.77	120.27	111.83
58	L	702	3PE	O31-C31-C32	2.76	120.24	111.83
67	AC	401	HEM	C4D-ND-C1D	2.76	108.47	105.21
57	I	301	PC1	C2-O21-C21	-2.72	111.28	117.80
68	AC	403	UQ6	C15-C14-C16	2.72	119.94	115.23
62	h	201	CDL	OB8-CB7-C71	2.71	120.11	111.83
66	n	201	EHZ	C10-S1-C9	2.71	109.85	101.84
66	n	201	EHZ	OP3-P1-O9	-2.70	100.33	110.83
58	H	402	3PE	O31-C31-C32	2.69	120.05	111.83
58	J	201	3PE	O31-C31-C32	2.69	120.03	111.83
67	AC	401	HEM	CHA-C1A-NA	2.68	128.72	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Y	201	CDL	CA4-OA6-CA5	-2.67	111.39	117.80
68	Ac	406	UQ6	C6-C7-C8	-2.67	107.50	112.06
67	Ac	402	HEM	CHA-C1A-NA	2.67	128.71	123.86
56	B	302	UQ1	C7-C6-C5	-2.67	120.31	124.89
67	Ac	402	HEM	C4D-ND-C1D	2.67	108.37	105.21
65	P	401	NDP	C5A-N7A-C8A	2.67	107.64	103.45
62	Y	201	CDL	OB8-CB7-C71	2.67	119.96	111.83
58	i	201	3PE	O31-C31-C32	2.65	119.91	111.83
62	L	703	CDL	CB4-OB6-CB5	-2.65	111.46	117.80
67	Ac	402	HEM	C1B-NB-C4B	2.64	108.33	105.21
62	L	703	CDL	OA8-CA7-C31	2.63	119.86	111.83
60	F	501	FMN	O4-C4-C4A	-2.63	119.60	126.53
70	Ac	405	U10	C7-C6-C5	2.62	121.56	118.52
62	h	201	CDL	OA8-CA7-C31	2.61	119.79	111.83
67	AC	402	HEM	C3B-C4B-NB	-2.61	107.60	109.47
67	Ac	403	HEM	C1B-NB-C4B	2.60	108.29	105.21
57	I	301	PC1	O31-C31-C32	2.60	119.75	111.83
70	Ac	405	U10	O4-C4-C5	-2.59	107.90	116.64
62	q	201	CDL	OA8-CA7-C31	2.59	119.72	111.83
62	L	703	CDL	OB8-CB7-C71	2.58	119.72	111.83
67	AC	402	HEM	C4C-CHD-C1D	-2.57	120.55	126.02
62	d	201	CDL	OB8-CB7-C71	2.57	119.66	111.83
58	L	705	3PE	C2-O21-C21	-2.56	111.66	117.80
67	AC	401	HEM	C1B-NB-C4B	2.54	108.21	105.21
67	AC	401	HEM	CHA-C4D-ND	2.53	127.50	124.37
68	AC	403	UQ6	C12-C13-C14	-2.53	121.84	127.62
57	B	303	PC1	O31-C31-C32	2.51	119.48	111.83
58	M	501	3PE	O31-C31-C32	2.51	119.47	111.83
58	D	501	3PE	O31-C31-C32	2.49	119.42	111.83
64	O	401	ADP	C5-N7-C8	2.49	107.36	103.45
67	Ac	402	HEM	CHA-C4D-ND	2.48	127.44	124.37
62	L	703	CDL	CA4-OA6-CA5	-2.48	111.86	117.80
67	Ac	403	HEM	CHB-C1B-C2B	-2.45	119.97	126.95
56	B	302	UQ1	CM5-C5-C6	-2.44	120.44	124.45
60	F	501	FMN	C4A-C10-N1	-2.44	118.61	124.59
67	Ac	403	HEM	C4A-CHB-C1B	-2.42	120.55	126.25
66	W	201	EHZ	C5-C6-C7	-2.41	108.03	114.68
68	AC	403	UQ6	C3M-O3-C3	2.41	121.28	114.74
66	W	201	EHZ	C10-S1-C9	2.40	108.94	101.84
56	B	302	UQ1	C11-C9-C10	2.40	120.10	114.59
62	M	503	CDL	OB8-CB7-C71	2.39	119.12	111.83
66	n	201	EHZ	C5-C6-C7	-2.36	108.17	114.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	303	PC1	C2-O21-C21	-2.35	112.18	117.80
58	Ac	401	3PE	C2-O21-C21	2.34	123.40	117.80
58	M	501	3PE	C2-O21-C21	-2.34	112.21	117.80
62	q	201	CDL	CA4-OA6-CA5	-2.33	112.21	117.80
62	Y	201	CDL	CB4-OB6-CB5	-2.33	112.23	117.80
65	P	401	NDP	N9A-C8A-N7A	-2.31	110.66	113.94
67	AC	402	HEM	CHA-C1A-NA	2.30	128.04	123.86
60	F	501	FMN	C4-C4A-N5	2.29	121.38	118.21
68	Ac	406	UQ6	C16-C14-C15	2.29	119.87	114.59
58	L	701	3PE	O31-C31-C32	2.28	118.78	111.83
62	d	201	CDL	CB4-OB6-CB5	-2.28	112.34	117.80
67	AC	402	HEM	C1A-CHA-C4D	-2.27	120.92	126.25
67	Ac	403	HEM	CHA-C1A-NA	2.26	127.97	123.86
67	AC	401	HEM	CHB-C1B-C2B	-2.26	120.53	126.95
68	AC	403	UQ6	C21-C19-C20	2.25	119.78	114.59
67	Ac	402	HEM	CHB-C1B-C2B	-2.25	120.54	126.95
62	h	201	CDL	CA4-OA6-CA5	-2.25	112.41	117.80
68	AC	403	UQ6	C17-C18-C19	-2.24	120.16	127.64
67	Ac	403	HEM	C1C-CHC-C4B	-2.24	121.25	126.02
67	Ac	403	HEM	C4C-CHD-C1D	-2.24	121.26	126.02
66	W	201	EHZ	O2-C9-S1	-2.23	119.84	122.68
67	Ac	403	HEM	C3B-C4B-NB	-2.23	107.86	109.47
56	B	302	UQ1	C7-C8-C9	-2.23	120.95	127.25
67	AC	402	HEM	CHA-C4D-C3D	-2.23	121.12	125.23
66	W	201	EHZ	O6-P1-O9	2.22	112.43	106.44
61	H	401	UQ9	C7-C6-C1	-2.21	121.10	124.89
67	Ac	403	HEM	C2A-C1A-NA	-2.20	107.72	110.15
65	P	401	NDP	C6A-C5A-N7A	2.18	136.30	132.09
67	Ac	403	HEM	CHA-C4D-ND	2.18	127.06	124.37
69	AD	401	HEC	C2A-C1A-NA	-2.17	108.23	110.32
66	W	201	EHZ	C11-N1-C12	-2.16	118.81	122.82
62	M	503	CDL	CA4-OA6-CA5	-2.16	112.63	117.80
67	Ac	402	HEM	C4B-C3B-C2B	-2.15	105.30	107.28
64	O	401	ADP	C6-C5-N7	2.15	136.24	132.09
64	O	401	ADP	N9-C8-N7	-2.14	110.90	113.94
67	AC	401	HEM	C4B-C3B-C2B	-2.13	105.32	107.28
69	AD	401	HEC	CAA-CBA-CGA	-2.13	108.02	113.67
62	M	503	CDL	OA6-CA5-OA7	-2.12	118.75	123.70
57	B	303	PC1	O21-C21-O22	-2.10	118.80	123.70
67	AC	401	HEM	C1C-CHC-C4B	-2.10	121.56	126.02
69	Ad	401	HEC	C2A-C1A-NA	-2.09	108.30	110.32
67	Ac	402	HEM	C1C-CHC-C4B	-2.09	121.57	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	D	501	3PE	C2-O21-C21	-2.09	112.80	117.80
60	F	501	FMN	C4-N3-C2	-2.09	121.94	125.64
60	F	501	FMN	C4A-C4-N3	2.08	118.54	113.25
62	Y	201	CDL	OB8-CB7-OB9	-2.07	118.44	123.63
65	P	401	NDP	C3D-C2D-C1D	2.07	105.38	101.46
69	Ad	401	HEC	CAA-CBA-CGA	-2.07	108.18	113.67
60	F	501	FMN	O2-C2-N1	-2.06	118.37	121.80
62	q	201	CDL	OA6-CA5-OA7	-2.06	118.88	123.70
62	d	201	CDL	OA6-CA5-OA7	-2.06	118.89	123.70
64	O	401	ADP	C3'-C2'-C1'	2.06	105.36	101.46
58	M	502	3PE	O21-C21-O22	-2.06	118.90	123.70
70	Ac	405	U10	C3M-O3-C3	2.05	123.69	116.47
60	F	501	FMN	C10-N1-C2	2.05	121.29	116.85
66	W	201	EHZ	O3-C12-N1	-2.05	119.01	123.03
68	AC	403	UQ6	C2-C3-C4	-2.05	117.19	119.97
62	h	201	CDL	OA8-CA7-OA9	-2.04	118.53	123.63
67	AC	402	HEM	O2A-CGA-CBA	2.04	120.44	114.00
67	Ac	402	HEM	C4A-CHB-C1B	-2.03	121.46	126.25
67	Ac	403	HEM	CAD-C3D-C4D	2.01	128.21	124.70
67	AC	401	HEM	C4A-CHB-C1B	-2.01	121.52	126.25
62	M	503	CDL	CB4-OB6-CB5	-2.01	112.99	117.80
67	AC	402	HEM	C1C-CHC-C4B	-2.00	121.76	126.02

There are no chirality outliers.

All (459) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	303	PC1	C1-O11-P-O12
57	B	303	PC1	C1-O11-P-O14
57	B	303	PC1	C1-O11-P-O13
57	B	303	PC1	O22-C21-O21-C2
58	D	501	3PE	C1-O11-P-O14
58	H	402	3PE	C1-O11-P-O12
58	H	402	3PE	C1-O11-P-O14
58	H	402	3PE	C11-O13-P-O11
58	H	402	3PE	C11-O13-P-O12
58	H	402	3PE	C11-O13-P-O14
58	H	402	3PE	O32-C31-O31-C3
58	H	402	3PE	C32-C31-O31-C3
58	H	403	3PE	C1-O11-P-O12
58	H	403	3PE	C1-O11-P-O13
58	H	403	3PE	C1-O11-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	H	403	3PE	C11-O13-P-O11
58	H	403	3PE	C11-O13-P-O14
58	J	201	3PE	C1-O11-P-O12
58	J	201	3PE	C1-O11-P-O13
58	J	201	3PE	C1-O11-P-O14
58	L	701	3PE	C1-O11-P-O12
58	L	701	3PE	C1-O11-P-O13
58	L	701	3PE	C22-C21-O21-C2
58	L	702	3PE	C1-O11-P-O12
58	L	702	3PE	C1-O11-P-O13
58	L	702	3PE	C1-O11-P-O14
58	L	702	3PE	C11-O13-P-O11
58	L	702	3PE	C11-O13-P-O12
58	L	702	3PE	C11-O13-P-O14
58	L	702	3PE	O22-C21-O21-C2
58	L	702	3PE	C22-C21-O21-C2
58	L	705	3PE	C1-O11-P-O12
58	L	705	3PE	C1-O11-P-O13
58	L	705	3PE	C11-O13-P-O11
58	L	705	3PE	C11-O13-P-O12
58	L	705	3PE	C11-O13-P-O14
58	L	705	3PE	O22-C21-O21-C2
58	L	705	3PE	C22-C21-O21-C2
58	M	501	3PE	C1-O11-P-O12
58	M	501	3PE	C11-O13-P-O11
58	M	501	3PE	C11-O13-P-O12
58	M	502	3PE	C1-O11-P-O13
58	M	502	3PE	C1-O11-P-O14
58	M	502	3PE	C32-C31-O31-C3
58	M	502	3PE	C22-C21-O21-C2
58	i	201	3PE	C1-O11-P-O12
58	i	201	3PE	C1-O11-P-O13
58	i	201	3PE	C1-O11-P-O14
58	i	201	3PE	C2-C1-O11-P
58	i	201	3PE	C22-C21-O21-C2
58	m	201	3PE	C1-O11-P-O14
58	m	201	3PE	C11-O13-P-O12
58	Ac	401	3PE	C11-O13-P-O11
58	Ac	401	3PE	C11-O13-P-O12
58	Ac	401	3PE	O13-C11-C12-N
58	Ac	404	3PE	O13-C11-C12-N
58	Ag	103	3PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	Ag	103	3PE	C1-O11-P-O13
58	Ag	103	3PE	C1-O11-P-O14
58	Ag	103	3PE	C11-O13-P-O11
58	Ag	103	3PE	C11-O13-P-O12
58	Ag	103	3PE	O13-C11-C12-N
61	H	401	UQ9	C17-C18-C19-C21
61	H	401	UQ9	C17-C18-C19-C20
61	H	401	UQ9	C12-C13-C14-C16
61	H	401	UQ9	C12-C13-C14-C15
61	H	401	UQ9	C7-C8-C9-C11
61	H	401	UQ9	C7-C8-C9-C10
61	H	401	UQ9	C6-C7-C8-C9
62	L	703	CDL	CA3-OA5-PA1-OA2
62	L	703	CDL	CA3-OA5-PA1-OA3
62	L	703	CDL	CA3-OA5-PA1-OA4
62	L	703	CDL	CB2-OB2-PB2-OB4
62	L	703	CDL	CB2-OB2-PB2-OB5
62	L	703	CDL	CB3-OB5-PB2-OB2
62	L	703	CDL	CB3-OB5-PB2-OB3
62	L	703	CDL	C51-CB5-OB6-CB4
62	M	503	CDL	CA2-OA2-PA1-OA3
62	M	503	CDL	CA2-OA2-PA1-OA4
62	M	503	CDL	CA2-OA2-PA1-OA5
62	M	503	CDL	CA3-OA5-PA1-OA2
62	M	503	CDL	C11-CA5-OA6-CA4
62	M	503	CDL	CB2-OB2-PB2-OB3
62	M	503	CDL	CB2-OB2-PB2-OB4
62	M	503	CDL	CB2-OB2-PB2-OB5
62	M	503	CDL	CB3-OB5-PB2-OB2
62	M	503	CDL	CB3-OB5-PB2-OB3
62	M	503	CDL	CB3-OB5-PB2-OB4
62	M	503	CDL	C51-CB5-OB6-CB4
62	Y	201	CDL	CA2-OA2-PA1-OA3
62	Y	201	CDL	CA2-OA2-PA1-OA4
62	Y	201	CDL	CA2-OA2-PA1-OA5
62	Y	201	CDL	CB3-OB5-PB2-OB2
62	Y	201	CDL	CB3-OB5-PB2-OB4
62	d	201	CDL	CA2-OA2-PA1-OA3
62	d	201	CDL	CA2-OA2-PA1-OA4
62	d	201	CDL	CA2-OA2-PA1-OA5
62	d	201	CDL	CA3-OA5-PA1-OA2
62	d	201	CDL	CB2-OB2-PB2-OB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	d	201	CDL	CB2-OB2-PB2-OB5
62	d	201	CDL	CB3-OB5-PB2-OB2
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB3-OB5-PB2-OB2
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	q	201	CDL	CA2-OA2-PA1-OA3
62	q	201	CDL	CA3-OA5-PA1-OA2
62	q	201	CDL	OA7-CA5-OA6-CA4
62	q	201	CDL	C11-CA5-OA6-CA4
62	q	201	CDL	CB2-OB2-PB2-OB3
62	q	201	CDL	CB2-OB2-PB2-OB4
62	q	201	CDL	CB2-OB2-PB2-OB5
62	q	201	CDL	CB3-OB5-PB2-OB2
62	q	201	CDL	CB3-OB5-PB2-OB4
62	Aa	501	CDL	CA2-OA2-PA1-OA3
62	Aa	501	CDL	CA2-OA2-PA1-OA4
62	Aa	501	CDL	CA2-OA2-PA1-OA5
62	Aa	501	CDL	CB2-OB2-PB2-OB4
62	Aa	501	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CA2-OA2-PA1-OA3
62	Ag	101	CDL	CA2-OA2-PA1-OA4
62	Ag	101	CDL	CA2-OA2-PA1-OA5
62	Ag	101	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	CB2-OB2-PB2-OB4
62	Ag	102	CDL	CB2-OB2-PB2-OB5
62	Ag	102	CDL	CB3-OB5-PB2-OB2
62	Ag	102	CDL	CB3-OB5-PB2-OB4
65	P	401	NDP	C2N-C3N-C7N-N7N
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	S1-C10-C11-N1
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	C20-O6-P1-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
66	W	201	EHZ	C20-O6-P1-O9
66	W	201	EHZ	C20-O6-P1-OP3
66	n	201	EHZ	O1-C7-C8-C9
66	n	201	EHZ	C7-C8-C9-S1
66	n	201	EHZ	C10-C11-N1-C12
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
66	n	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C20-O6-P1-O7
66	n	201	EHZ	C20-O6-P1-O9
66	n	201	EHZ	C20-O6-P1-OP3
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	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
67	Ac	402	HEM	C2C-C3C-CAC-CBC
67	Ac	402	HEM	C4C-C3C-CAC-CBC
67	Ac	403	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C4B-C3B-CAB-CBB
67	Ac	403	HEM	C2C-C3C-CAC-CBC
68	AC	403	UQ6	C1-C6-C7-C8
69	AD	401	HEC	C2B-C3B-CAB-CBB
69	AD	401	HEC	C2C-C3C-CAC-CBC
69	Ad	401	HEC	C2B-C3B-CAB-CBB
69	Ad	401	HEC	C2C-C3C-CAC-CBC
70	Ac	405	U10	C7-C8-C9-C10
70	Ac	405	U10	C7-C8-C9-C11
58	M	502	3PE	O32-C31-O31-C3
58	m	201	3PE	O32-C31-O31-C3
70	Ac	405	U10	C12-C13-C14-C15
70	Ac	405	U10	C12-C13-C14-C16
58	m	201	3PE	C32-C31-O31-C3
57	I	301	PC1	O22-C21-O21-C2
58	D	501	3PE	O22-C21-O21-C2
58	L	701	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	M	502	3PE	O22-C21-O21-C2
62	L	703	CDL	OB7-CB5-OB6-CB4
62	M	503	CDL	OA7-CA5-OA6-CA4
62	h	201	CDL	OB7-CB5-OB6-CB4
58	M	501	3PE	C2-C3-O31-C31
57	B	303	PC1	C22-C21-O21-C2
57	I	301	PC1	C22-C21-O21-C2
58	D	501	3PE	C22-C21-O21-C2
68	AC	403	UQ6	C15-C14-C16-C17
68	AC	403	UQ6	C13-C14-C16-C17
58	i	201	3PE	C32-C31-O31-C3
58	i	201	3PE	O22-C21-O21-C2
62	M	503	CDL	OB7-CB5-OB6-CB4
58	H	402	3PE	C22-C21-O21-C2
62	L	703	CDL	C11-CA5-OA6-CA4
68	Ac	406	UQ6	C12-C11-C9-C10
58	i	201	3PE	O32-C31-O31-C3
61	H	401	UQ9	C14-C16-C17-C18
61	H	401	UQ9	C9-C11-C12-C13
68	AC	403	UQ6	C9-C11-C12-C13
58	Ac	404	3PE	C23-C24-C25-C26
58	H	403	3PE	C32-C31-O31-C3
62	Y	201	CDL	C31-CA7-OA8-CA6
62	Y	201	CDL	C71-CB7-OB8-CB6
62	h	201	CDL	C71-CB7-OB8-CB6
62	q	201	CDL	C31-CA7-OA8-CA6
58	Ac	404	3PE	C2C-C2D-C2E-C2F
61	H	401	UQ9	C25-C24-C26-C27
61	H	401	UQ9	C23-C24-C26-C27
68	Ac	406	UQ6	C12-C11-C9-C8
58	H	403	3PE	O32-C31-O31-C3
62	h	201	CDL	OB9-CB7-OB8-CB6
62	Y	201	CDL	OB9-CB7-OB8-CB6
58	H	402	3PE	O22-C21-O21-C2
58	m	201	3PE	C22-C21-O21-C2
62	q	201	CDL	C51-CB5-OB6-CB4
62	Y	201	CDL	OA9-CA7-OA8-CA6
62	h	201	CDL	CA4-CA3-OA5-PA1
58	Ac	404	3PE	C21-C22-C23-C24
62	q	201	CDL	OA9-CA7-OA8-CA6
58	Ac	404	3PE	C2A-C2B-C2C-C2D
62	d	201	CDL	O1-C1-CB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	I	301	PC1	C32-C31-O31-C3
62	L	703	CDL	OA7-CA5-OA6-CA4
62	q	201	CDL	OB7-CB5-OB6-CB4
58	Ag	103	3PE	C32-C33-C34-C35
62	L	703	CDL	C71-CB7-OB8-CB6
62	d	201	CDL	C11-CA5-OA6-CA4
58	m	201	3PE	O22-C21-O21-C2
62	d	201	CDL	CA2-C1-CB2-OB2
62	d	201	CDL	C54-C55-C56-C57
62	d	201	CDL	OA7-CA5-OA6-CA4
62	q	201	CDL	CB6-CB4-OB6-CB5
62	L	703	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	C71-CB7-OB8-CB6
57	I	301	PC1	O32-C31-O31-C3
58	J	201	3PE	C32-C31-O31-C3
58	M	501	3PE	C32-C31-O31-C3
58	Ag	103	3PE	C3C-C3D-C3E-C3F
62	L	703	CDL	C11-C12-C13-C14
58	M	501	3PE	C32-C33-C34-C35
58	Ag	103	3PE	C37-C38-C39-C3A
62	M	503	CDL	C71-CB7-OB8-CB6
62	M	503	CDL	C62-C63-C64-C65
62	Ag	102	CDL	C74-C75-C76-C77
58	Ac	404	3PE	C22-C21-O21-C2
62	d	201	CDL	C31-CA7-OA8-CA6
58	M	501	3PE	C23-C24-C25-C26
58	J	201	3PE	O32-C31-O31-C3
62	d	201	CDL	OB9-CB7-OB8-CB6
62	h	201	CDL	C14-C15-C16-C17
62	L	703	CDL	C31-CA7-OA8-CA6
58	M	501	3PE	O32-C31-O31-C3
58	J	201	3PE	C22-C21-O21-C2
58	J	201	3PE	O22-C21-O21-C2
62	Ag	101	CDL	OB5-CB3-CB4-OB6
57	B	303	PC1	C23-C24-C25-C26
58	M	502	3PE	C2-C3-O31-C31
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
67	Ac	403	HEM	C4C-C3C-CAC-CBC
62	M	503	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	OA9-CA7-OA8-CA6
57	B	303	PC1	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	Ag	102	CDL	C1-CB2-OB2-PB2
62	L	703	CDL	OA9-CA7-OA8-CA6
58	Ac	404	3PE	O22-C21-O21-C2
61	H	401	UQ9	C13-C14-C16-C17
61	H	401	UQ9	C12-C11-C9-C8
58	J	201	3PE	C2A-C2B-C2C-C2D
58	L	702	3PE	C24-C25-C26-C27
58	H	402	3PE	C2E-C2F-C2G-C2H
58	H	402	3PE	C31-C32-C33-C34
61	H	401	UQ9	C15-C14-C16-C17
67	AC	401	HEM	C2A-CAA-CBA-CGA
67	Ac	402	HEM	C2A-CAA-CBA-CGA
58	H	402	3PE	C3-C2-O21-C21
58	L	705	3PE	C3C-C3D-C3E-C3F
58	i	201	3PE	C27-C28-C29-C2A
61	H	401	UQ9	C12-C11-C9-C10
62	L	703	CDL	C74-C75-C76-C77
58	H	403	3PE	C3E-C3F-C3G-C3H
62	Ag	101	CDL	OB5-CB3-CB4-CB6
62	Ag	102	CDL	OB5-CB3-CB4-CB6
58	L	702	3PE	C28-C29-C2A-C2B
66	W	201	EHZ	N2-C15-C16-C17
62	h	201	CDL	C18-C19-C20-C21
66	n	201	EHZ	C3-C4-C5-C6
58	Ac	404	3PE	C29-C2A-C2B-C2C
66	n	201	EHZ	C5-C6-C7-O1
58	D	501	3PE	C24-C25-C26-C27
62	Ag	102	CDL	OB5-CB3-CB4-OB6
58	Ac	404	3PE	C2B-C2C-C2D-C2E
58	H	403	3PE	C37-C38-C39-C3A
66	W	201	EHZ	C3-C4-C5-C6
66	n	201	EHZ	C6-C7-C8-C9
58	Ac	404	3PE	C32-C31-O31-C3
62	Aa	501	CDL	OB5-CB3-CB4-CB6
67	AC	402	HEM	C2C-C3C-CAC-CBC
58	L	701	3PE	C3-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5
62	Aa	501	CDL	OB5-CB3-CB4-OB6
58	Ac	404	3PE	O32-C31-O31-C3
57	I	301	PC1	C11-C12-N-C13
58	L	705	3PE	C27-C28-C29-C2A
65	P	401	NDP	PN-O3-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	L	705	3PE	C32-C31-O31-C3
62	M	503	CDL	C31-CA7-OA8-CA6
57	I	301	PC1	C11-C12-N-C15
66	W	201	EHZ	O4-C15-C16-O5
66	n	201	EHZ	O4-C15-C16-O5
65	P	401	NDP	O4D-C1D-N1N-C6N
66	W	201	EHZ	C18-C17-C20-O6
66	W	201	EHZ	C19-C17-C20-O6
62	Ag	102	CDL	CB4-CB3-OB5-PB2
66	W	201	EHZ	C11-C10-S1-C9
69	AD	401	HEC	C4B-C3B-CAB-CBB
69	AD	401	HEC	C4C-C3C-CAC-CBC
69	Ad	401	HEC	C4B-C3B-CAB-CBB
69	Ad	401	HEC	C4C-C3C-CAC-CBC
62	d	201	CDL	C51-CB5-OB6-CB4
58	L	705	3PE	O32-C31-O31-C3
62	M	503	CDL	OA9-CA7-OA8-CA6
58	L	701	3PE	C36-C37-C38-C39
58	H	402	3PE	C1-O11-P-O13
58	H	403	3PE	C11-O13-P-O12
58	L	701	3PE	C1-O11-P-O14
58	L	705	3PE	C1-O11-P-O14
58	M	501	3PE	C1-O11-P-O13
58	M	501	3PE	C1-O11-P-O14
58	M	502	3PE	C1-O11-P-O12
58	M	502	3PE	C11-O13-P-O11
58	M	502	3PE	C11-O13-P-O12
58	M	502	3PE	C11-O13-P-O14
58	m	201	3PE	C1-O11-P-O13
58	m	201	3PE	C11-O13-P-O11
58	m	201	3PE	C11-O13-P-O14
58	Ac	401	3PE	C11-O13-P-O14
62	L	703	CDL	CB3-OB5-PB2-OB4
62	M	503	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	CA3-OA5-PA1-OA2
62	h	201	CDL	CB3-OB5-PB2-OB4
62	q	201	CDL	CA3-OA5-PA1-OA3
62	q	201	CDL	CB3-OB5-PB2-OB3
62	Aa	501	CDL	CB2-OB2-PB2-OB3
62	Aa	501	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	Aa	501	CDL	CB3-OB5-PB2-OB3
62	Aa	501	CDL	CB3-OB5-PB2-OB4
58	L	702	3PE	C33-C34-C35-C36
58	L	701	3PE	C2-C1-O11-P
62	Y	201	CDL	C1-CA2-OA2-PA1
62	q	201	CDL	C1-CA2-OA2-PA1
62	L	703	CDL	C32-C33-C34-C35
58	M	502	3PE	C2D-C2E-C2F-C2G
60	F	501	FMN	C5'-O5'-P-O1P
66	W	201	EHZ	C5-C6-C7-O1
66	n	201	EHZ	C5-C6-C7-C8
62	h	201	CDL	CB4-CB3-OB5-PB2
58	L	705	3PE	C36-C37-C38-C39
62	d	201	CDL	OB7-CB5-OB6-CB4
70	Ac	405	U10	C12-C11-C9-C10
66	n	201	EHZ	C7-C8-C9-O2
62	Y	201	CDL	C55-C56-C57-C58
58	J	201	3PE	C36-C37-C38-C39
65	P	401	NDP	C2B-O2B-P2B-O2X
58	Ag	103	3PE	C35-C36-C37-C38
66	n	201	EHZ	C2-C3-C4-C5
66	W	201	EHZ	C2-C3-C4-C5
58	D	501	3PE	C32-C31-O31-C3
70	Ac	405	U10	C12-C11-C9-C8
58	D	501	3PE	O32-C31-O31-C3
62	M	503	CDL	C58-C59-C60-C61
58	H	403	3PE	C24-C25-C26-C27
67	AC	401	HEM	CAA-CBA-CGA-O2A
67	Ac	402	HEM	CAA-CBA-CGA-O2A
62	M	503	CDL	CB4-CB3-OB5-PB2
57	I	301	PC1	C11-C12-N-C14
67	AC	402	HEM	CAA-CBA-CGA-O1A
66	W	201	EHZ	N2-C15-C16-O5
58	m	201	3PE	C3-C2-O21-C21
62	Y	201	CDL	C56-C57-C58-C59
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	Ac	402	HEM	CAA-CBA-CGA-O1A
62	Ag	101	CDL	C72-C71-CB7-OB8
62	Ag	102	CDL	C1-CA2-OA2-PA1
66	W	201	EHZ	O2-C9-S1-C10
67	AC	402	HEM	CAA-CBA-CGA-O2A
67	Ac	402	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-O1D
67	AC	402	HEM	CAD-CBD-CGD-O1D
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O2D
67	Ac	403	HEM	CAA-CBA-CGA-O2A
67	Ac	403	HEM	CAD-CBD-CGD-O1D
62	M	503	CDL	C36-C37-C38-C39
67	Ac	403	HEM	CAD-CBD-CGD-O2D
57	B	303	PC1	C1-C2-C3-O31
62	L	703	CDL	CA3-CA4-CA6-OA8
62	M	503	CDL	CB3-CB4-CB6-OB8
67	AC	402	HEM	CAD-CBD-CGD-O2D
58	J	201	3PE	O11-C1-C2-O21
58	M	502	3PE	C34-C35-C36-C37
62	Ag	102	CDL	C72-C73-C74-C75
62	Ag	102	CDL	C52-C51-CB5-OB6
58	J	201	3PE	O21-C2-C3-O31
58	L	702	3PE	C2-C1-O11-P
64	O	401	ADP	C4'-C5'-O5'-PA
57	I	301	PC1	C32-C33-C34-C35
62	Ag	101	CDL	C72-C71-CB7-OB9
67	Ac	403	HEM	CAA-CBA-CGA-O1A
58	M	502	3PE	C32-C33-C34-C35
58	J	201	3PE	C38-C39-C3A-C3B
62	d	201	CDL	CB4-CB3-OB5-PB2
62	q	201	CDL	CA4-CA3-OA5-PA1
67	AC	402	HEM	C4C-C3C-CAC-CBC
66	W	201	EHZ	C15-C16-C17-C18
58	D	501	3PE	C32-C33-C34-C35
62	Y	201	CDL	OA7-CA5-OA6-CA4
58	J	201	3PE	O11-C1-C2-C3
61	H	401	UQ9	C20-C19-C21-C22
62	Aa	501	CDL	C32-C31-CA7-OA8
62	Y	201	CDL	C11-CA5-OA6-CA4
66	W	201	EHZ	O5-C16-C17-C18
61	H	401	UQ9	C18-C19-C21-C22
66	W	201	EHZ	O4-C15-C16-C17
58	L	702	3PE	C26-C27-C28-C29
58	D	501	3PE	C34-C35-C36-C37
64	O	401	ADP	O4'-C4'-C5'-O5'
58	Ac	401	3PE	O31-C31-C32-C33
62	Aa	501	CDL	CB3-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
62	d	201	CDL	C32-C31-CA7-OA8
62	d	201	CDL	C57-C58-C59-C60
57	B	303	PC1	O32-C31-O31-C3
66	W	201	EHZ	C15-C16-C17-C20
57	B	303	PC1	C32-C31-O31-C3
57	B	303	PC1	C3-C2-O21-C21
62	Ag	101	CDL	C32-C31-CA7-OA8
62	d	201	CDL	C1-CB2-OB2-PB2
62	q	201	CDL	CB4-CB3-OB5-PB2
58	L	701	3PE	C22-C23-C24-C25
62	Aa	501	CDL	C32-C31-CA7-OA9
62	d	201	CDL	C56-C57-C58-C59
62	h	201	CDL	C11-C12-C13-C14
58	Ac	404	3PE	O21-C21-C22-C23
65	P	401	NDP	C2N-C3N-C7N-O7N
66	n	201	EHZ	N2-C15-C16-O5
62	d	201	CDL	C34-C35-C36-C37
62	h	201	CDL	C16-C17-C18-C19
58	H	403	3PE	C33-C34-C35-C36
62	Aa	501	CDL	C12-C11-CA5-OA6
62	Y	201	CDL	C54-C55-C56-C57
58	L	701	3PE	O32-C31-O31-C3
65	P	401	NDP	PN-O3-PA-O1A
62	d	201	CDL	C32-C31-CA7-OA9

There are no ring outliers.

44 monomers are involved in 338 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	B	301	SF4	3	0
58	H	402	3PE	7	0
68	Ac	406	UQ6	10	0
58	M	502	3PE	5	0
61	H	401	UQ9	28	0
65	P	401	NDP	5	0
67	Ac	402	HEM	1	0
55	F	502	SF4	6	0
58	Ac	404	3PE	1	0
58	L	701	3PE	5	0
62	q	201	CDL	22	0
70	Ac	405	U10	11	0
58	M	501	3PE	10	0

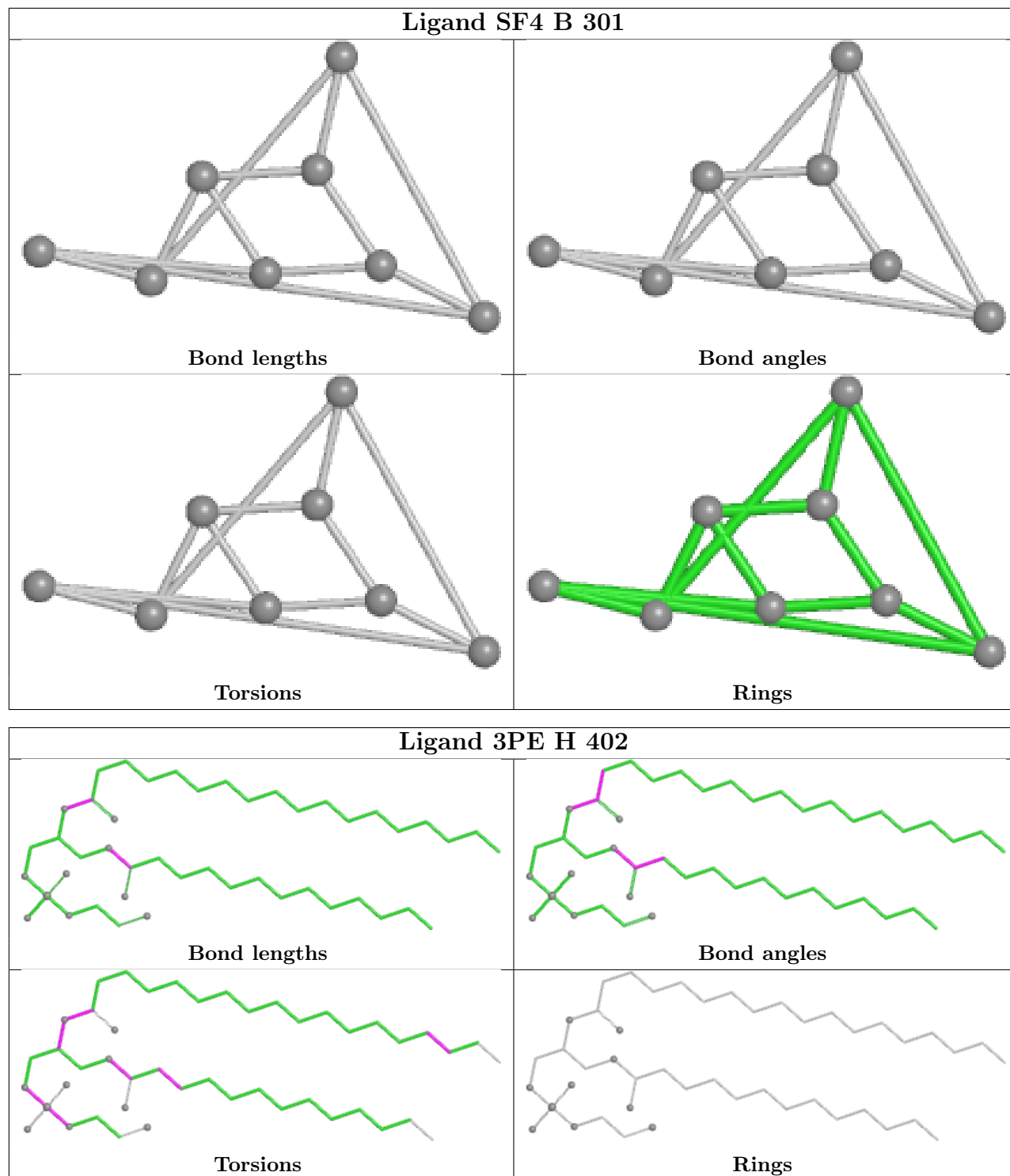
Continued on next page...

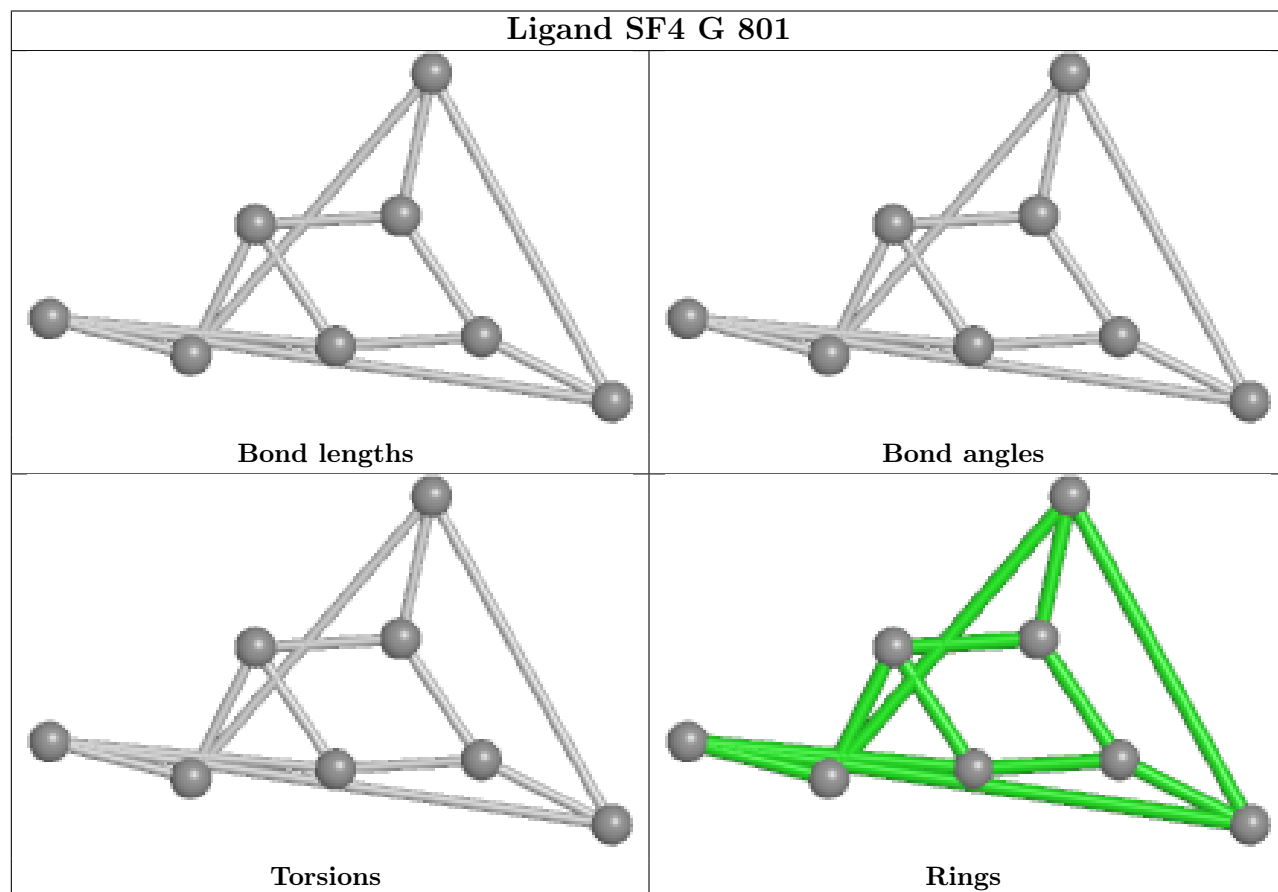
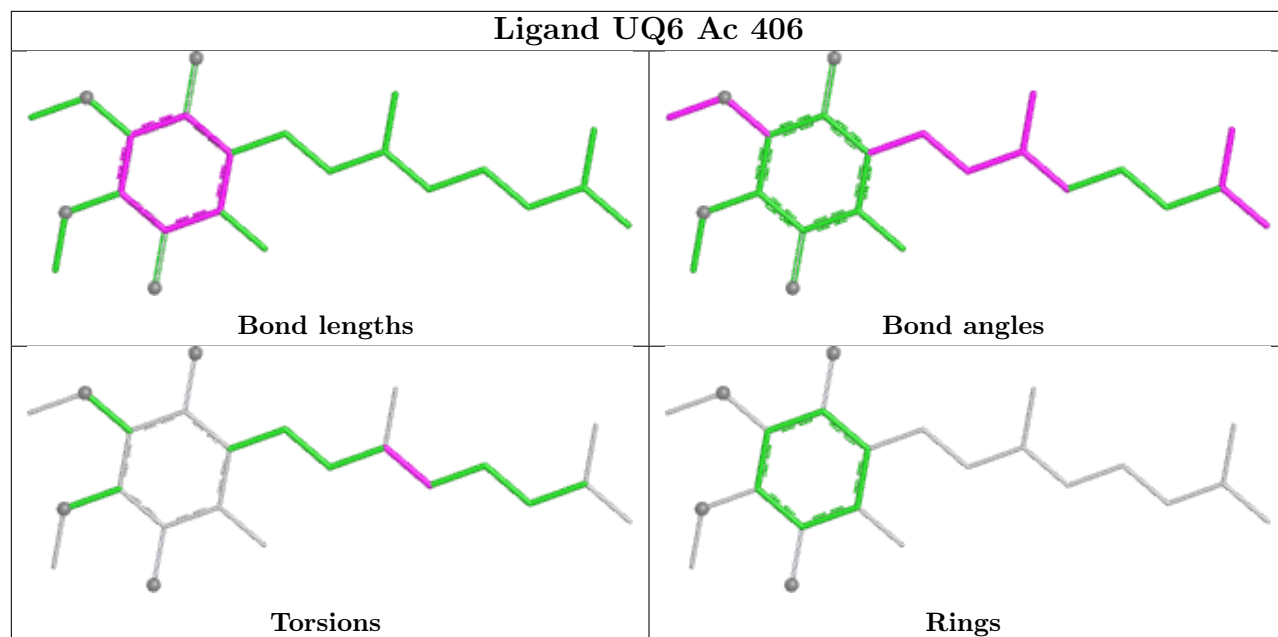
Continued from previous page...

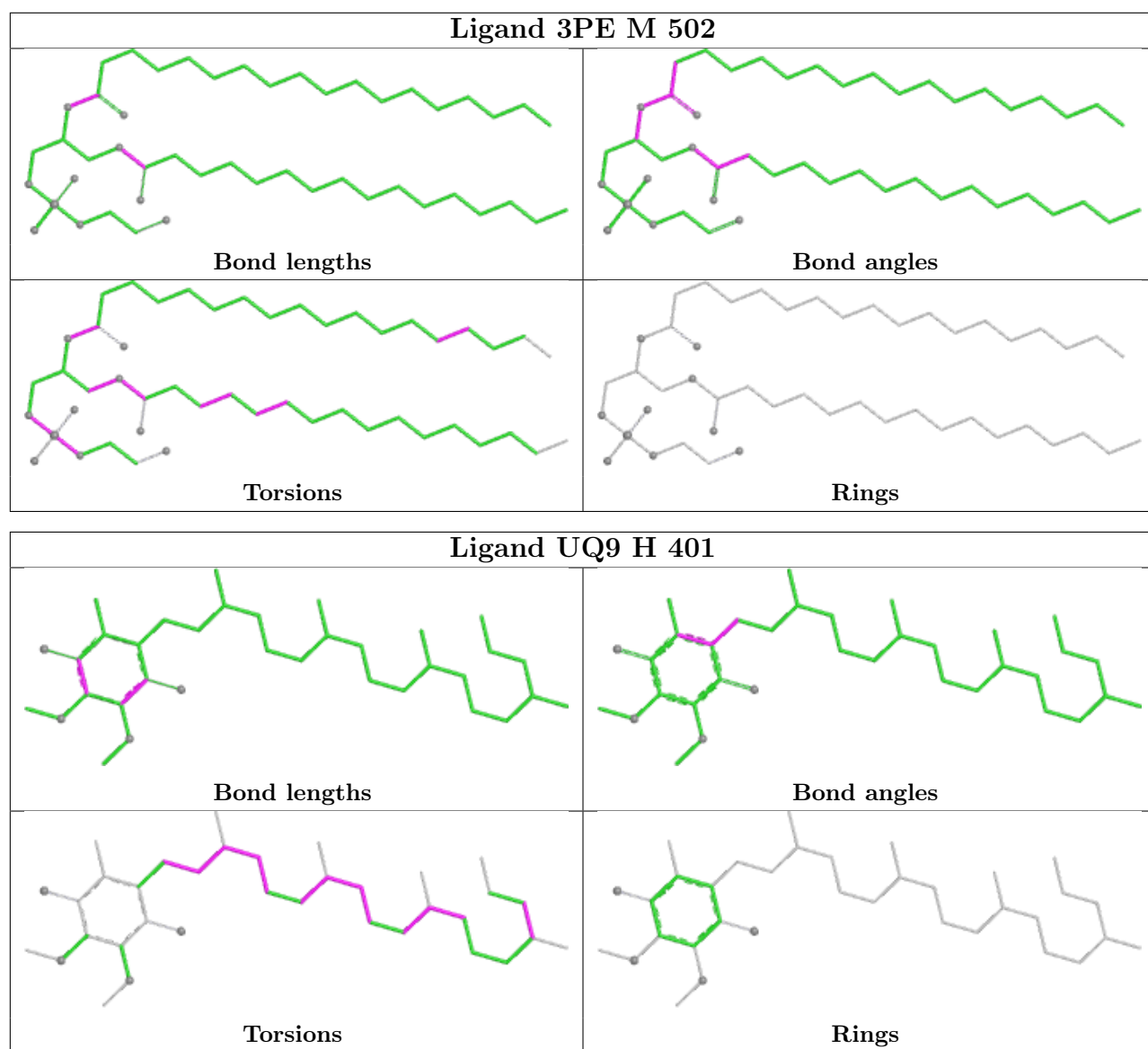
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	h	201	CDL	13	0
58	D	501	3PE	6	0
68	AC	403	UQ6	29	0
62	Y	201	CDL	5	0
62	Aa	501	CDL	1	0
58	L	702	3PE	9	0
59	E	301	FES	4	0
67	AC	402	HEM	30	0
69	AD	401	HEC	13	0
58	J	201	3PE	1	0
67	AC	401	HEM	1	0
62	L	703	CDL	12	0
56	B	302	UQ1	3	0
66	n	201	EHZ	1	0
59	G	803	FES	5	0
66	W	201	EHZ	4	0
57	B	303	PC1	6	0
62	M	503	CDL	12	0
58	L	705	3PE	4	0
62	d	201	CDL	8	0
62	Ag	102	CDL	3	0
58	Ac	401	3PE	2	0
69	Ad	401	HEC	12	0
58	i	201	3PE	11	0
57	I	301	PC1	8	0
64	O	401	ADP	3	0
67	Ac	403	HEM	8	0
58	H	403	3PE	11	0
58	m	201	3PE	9	0
55	G	802	SF4	2	0
55	I	303	SF4	5	0

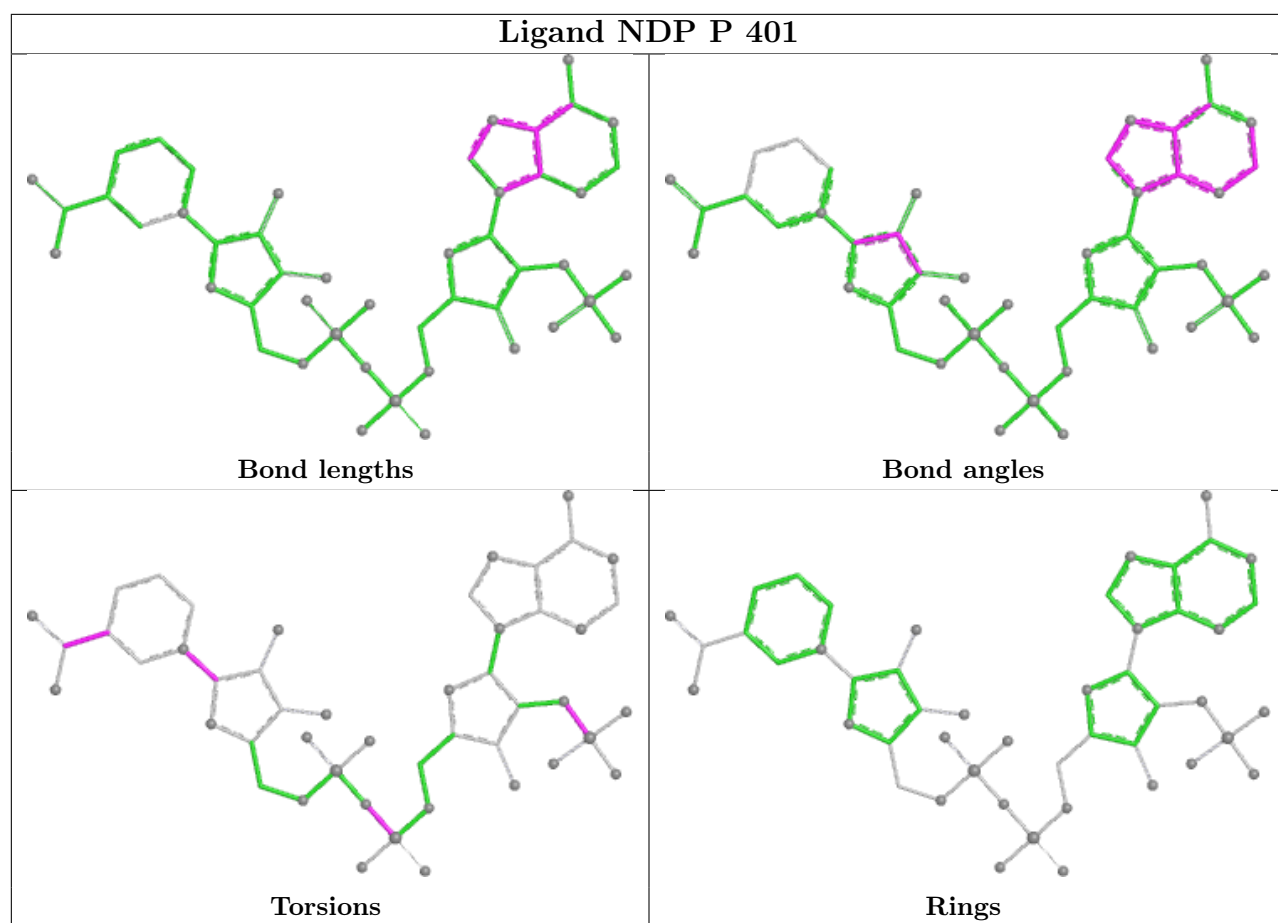
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

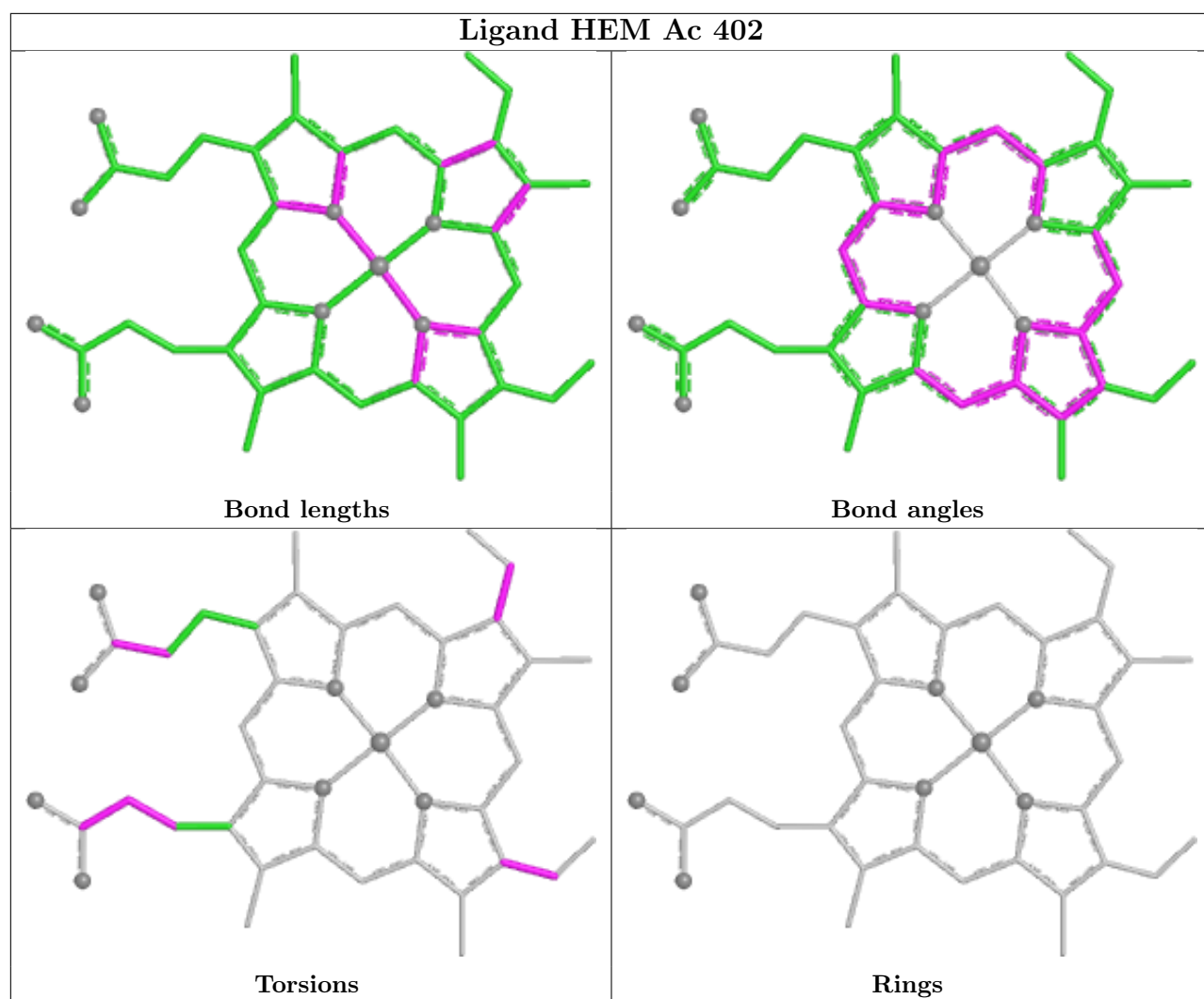
equivalents in the CSD to analyse the geometry.

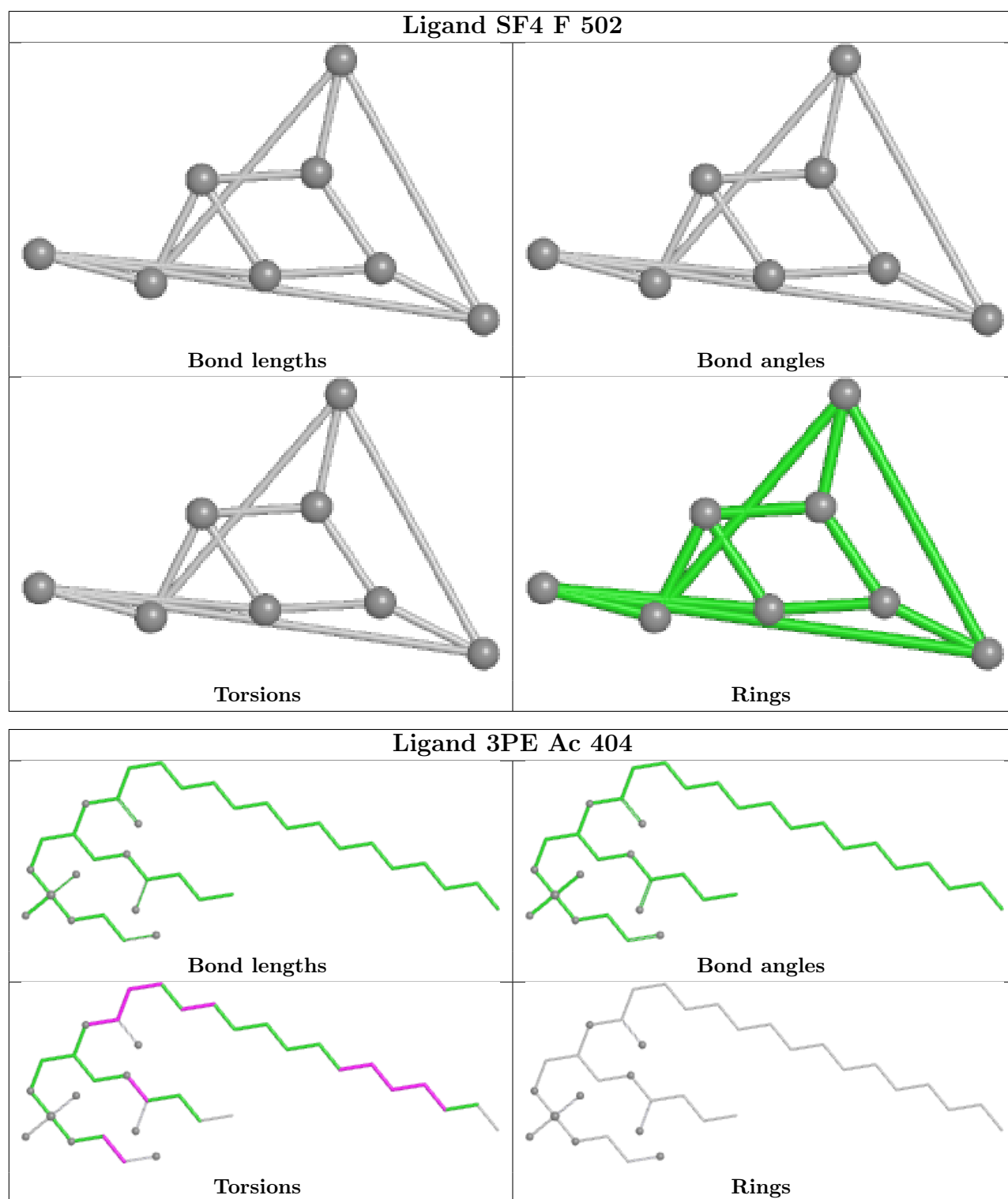


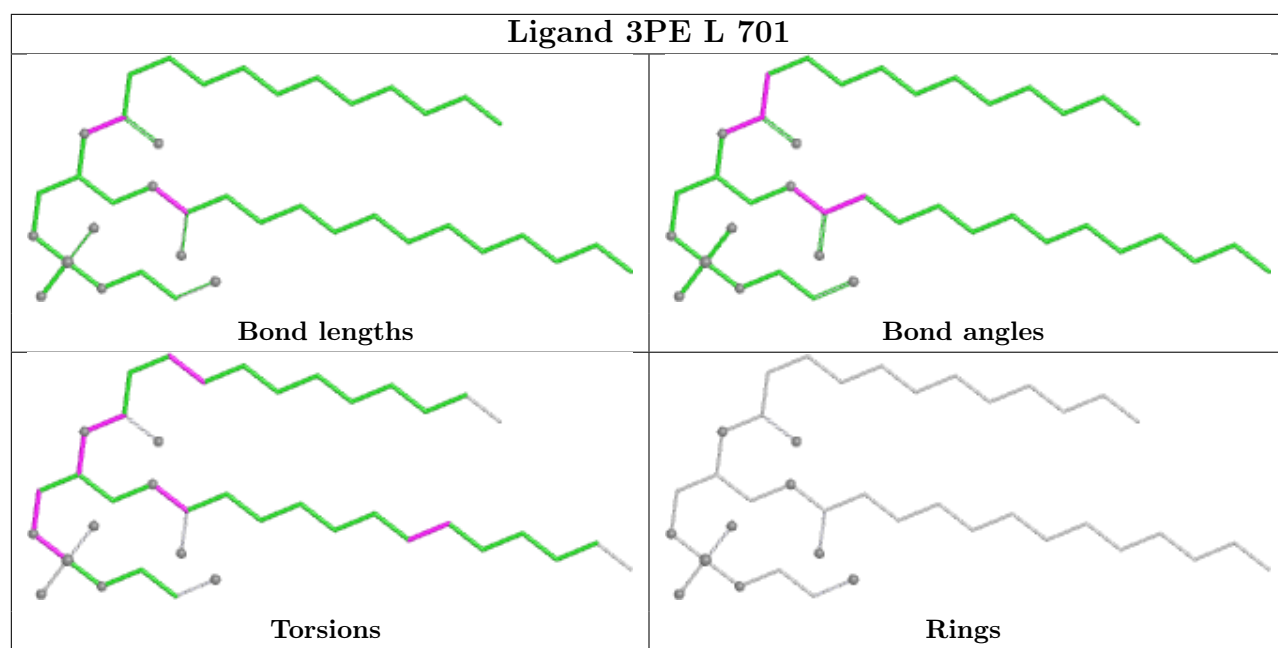


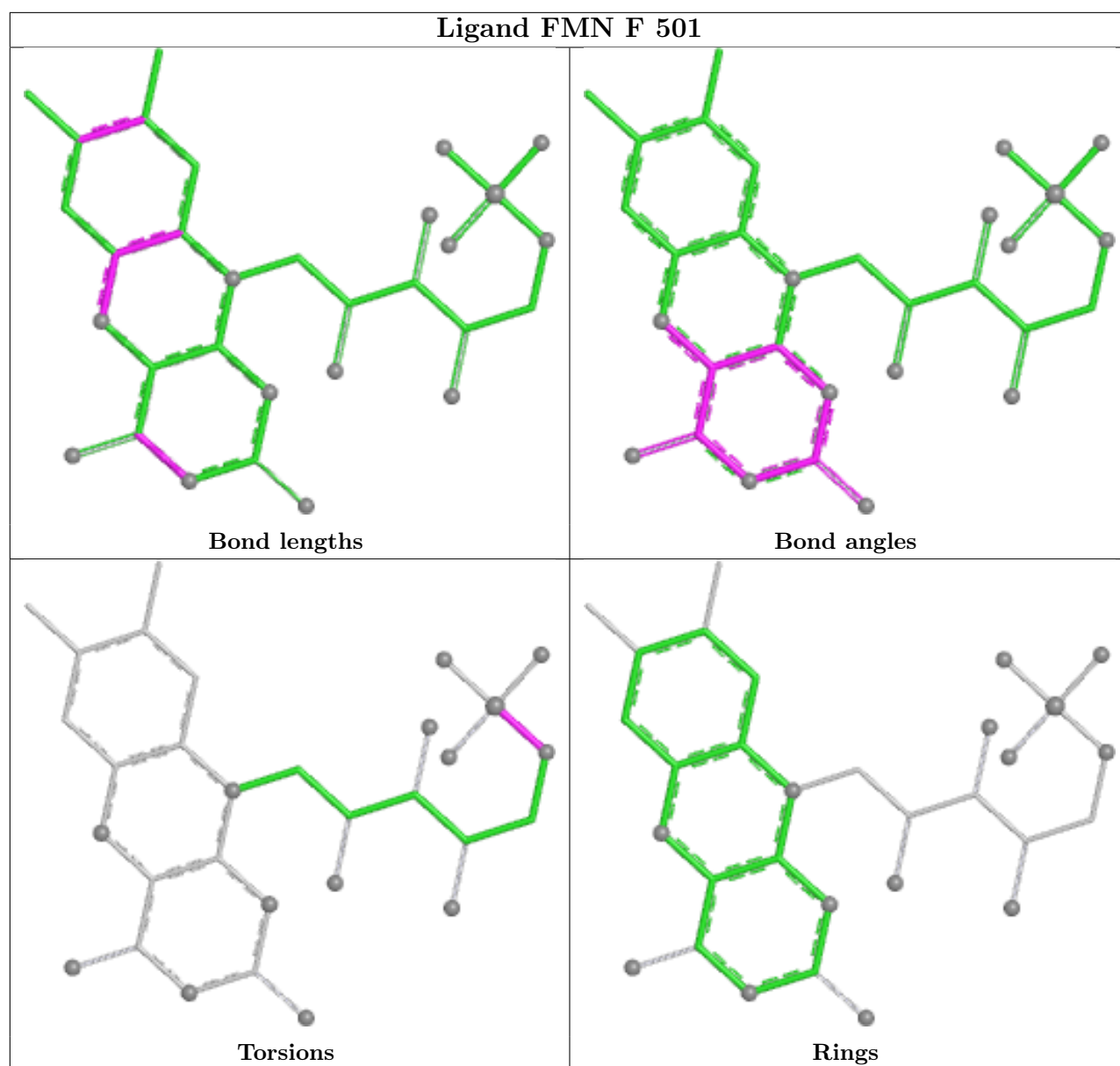


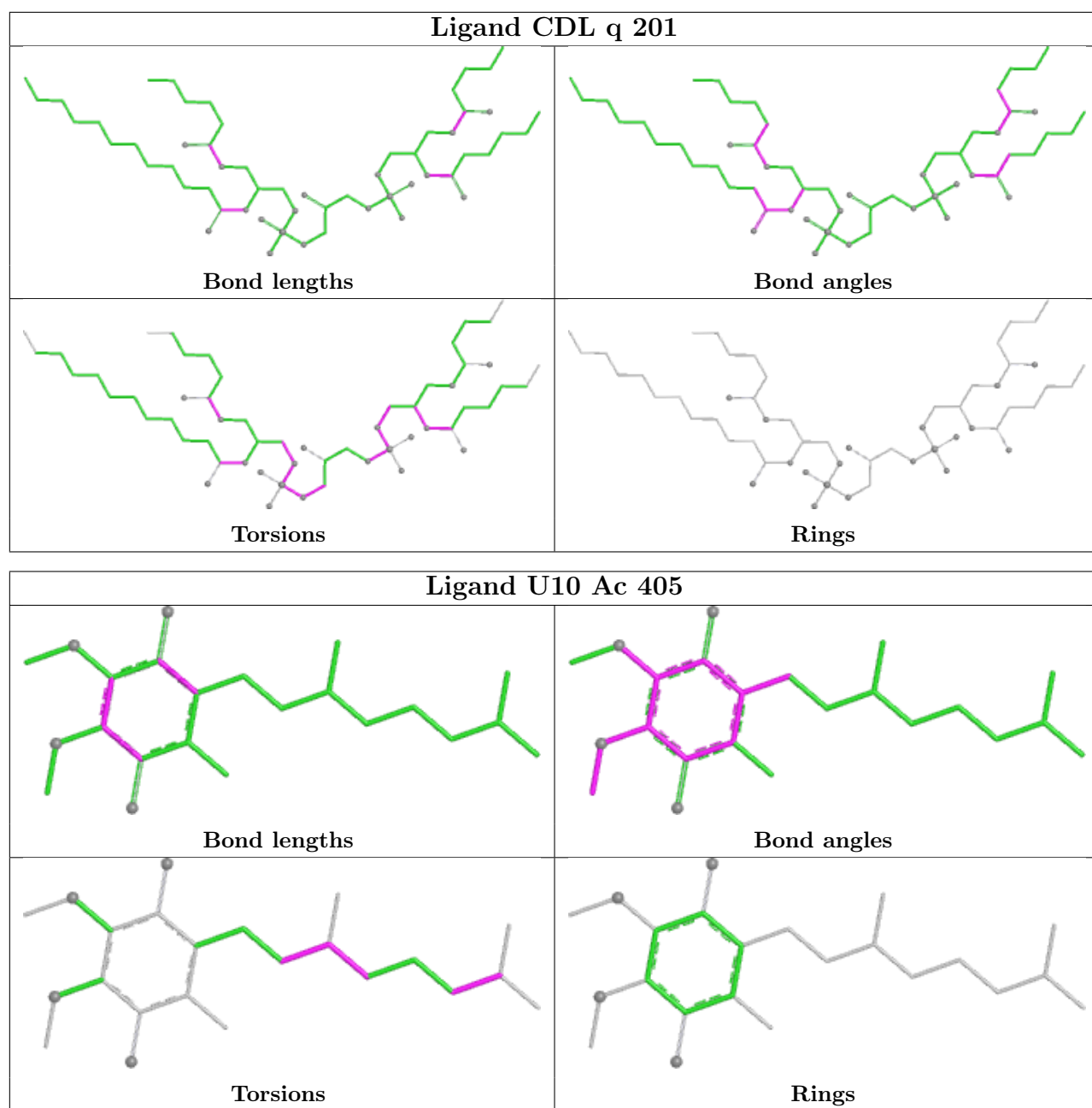


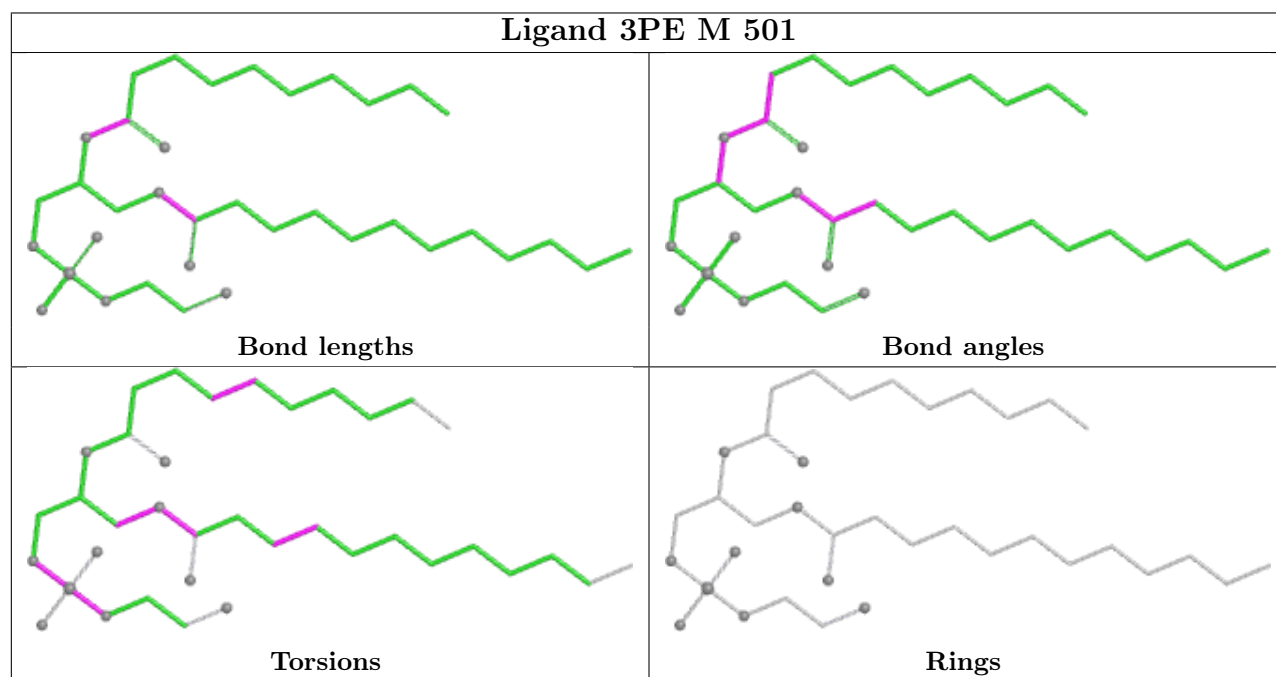
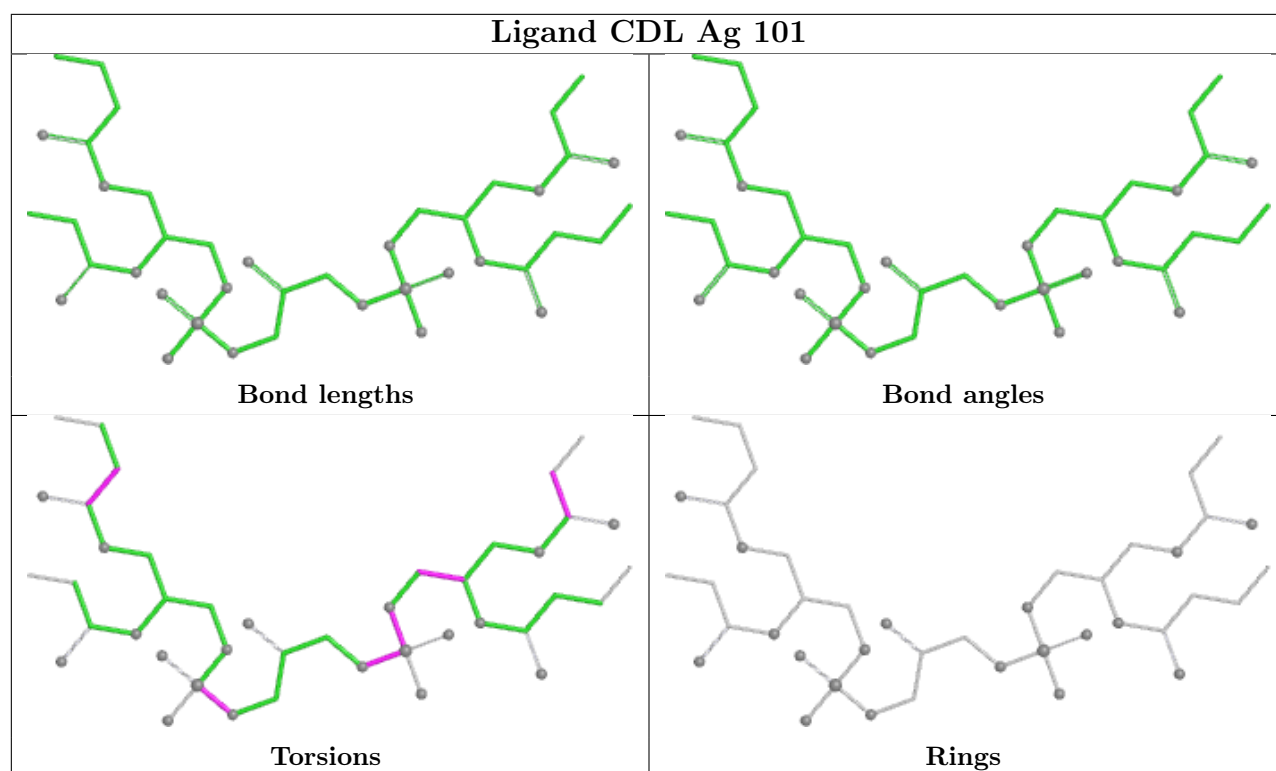


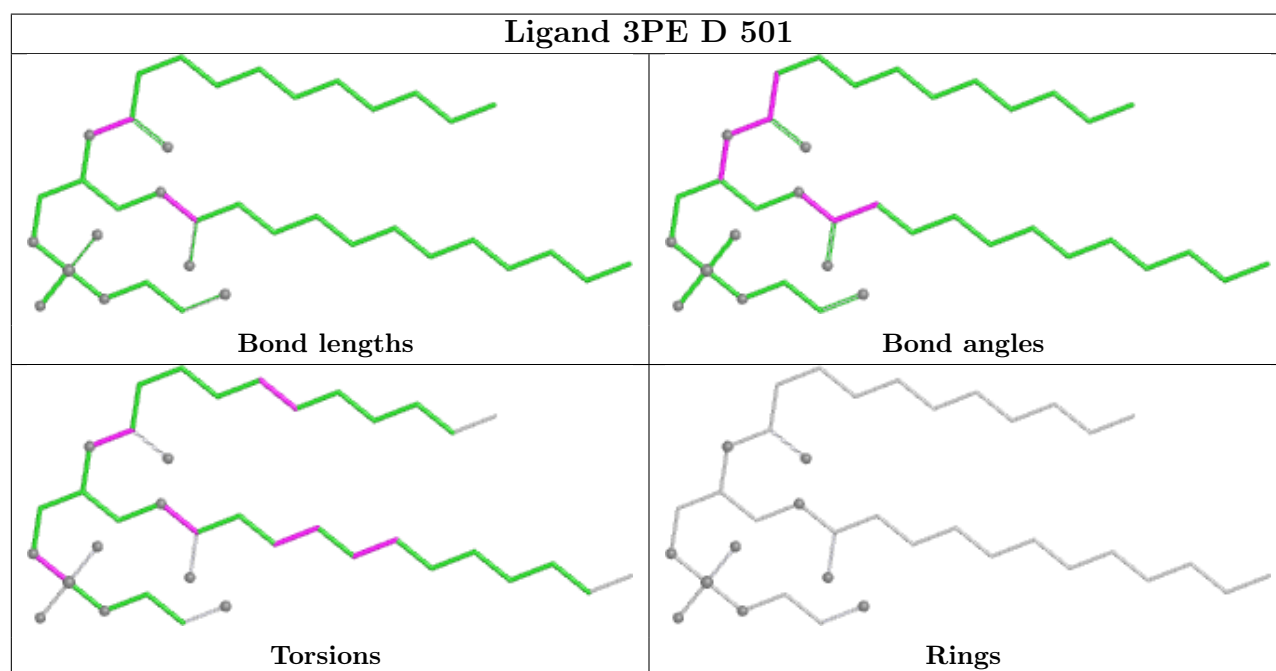
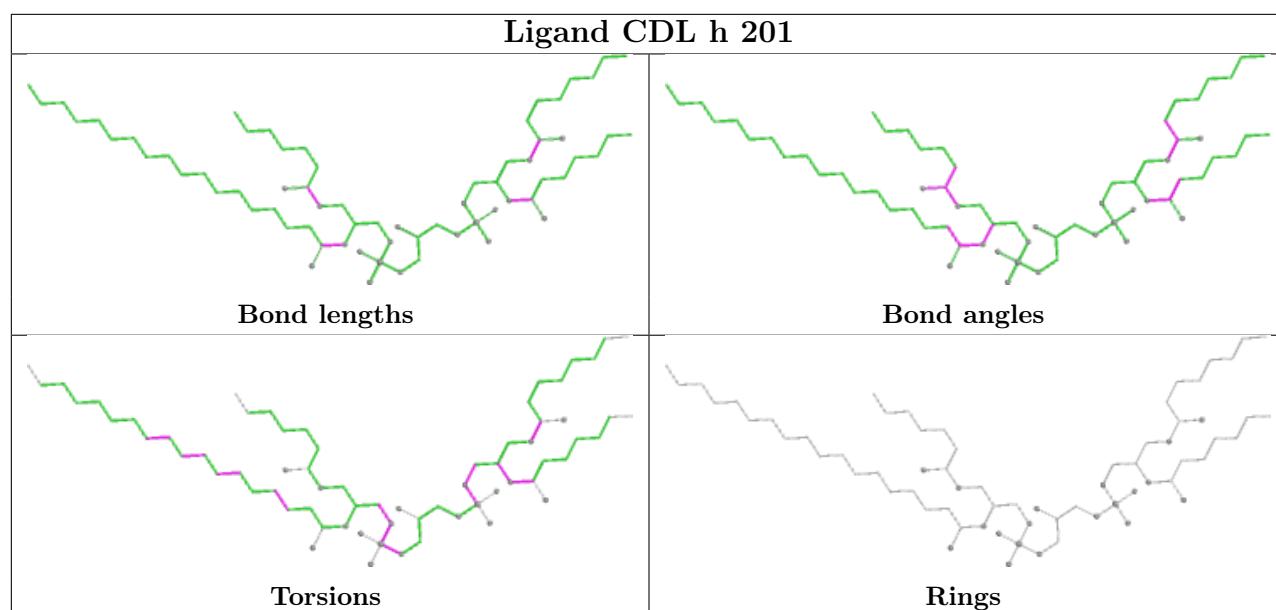


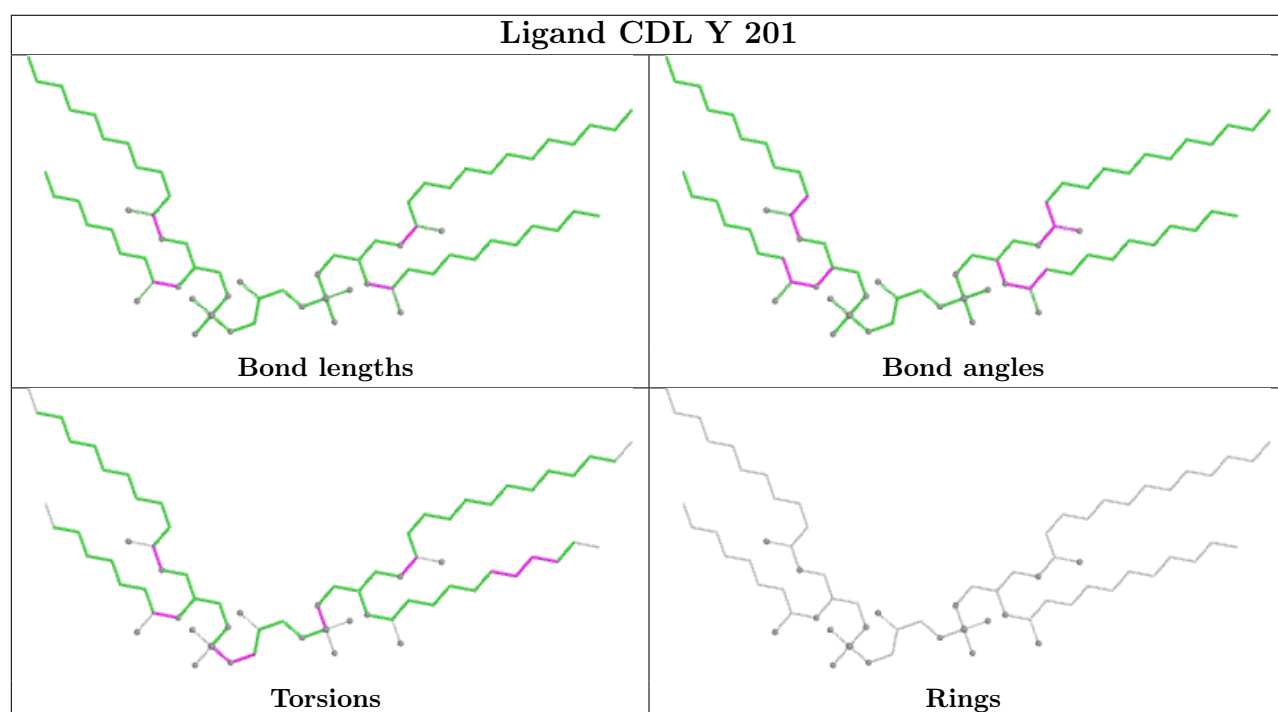
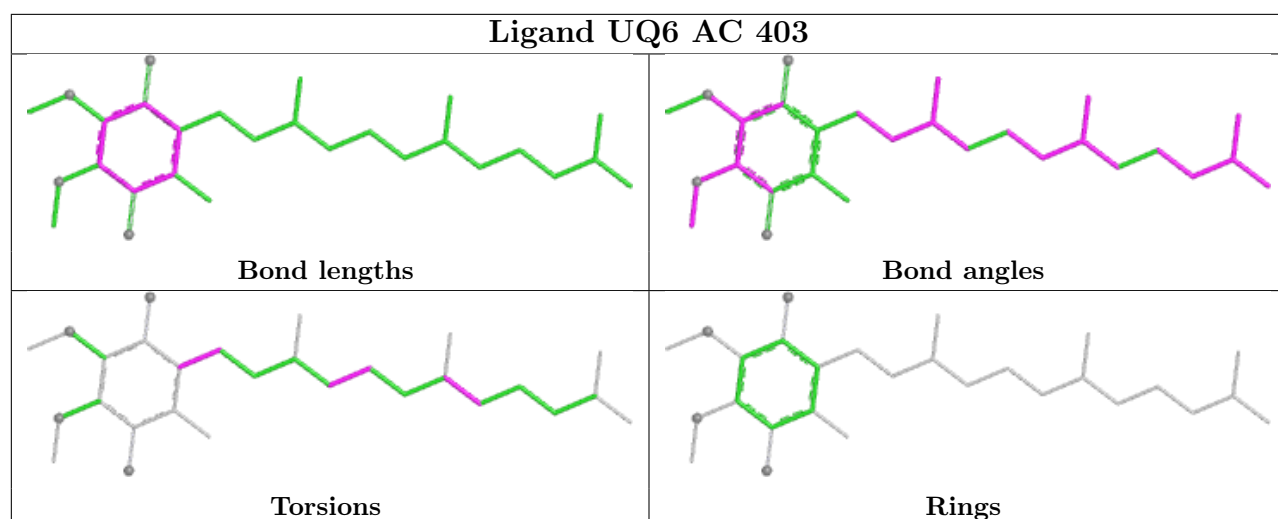


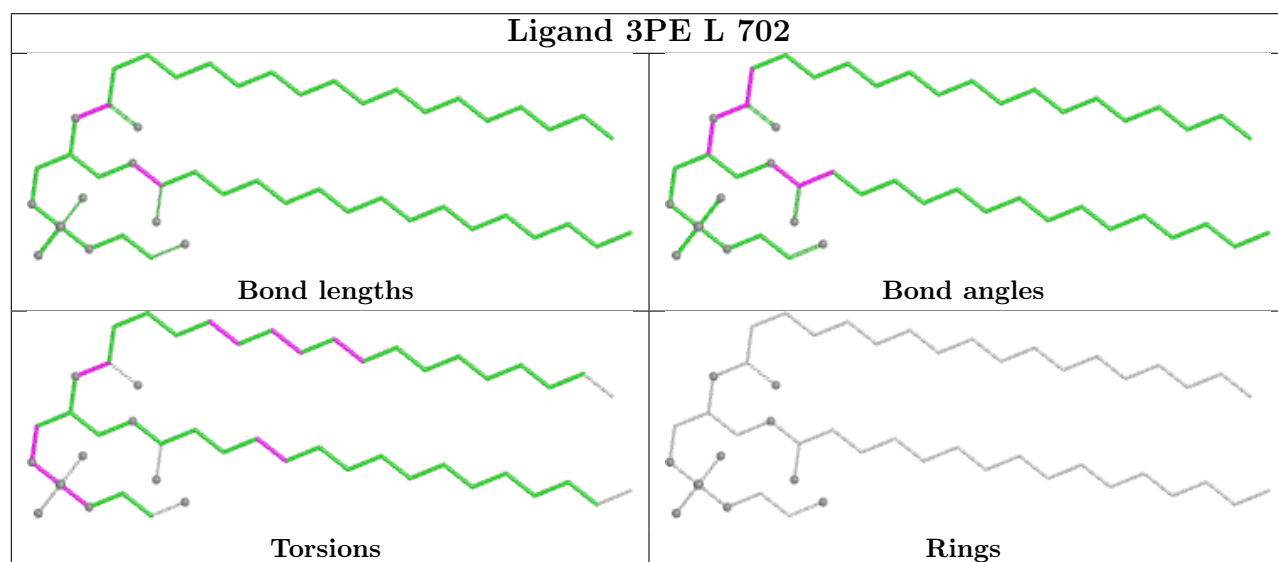
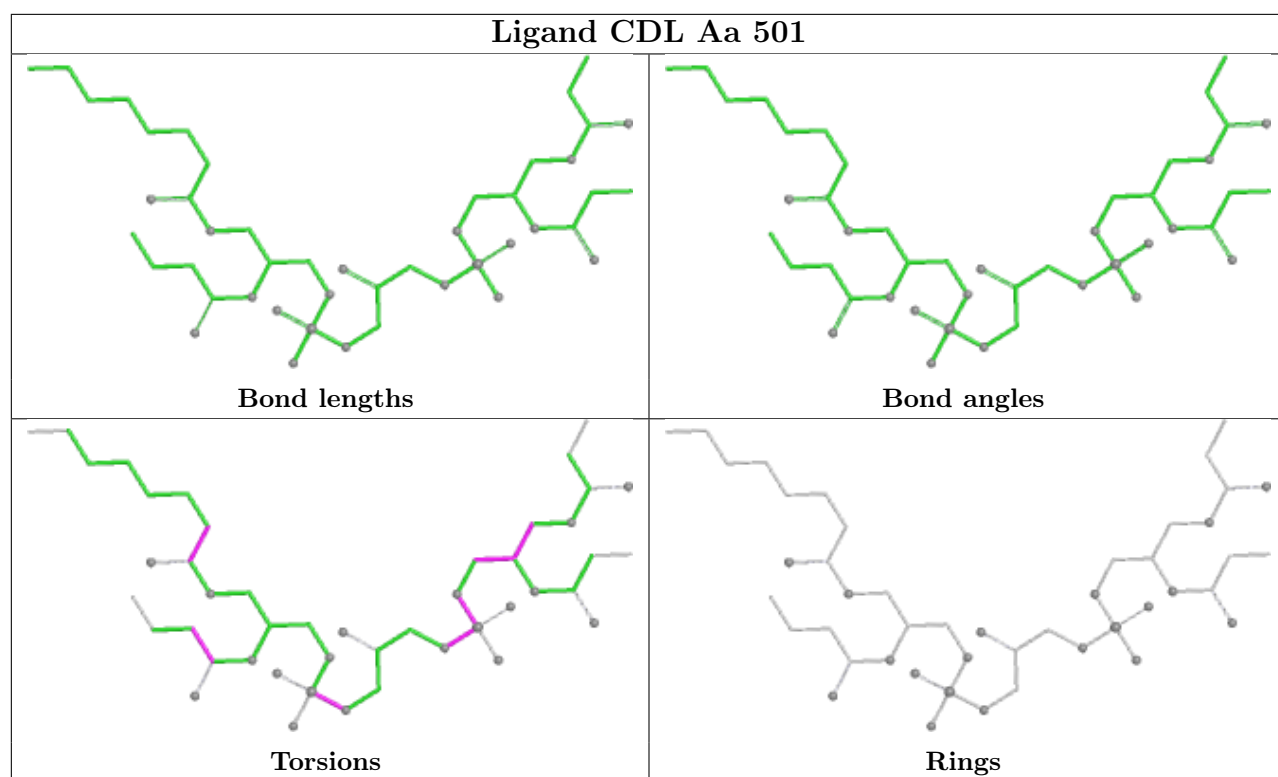


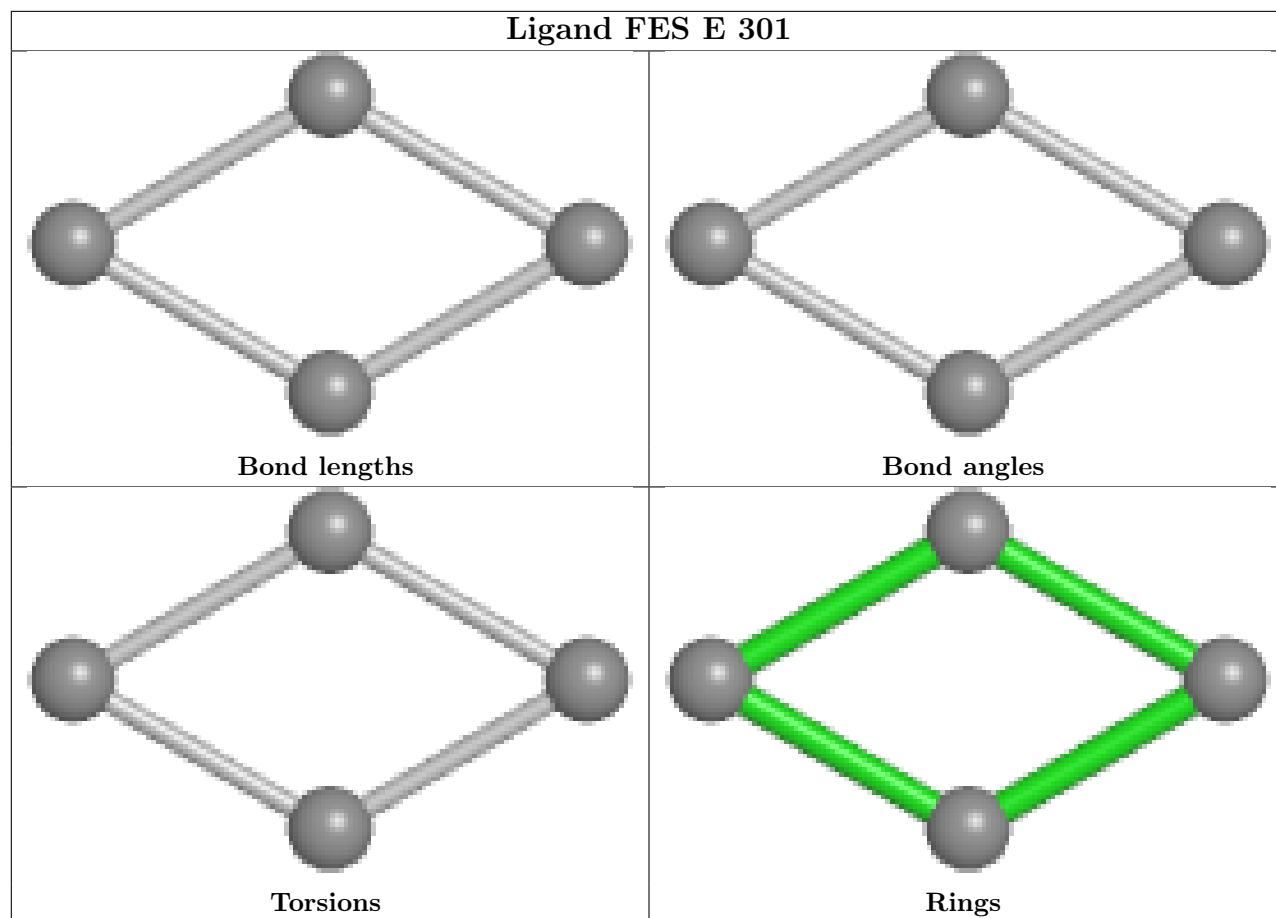




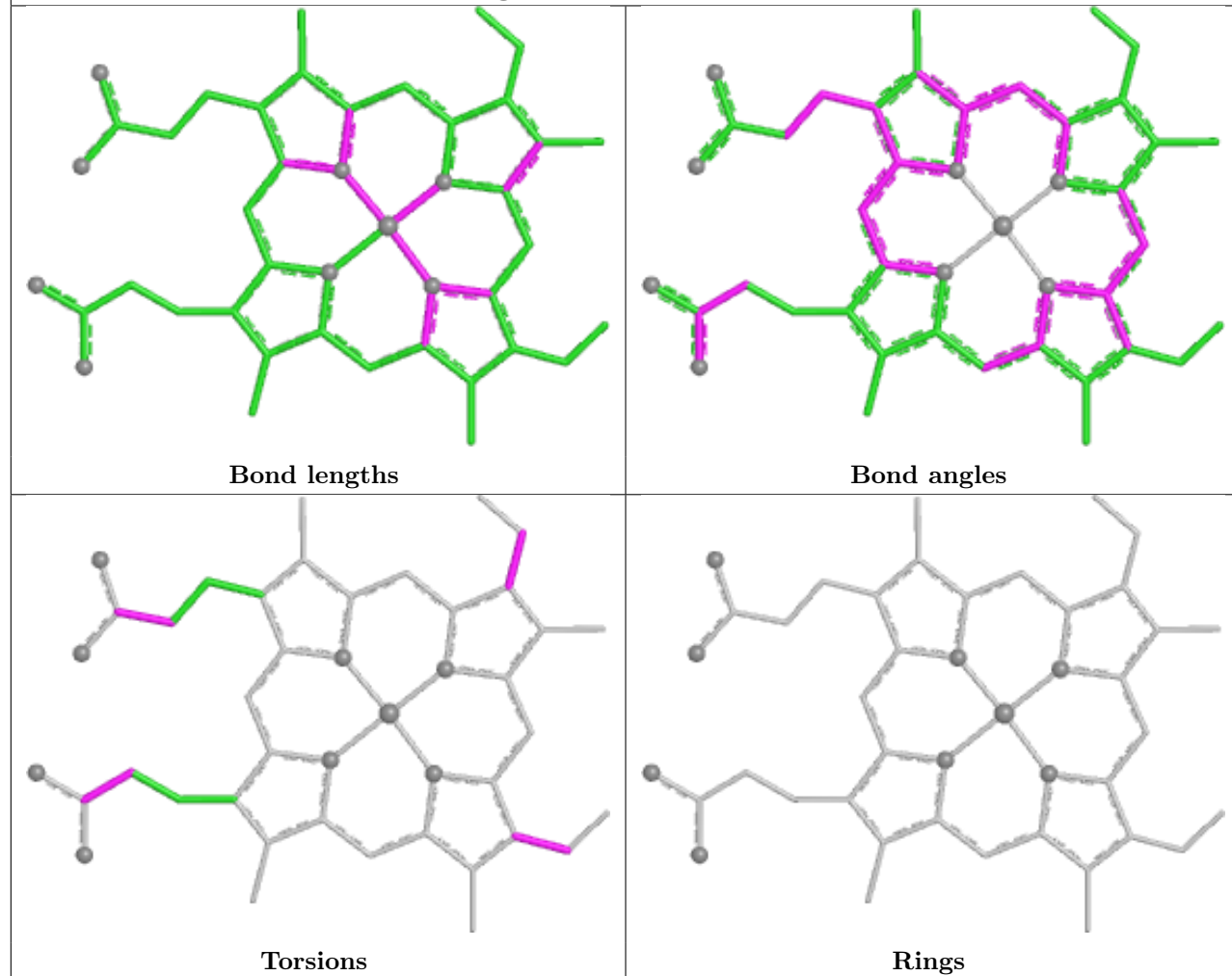




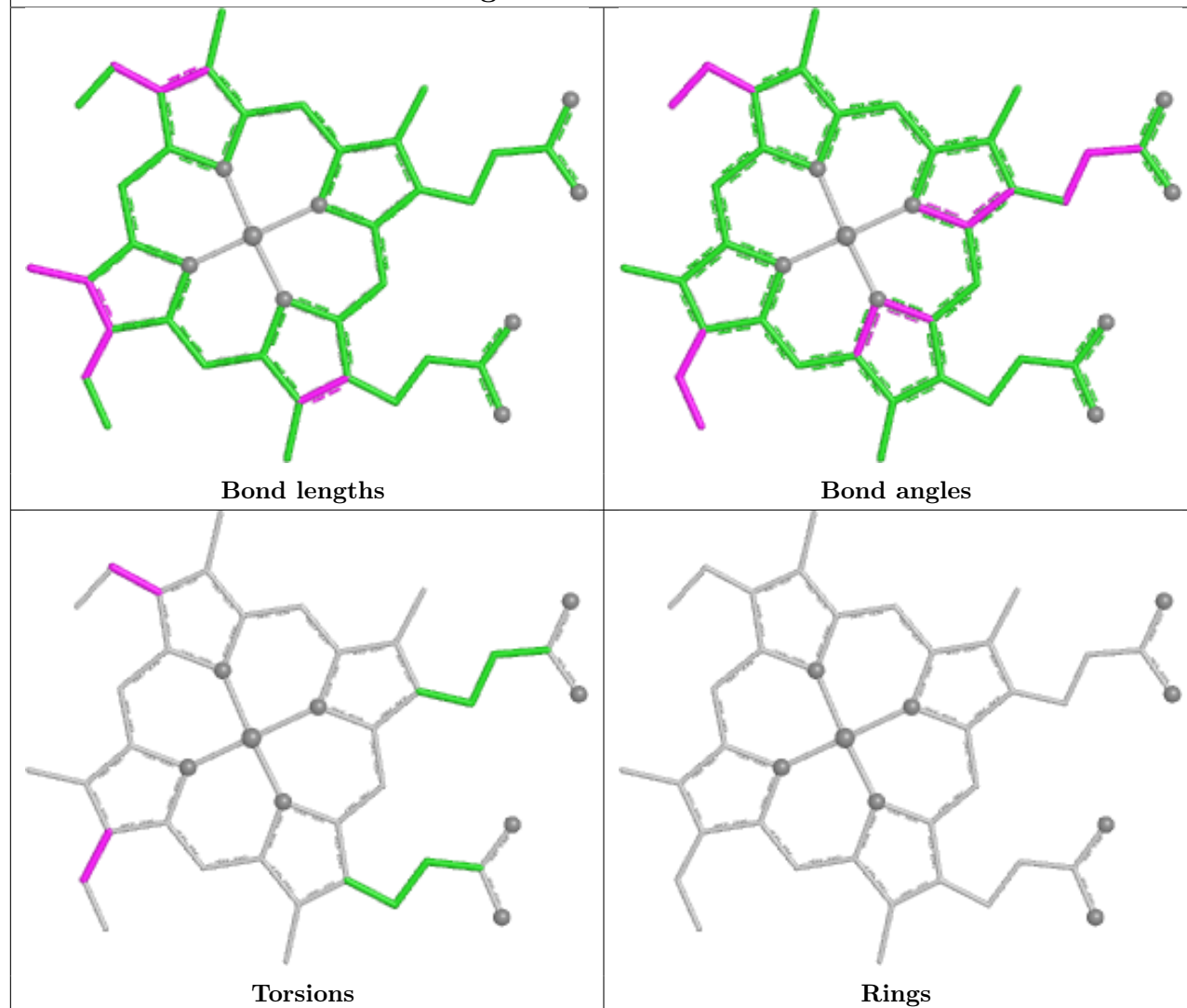




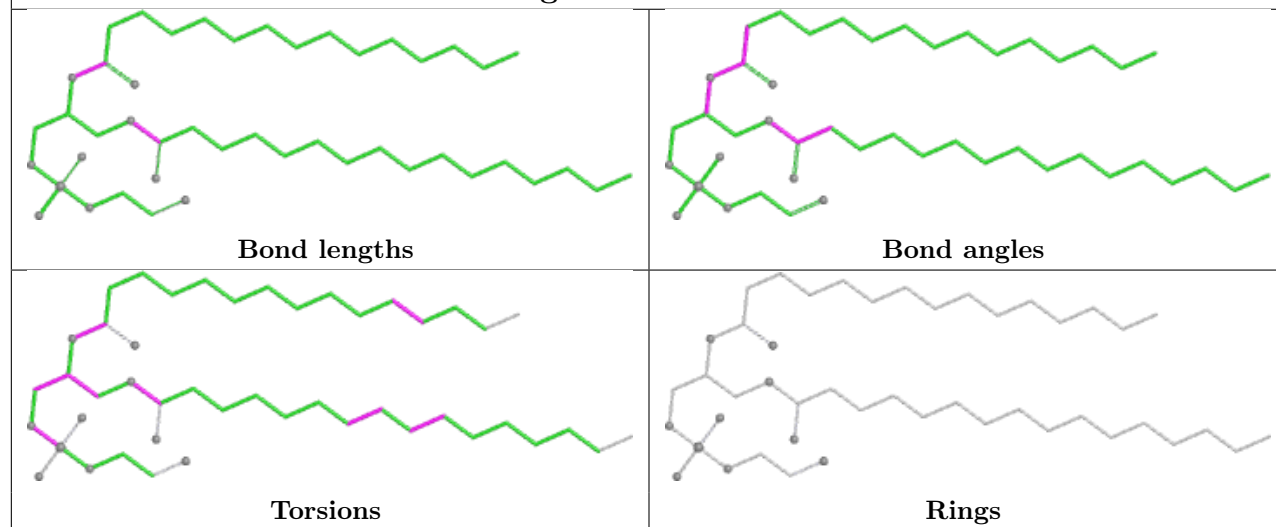
Ligand HEM AC 402



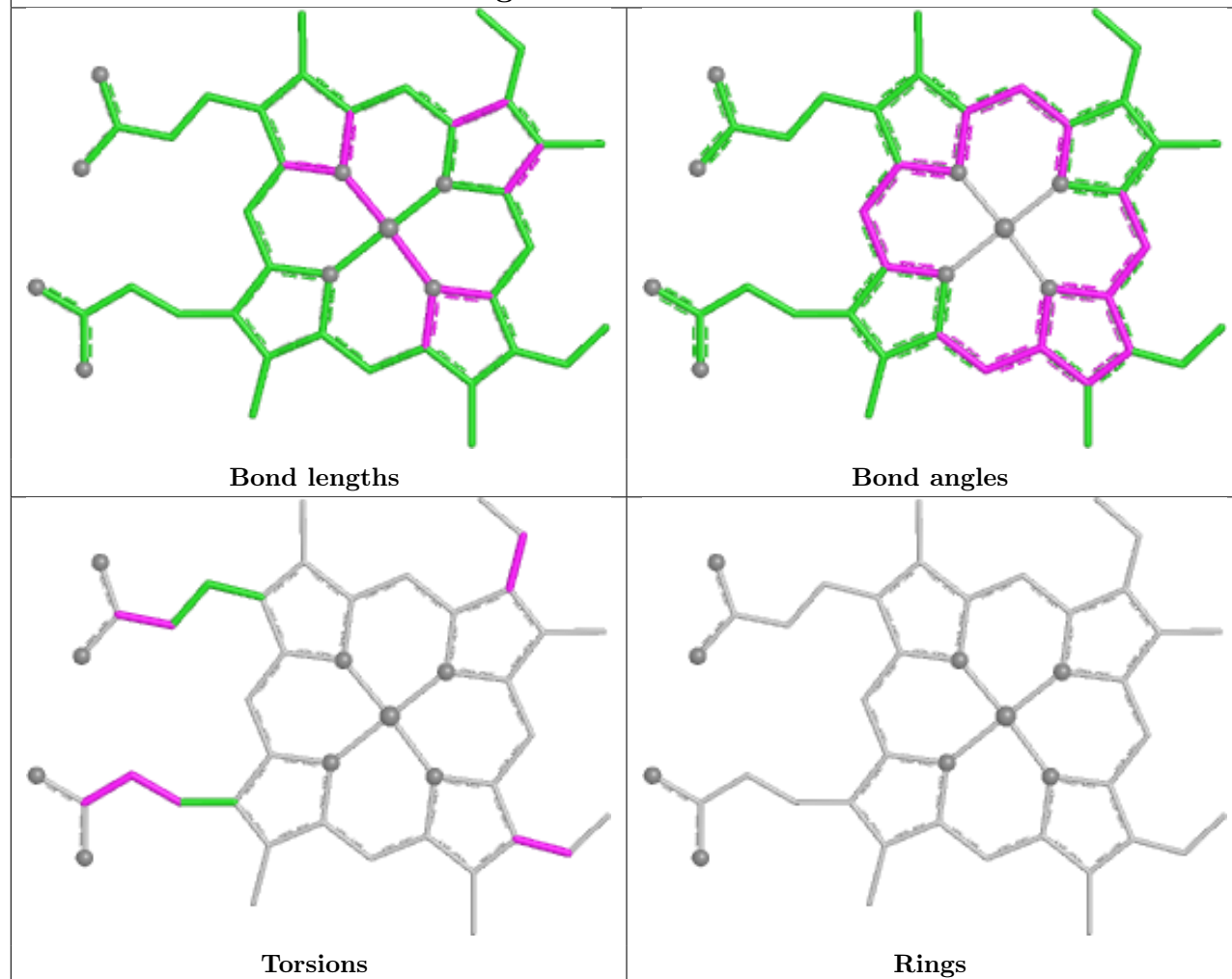
Ligand HEC AD 401



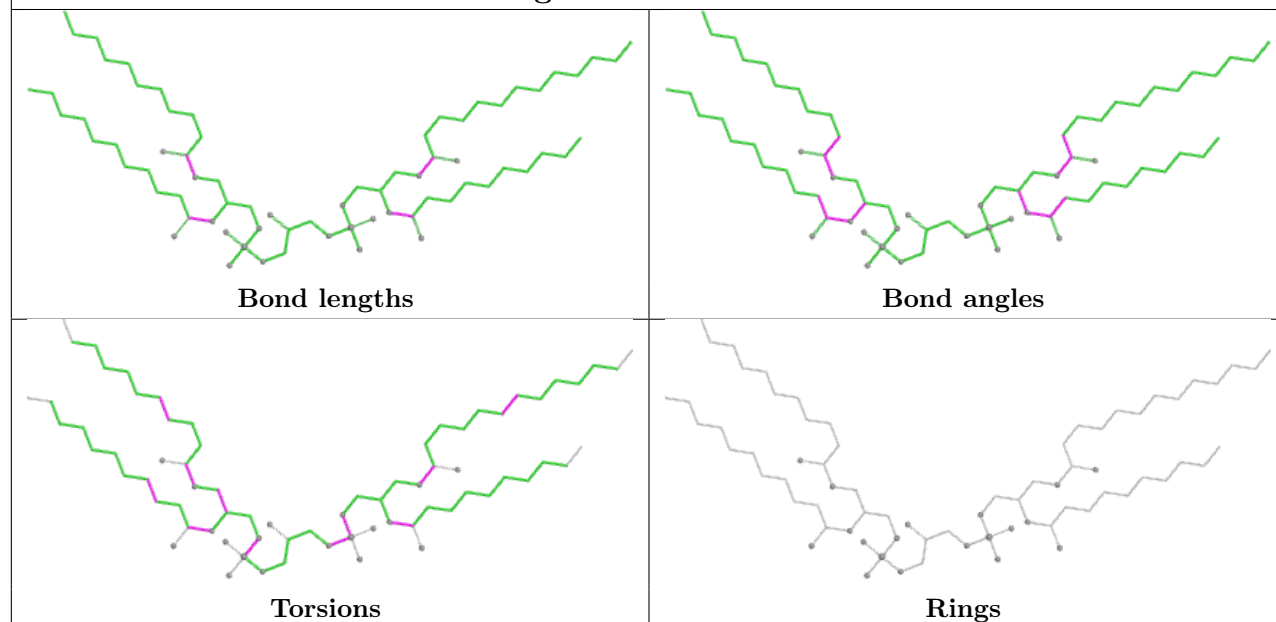
Ligand 3PE J 201



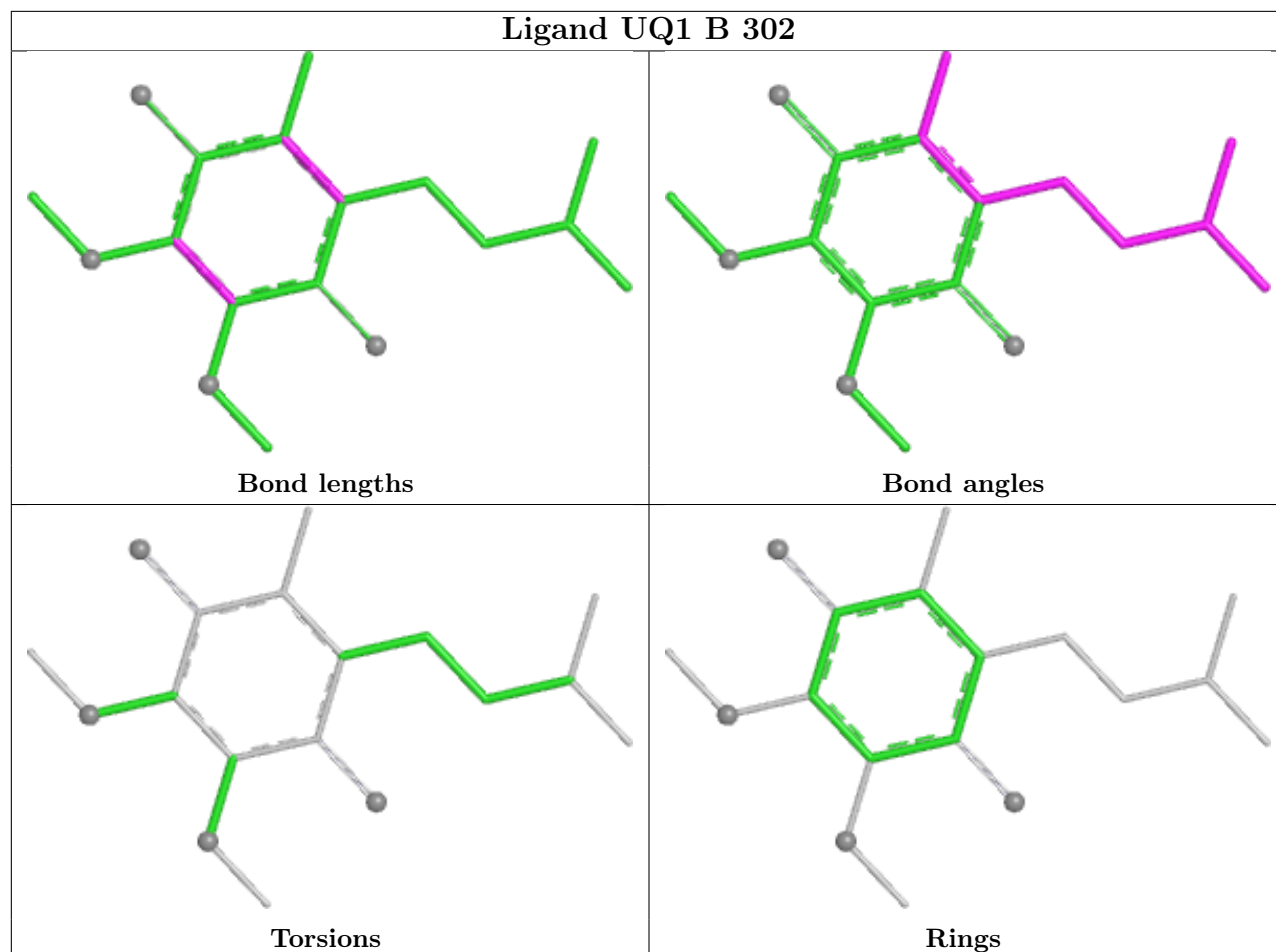
Ligand HEM AC 401



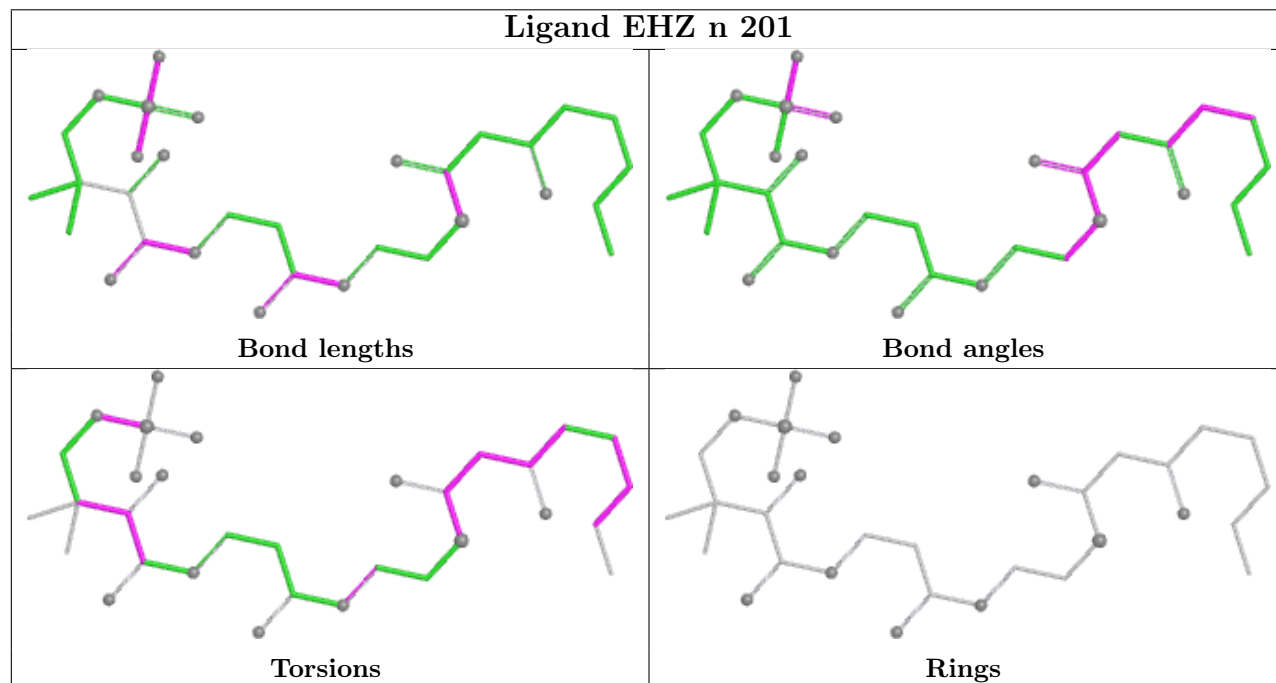
Ligand CDL L 703

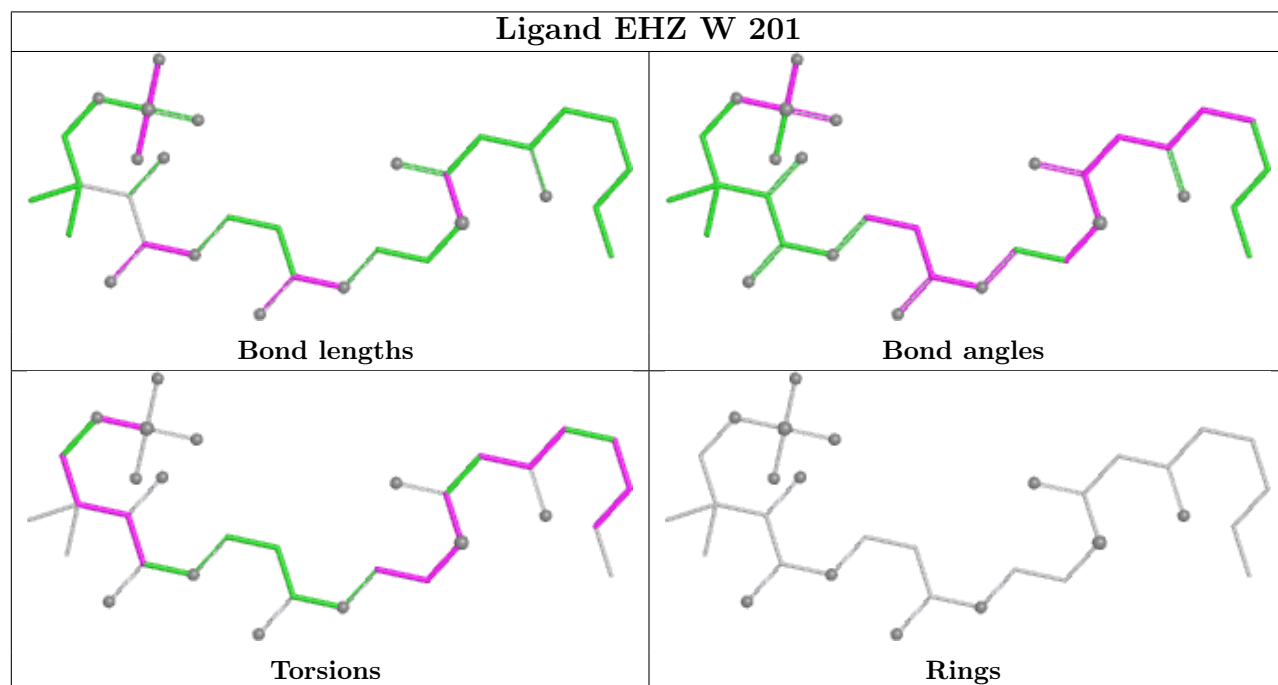
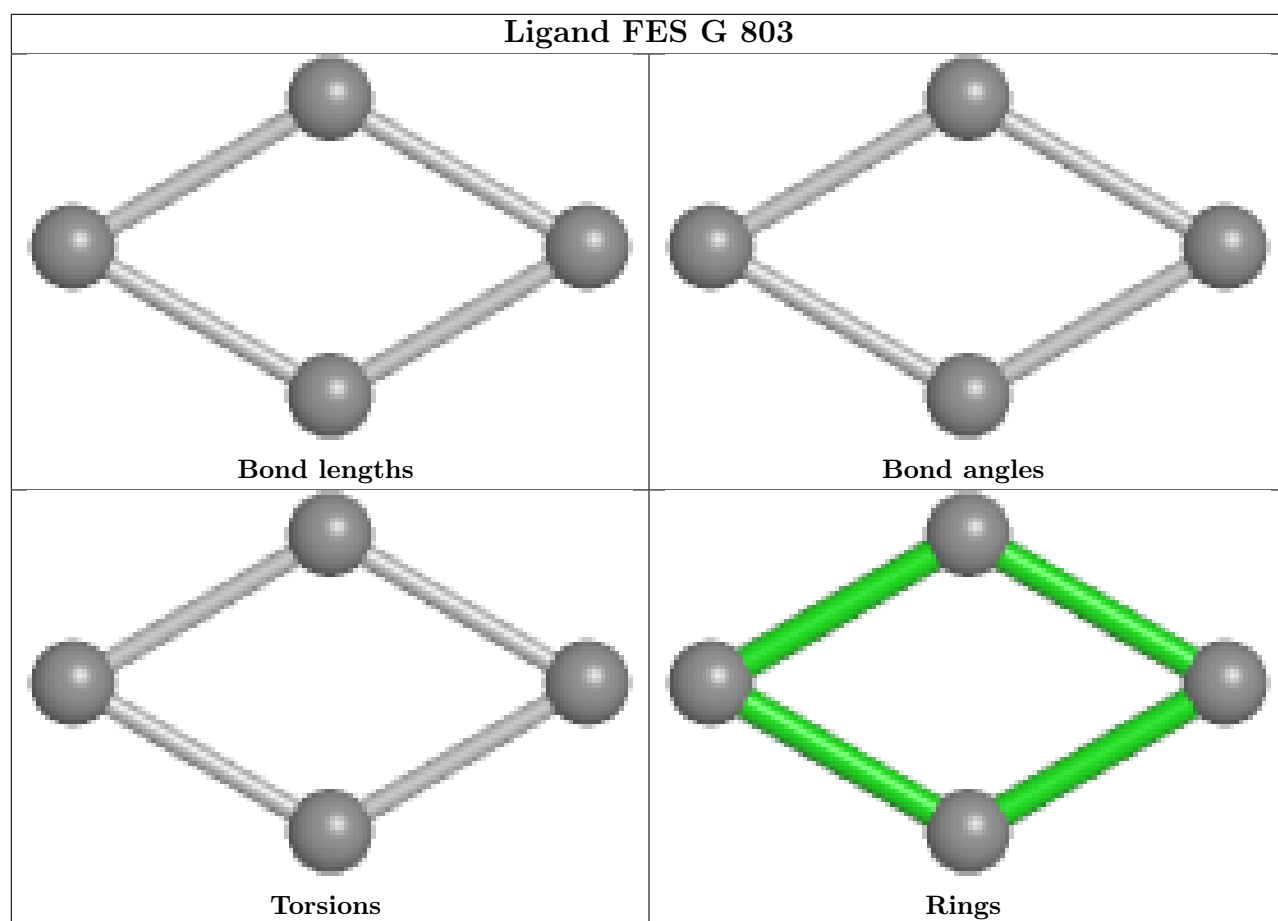


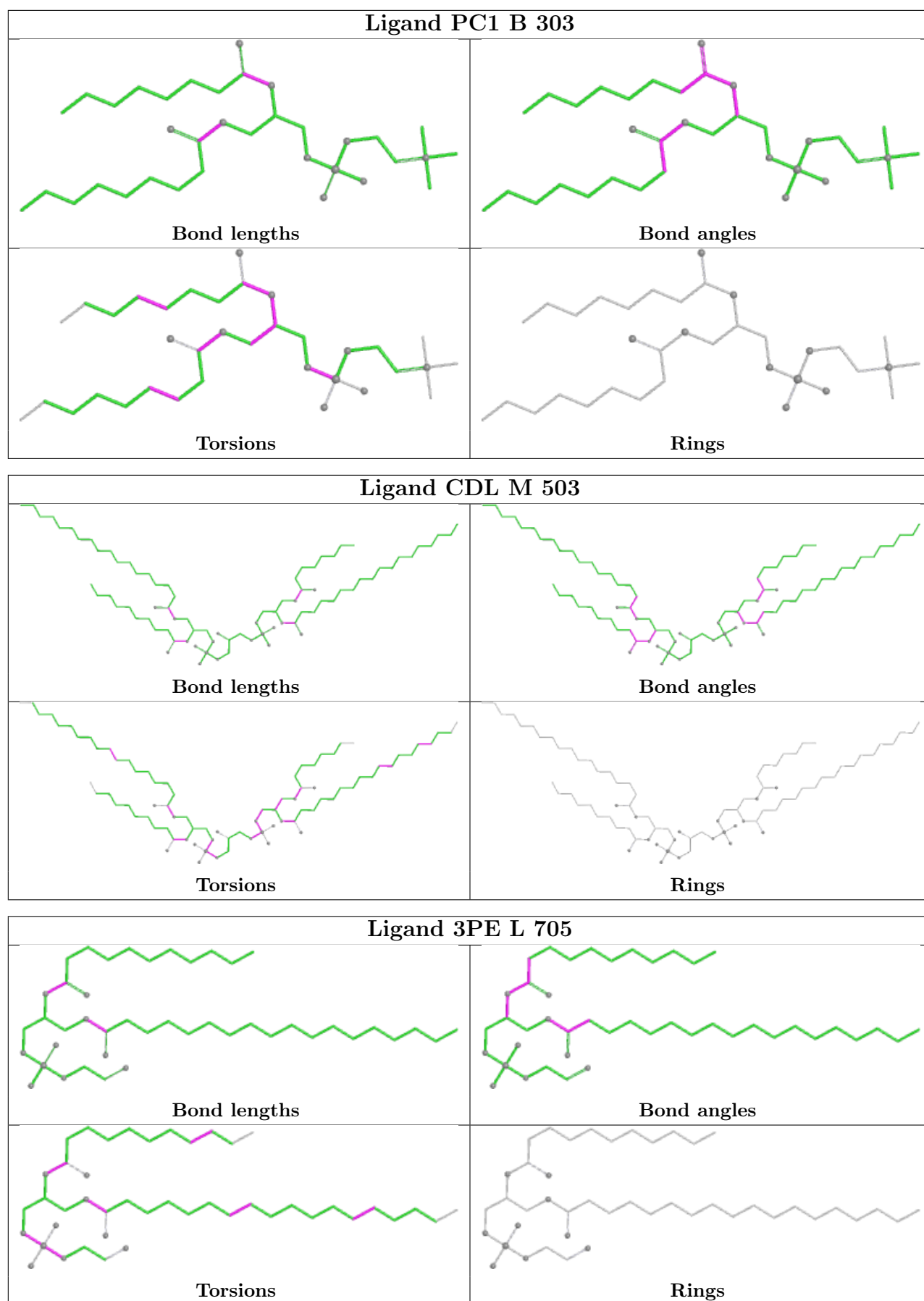
Ligand UQ1 B 302

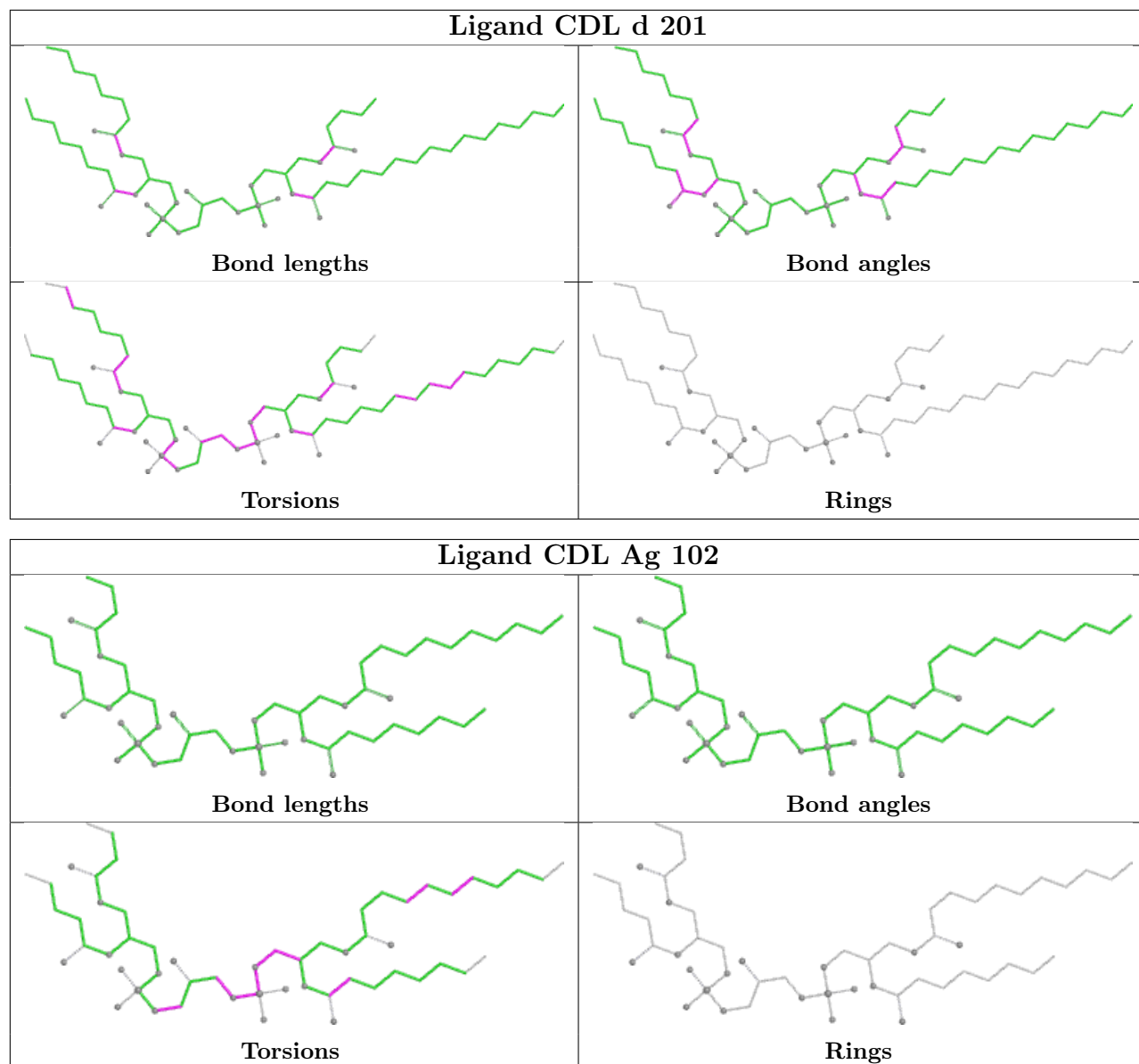


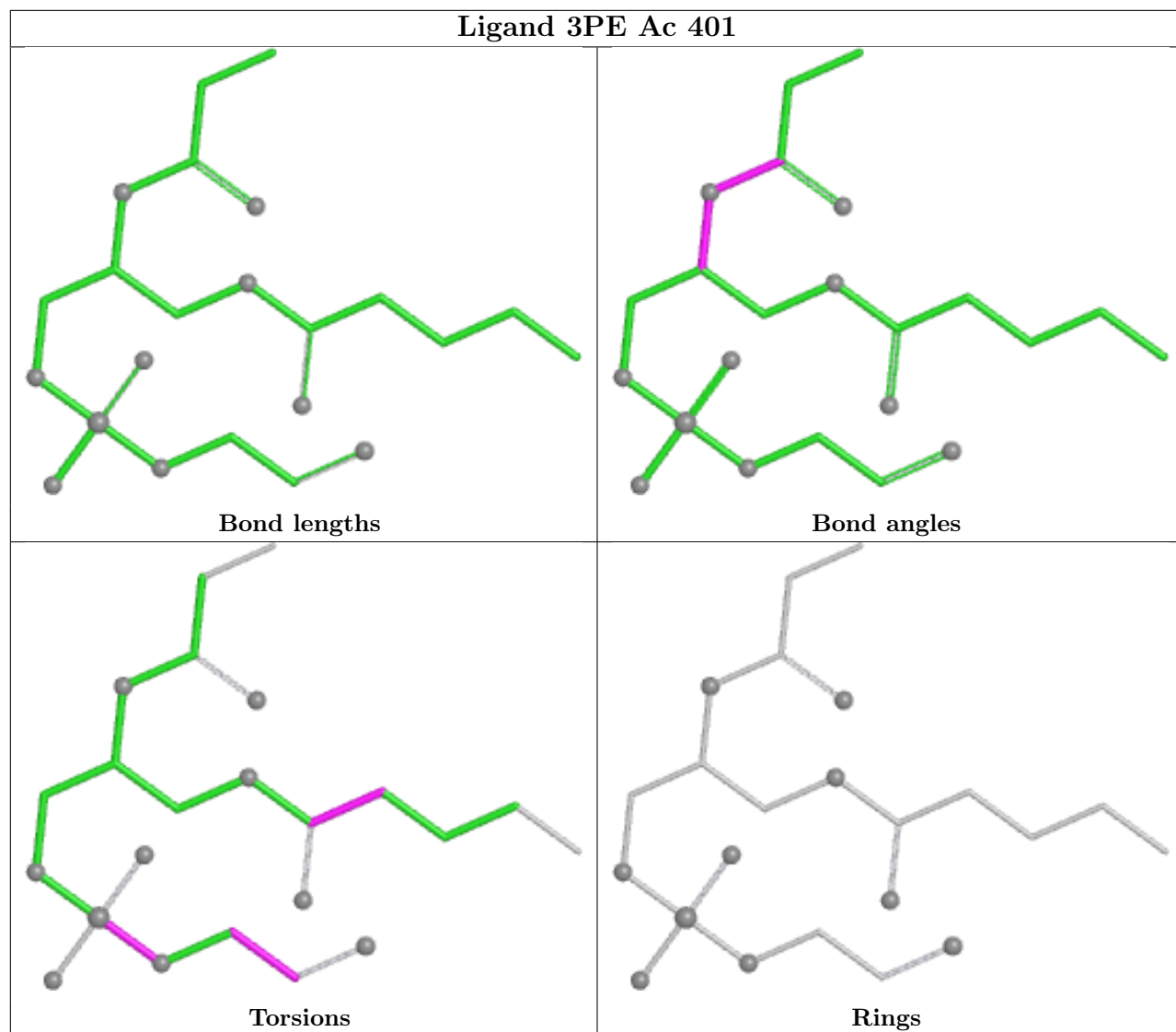
Ligand EHZ n 201



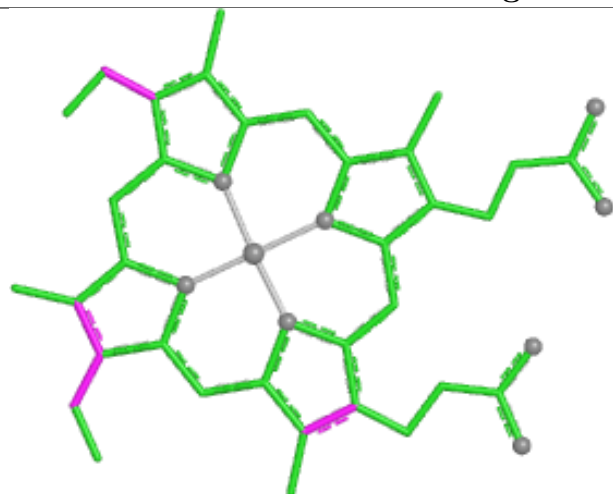




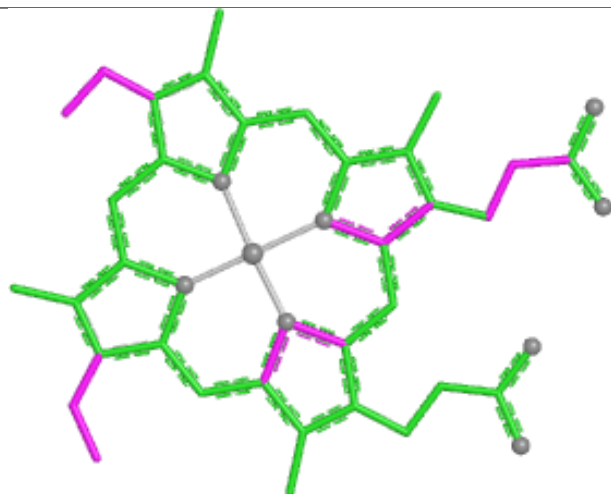




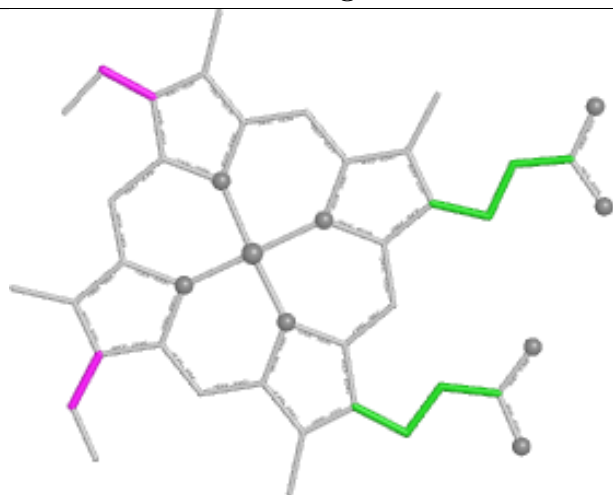
Ligand HEC Ad 401



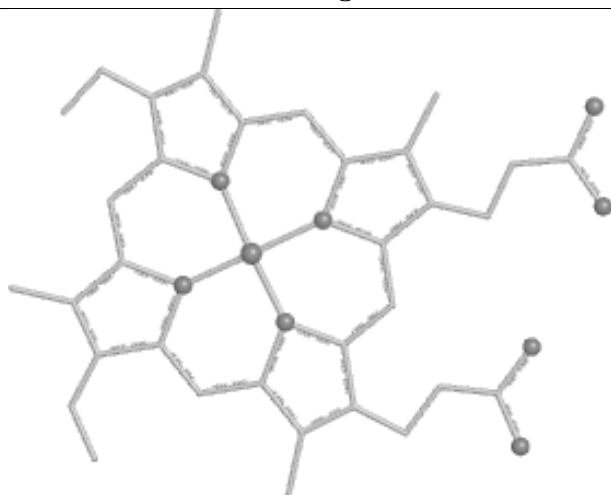
Bond lengths



Bond angles

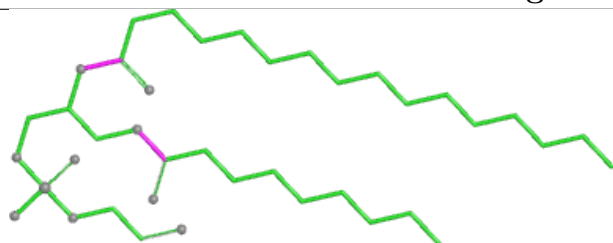


Torsions

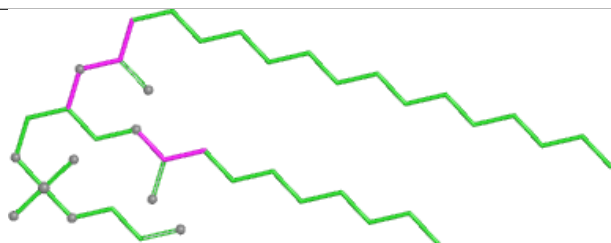


Rings

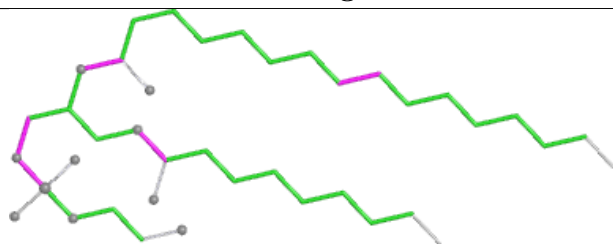
Ligand 3PE i 201



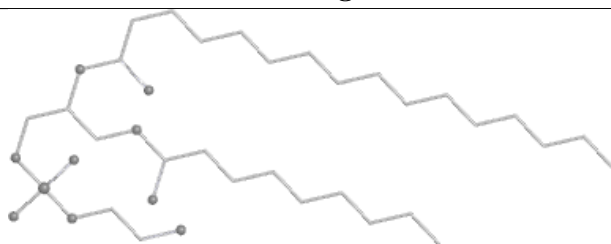
Bond lengths



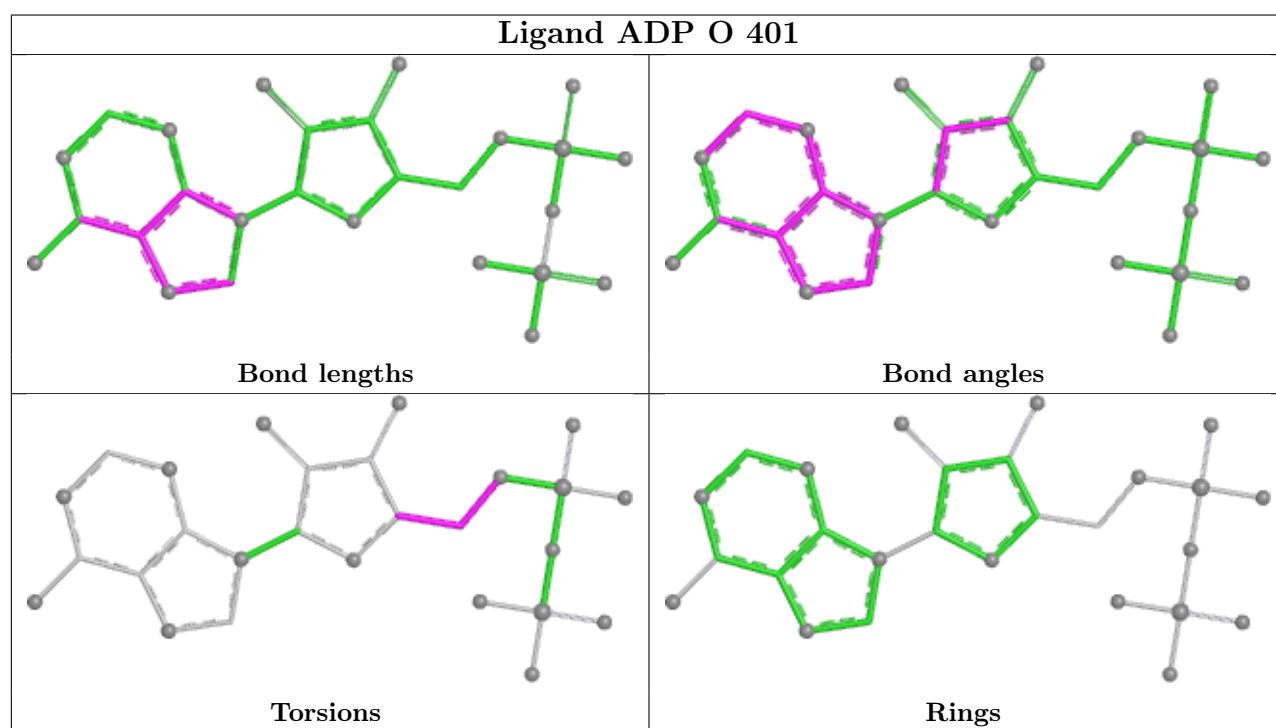
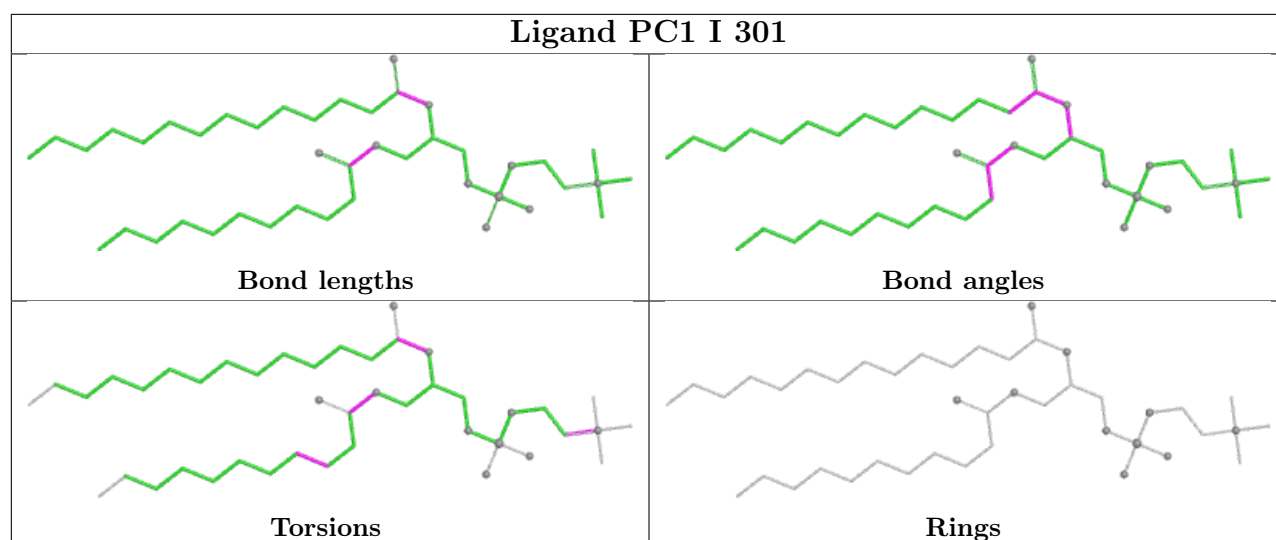
Bond angles



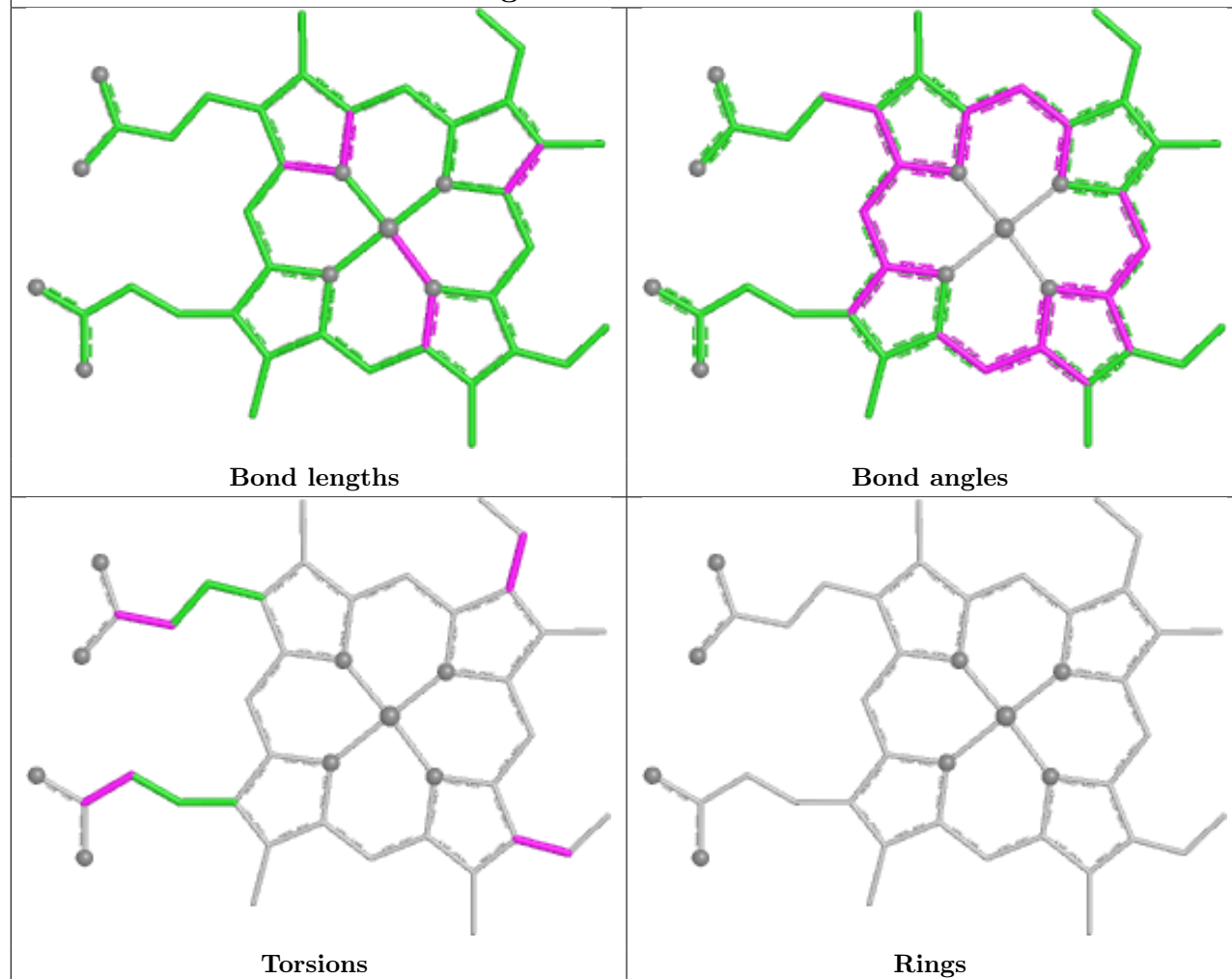
Torsions



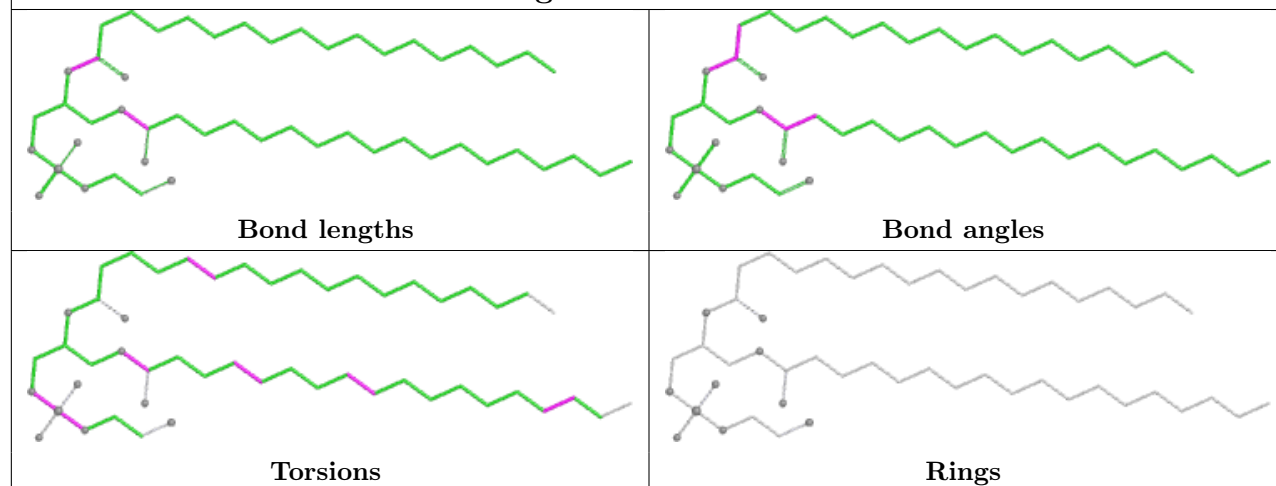
Rings

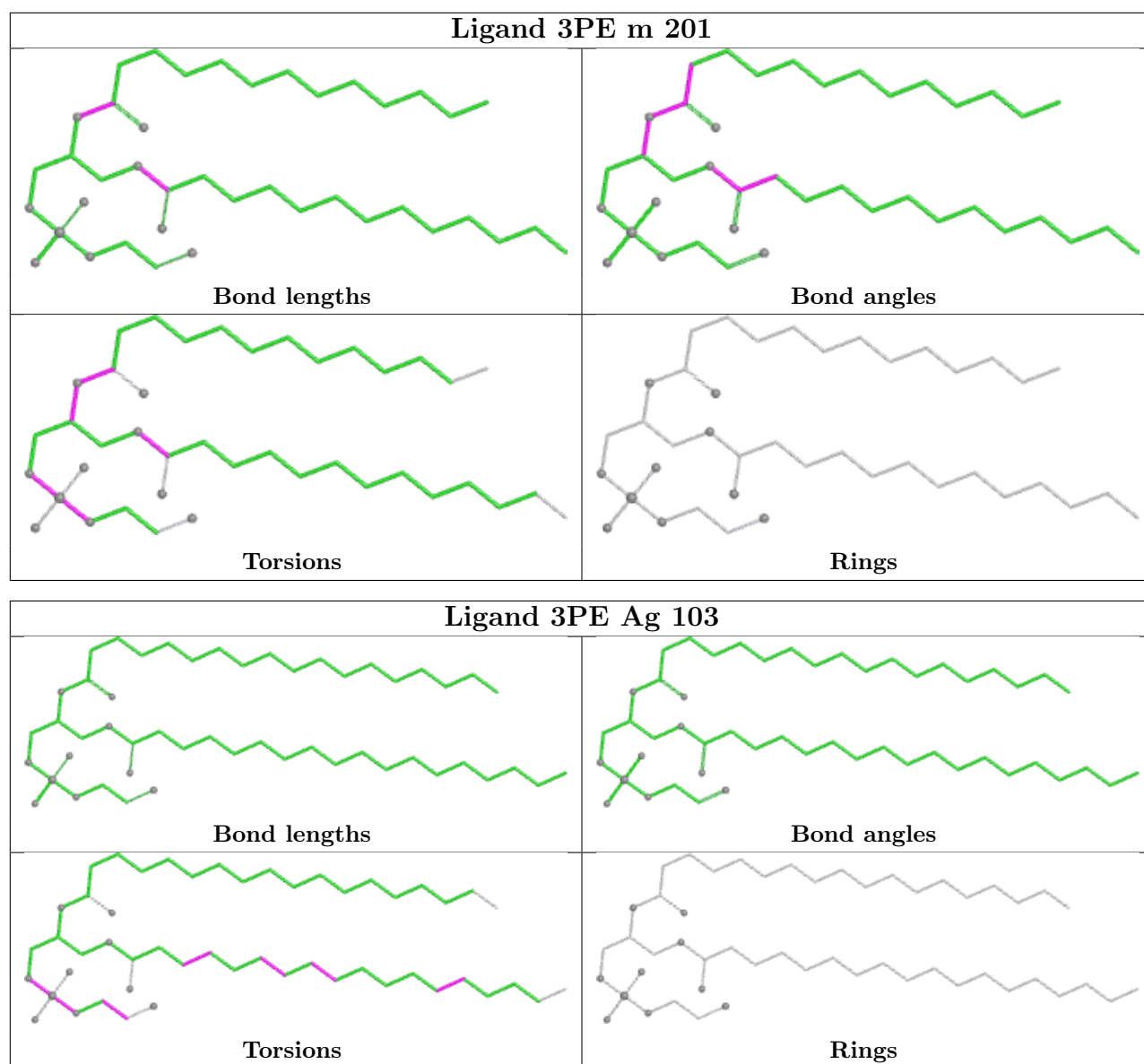


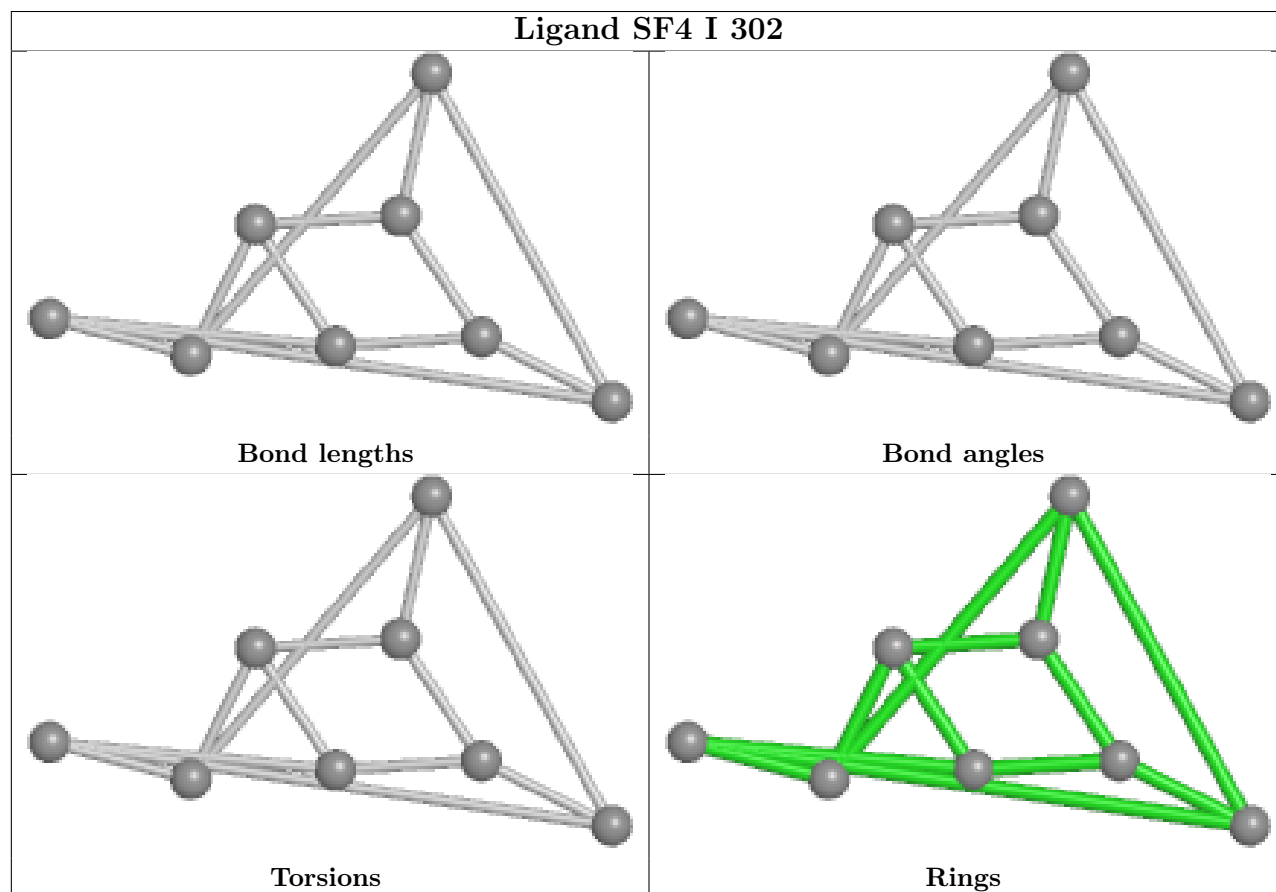
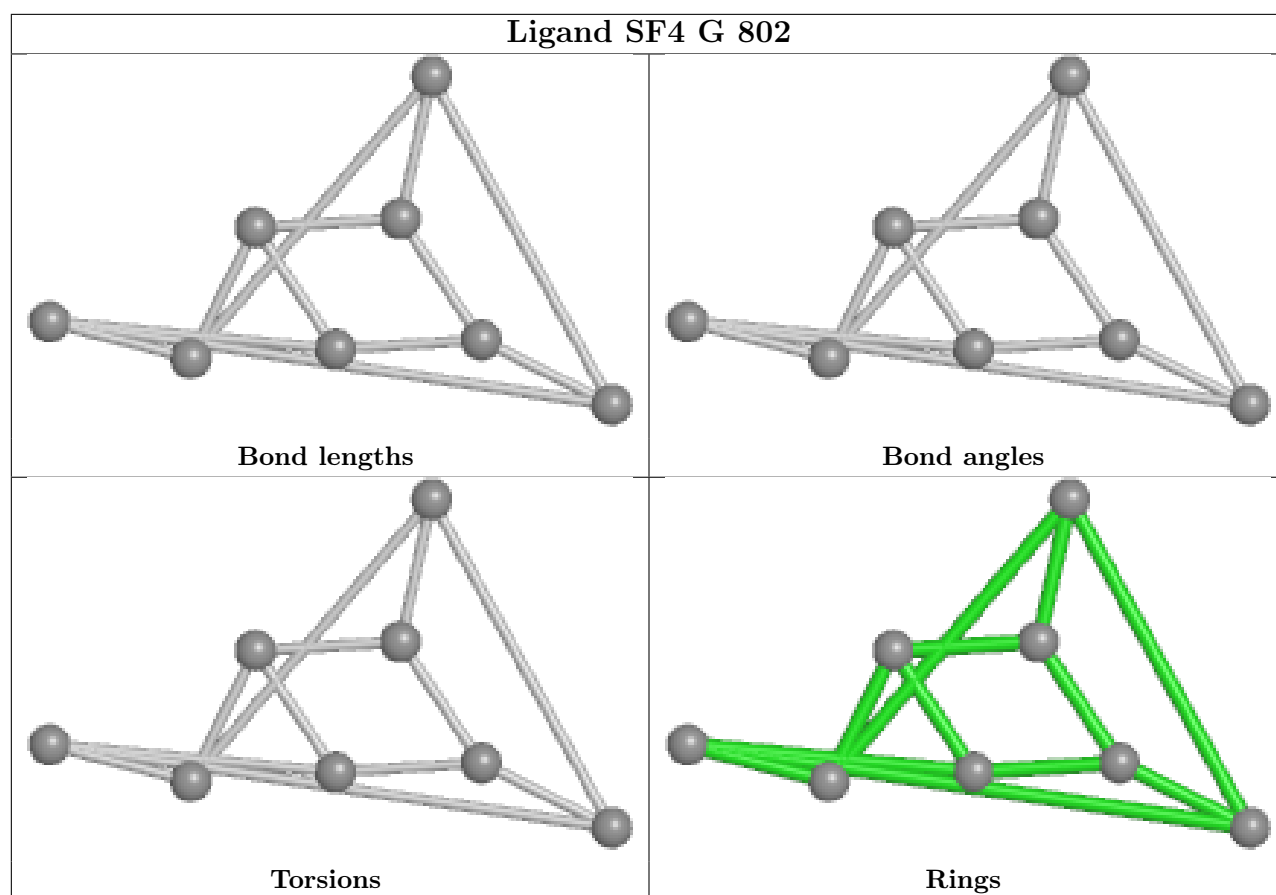
Ligand HEM Ac 403

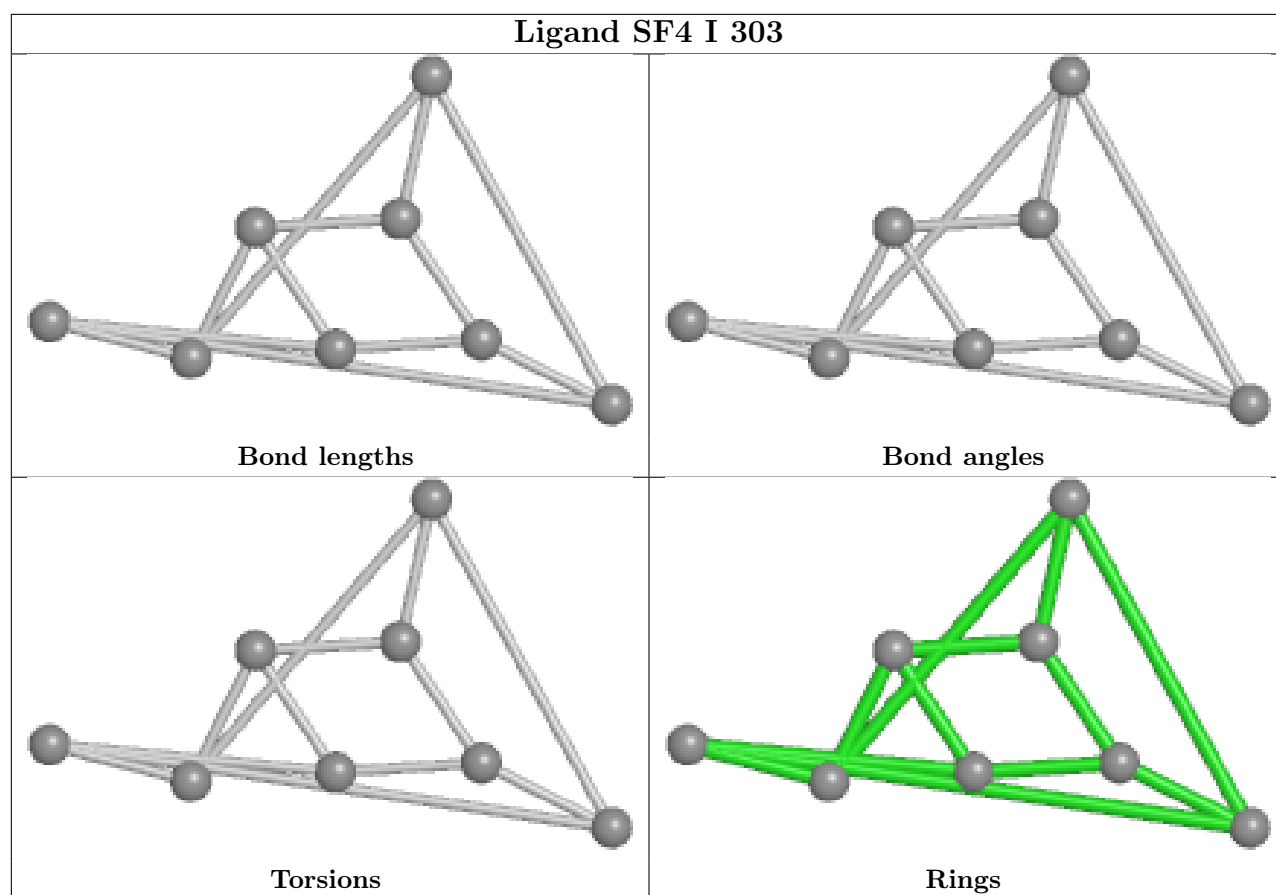


Ligand 3PE H 403









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.

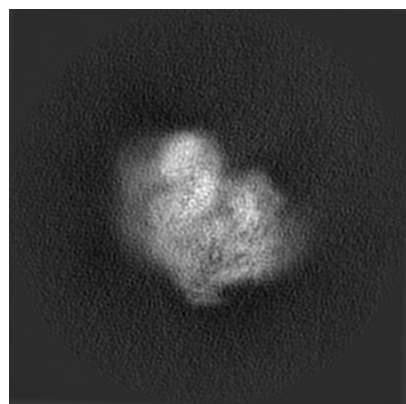
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35352. These allow visual inspection of the internal detail of the map and identification of artifacts.

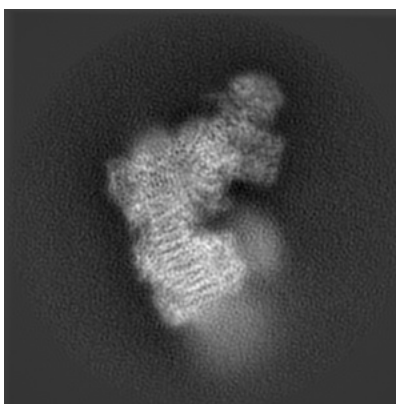
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

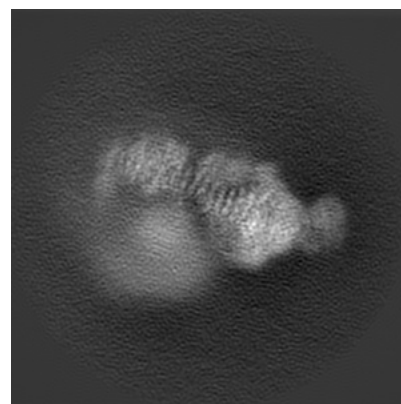
6.1.1 Primary map



X

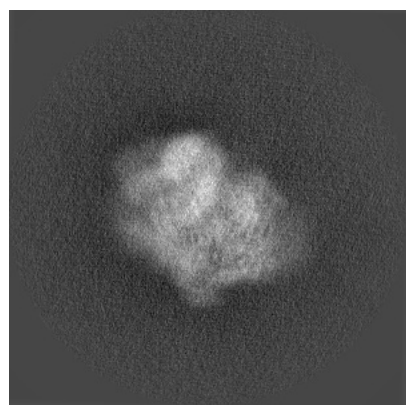


Y

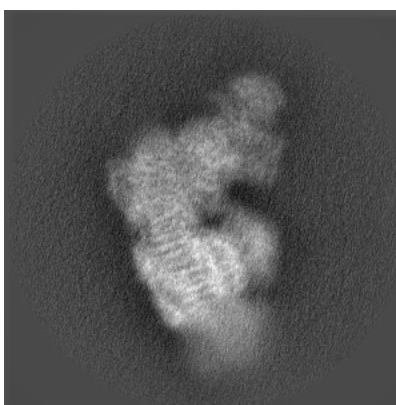


Z

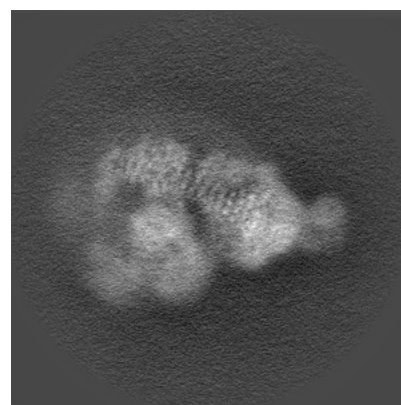
6.1.2 Raw map



X



Y

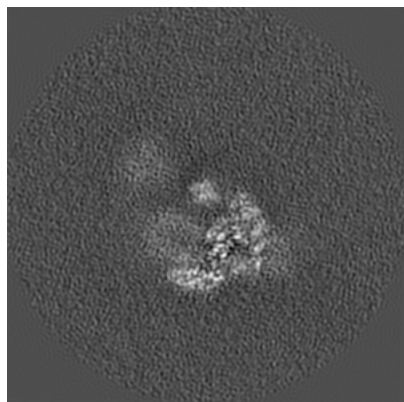


Z

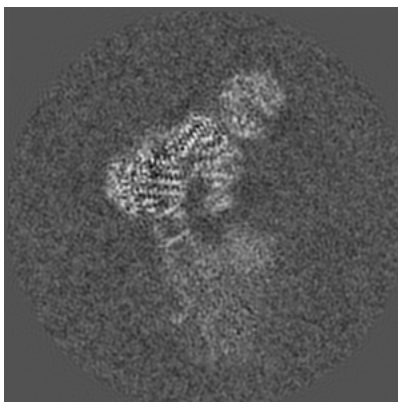
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

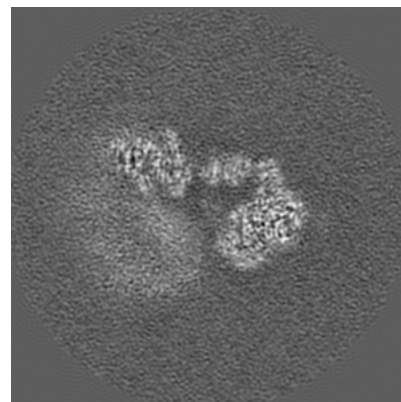
6.2.1 Primary map



X Index: 256

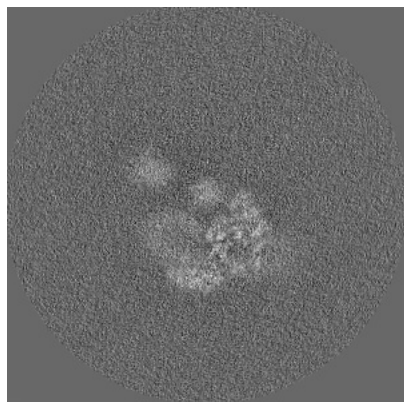


Y Index: 256

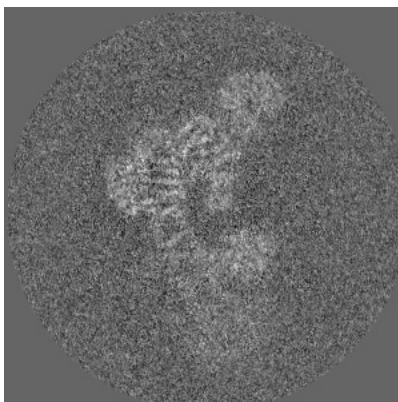


Z Index: 256

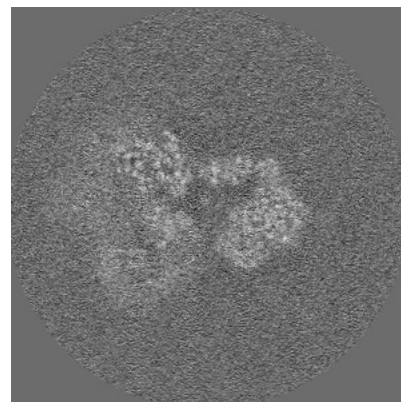
6.2.2 Raw map



X Index: 256



Y Index: 256

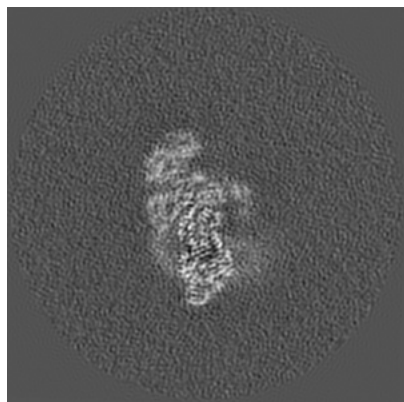


Z Index: 256

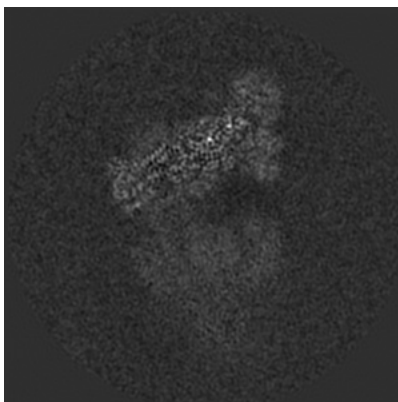
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

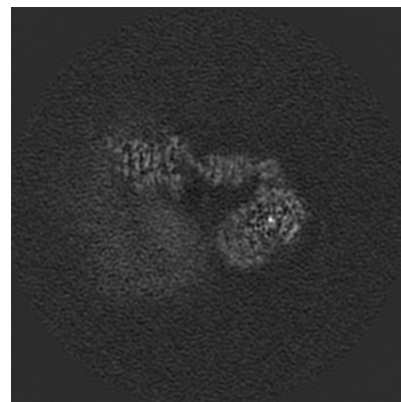
6.3.1 Primary map



X Index: 310

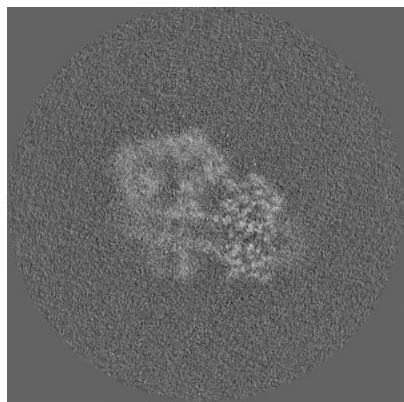


Y Index: 232

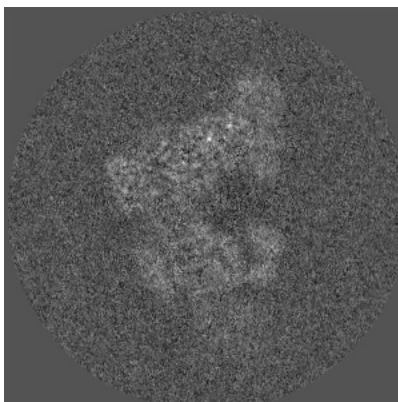


Z Index: 252

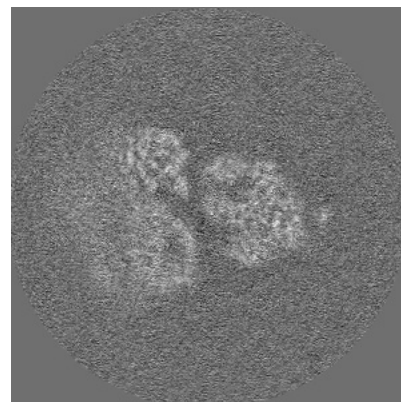
6.3.2 Raw map



X Index: 205



Y Index: 234

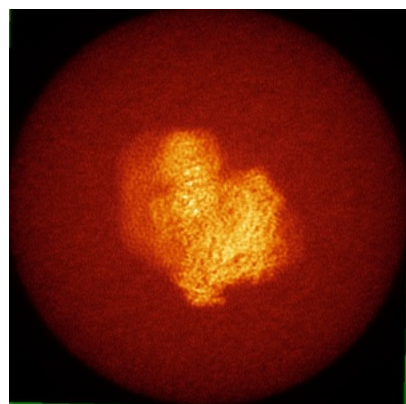


Z Index: 268

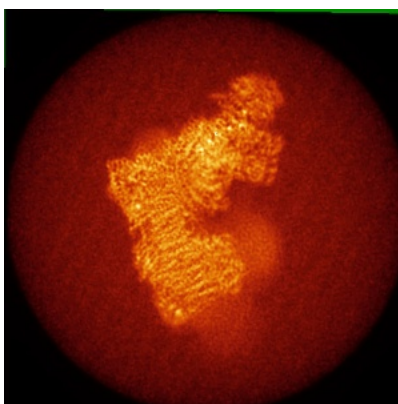
The images above show the largest variance slices of the map in three orthogonal directions.

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

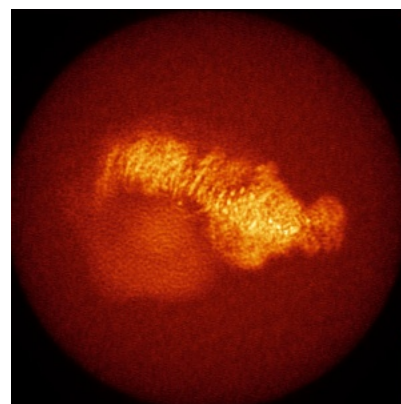
6.4.1 Primary map



X

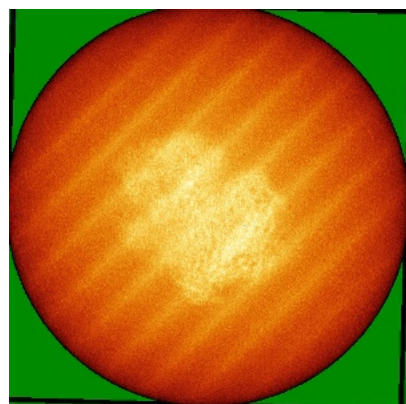


Y

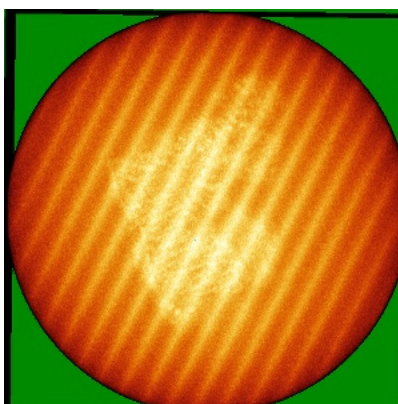


Z

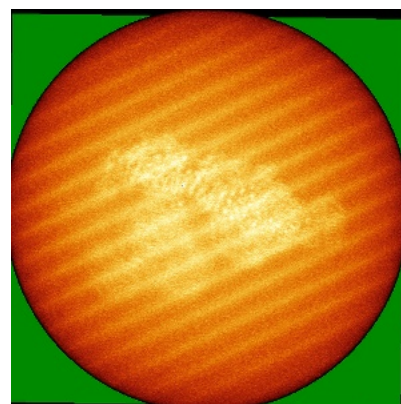
6.4.2 Raw map



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](#)

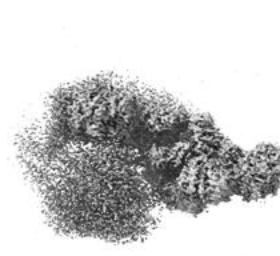
6.5.1 Primary map



X



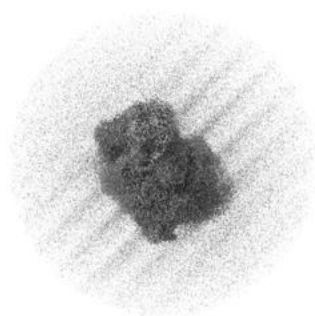
Y



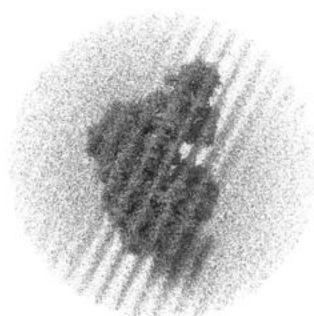
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0082. 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.

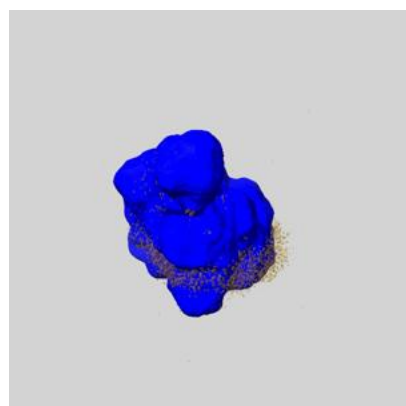
6.6 Mask visualisation [i](#)

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

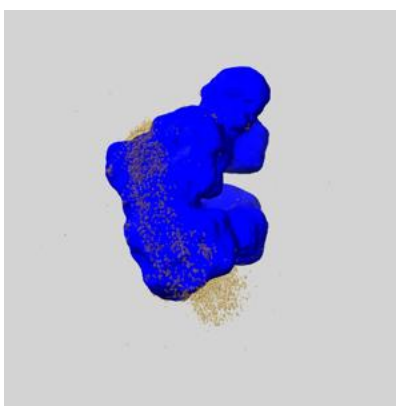
A mask typically either:

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

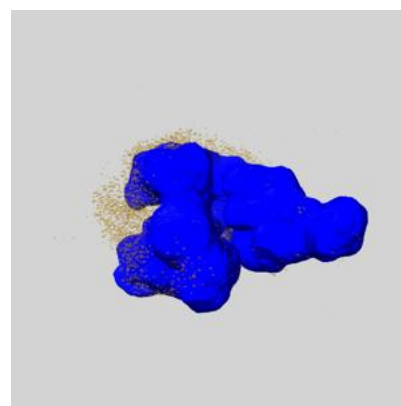
6.6.1 emd_35352_msk_1.map [i](#)



X



Y

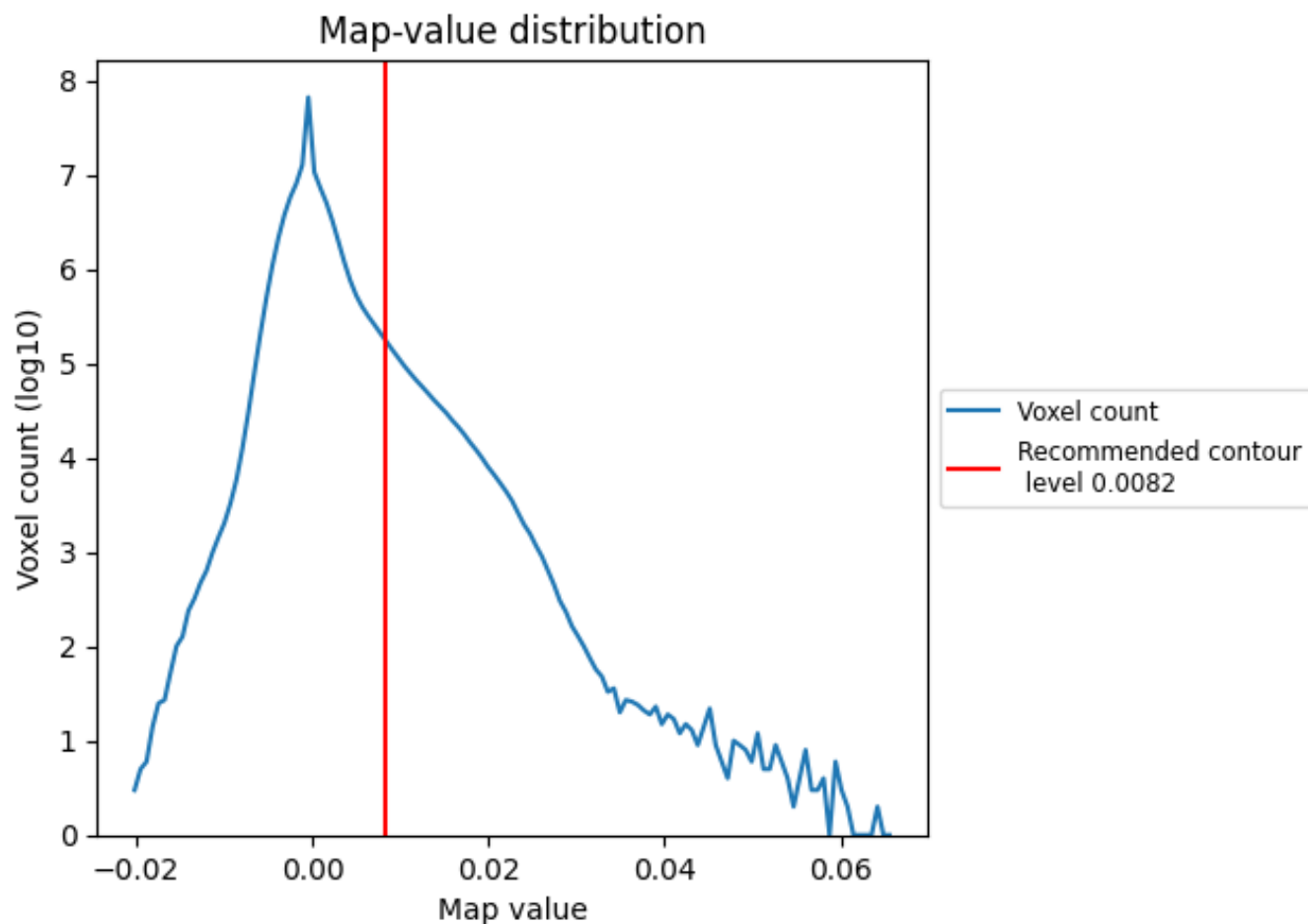


Z

7 Map analysis [i](#)

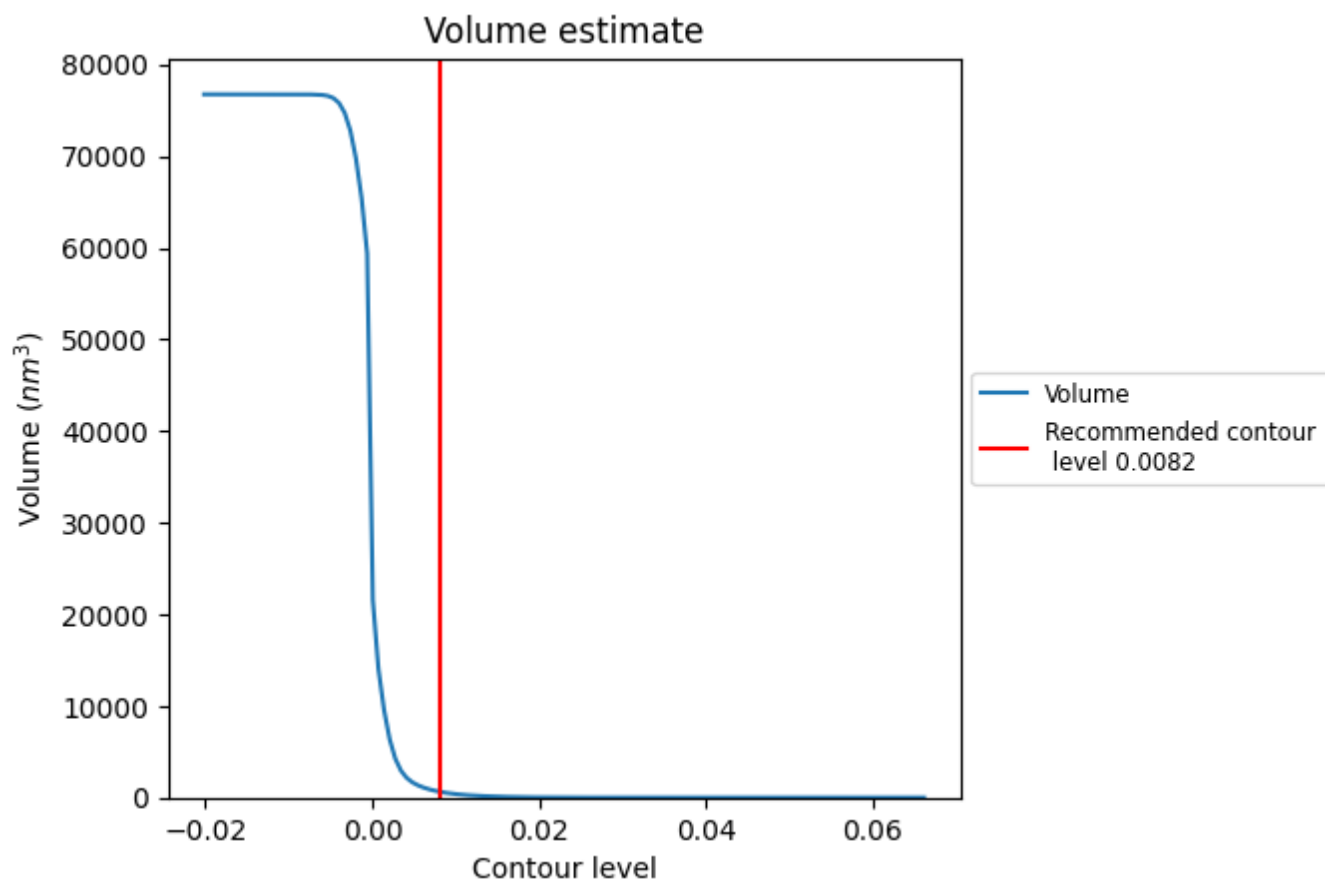
This section contains the results of statistical analysis of the map.

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.

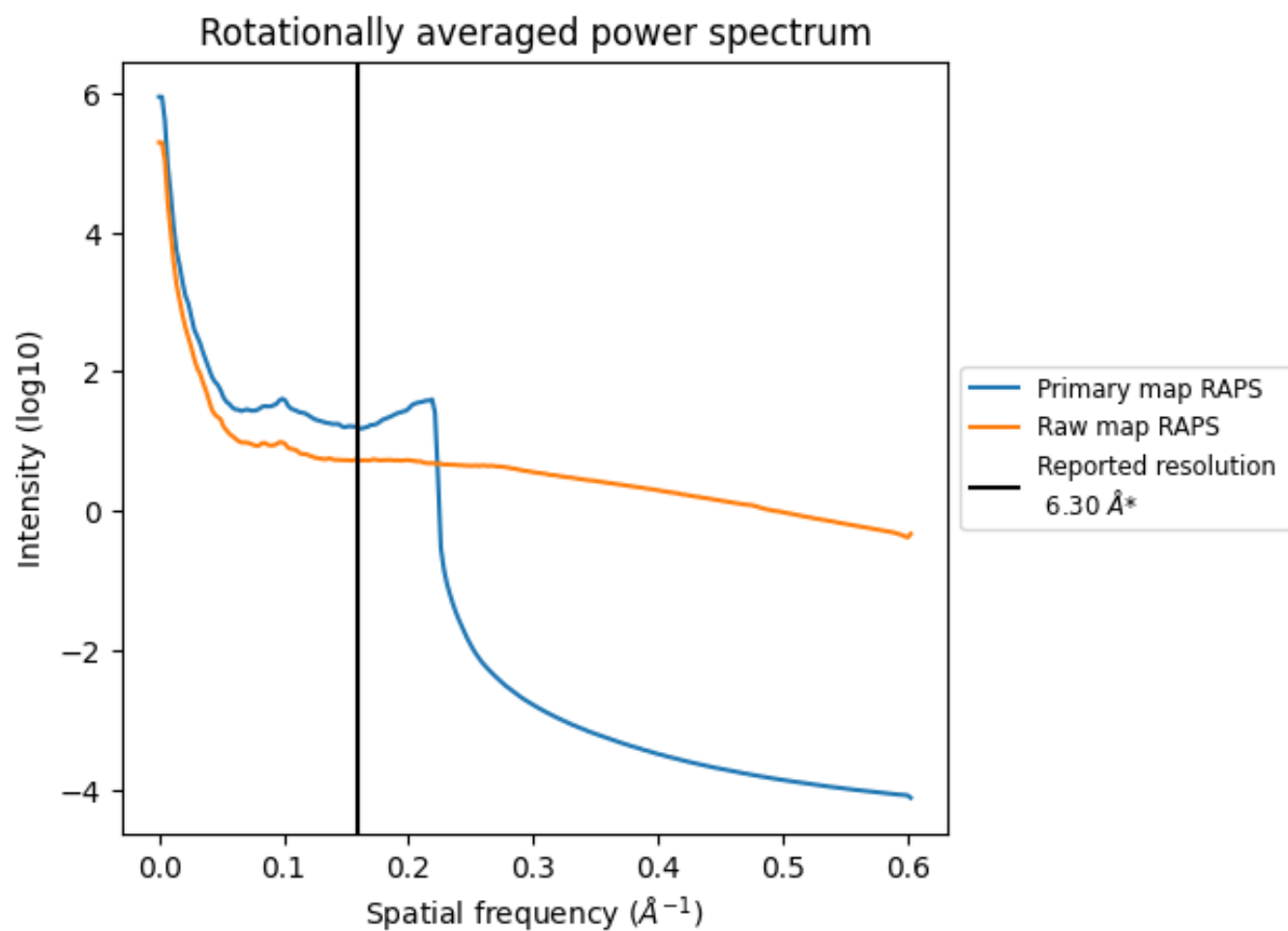
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm^3 ; this corresponds to an approximate mass of 557 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 ⓘ

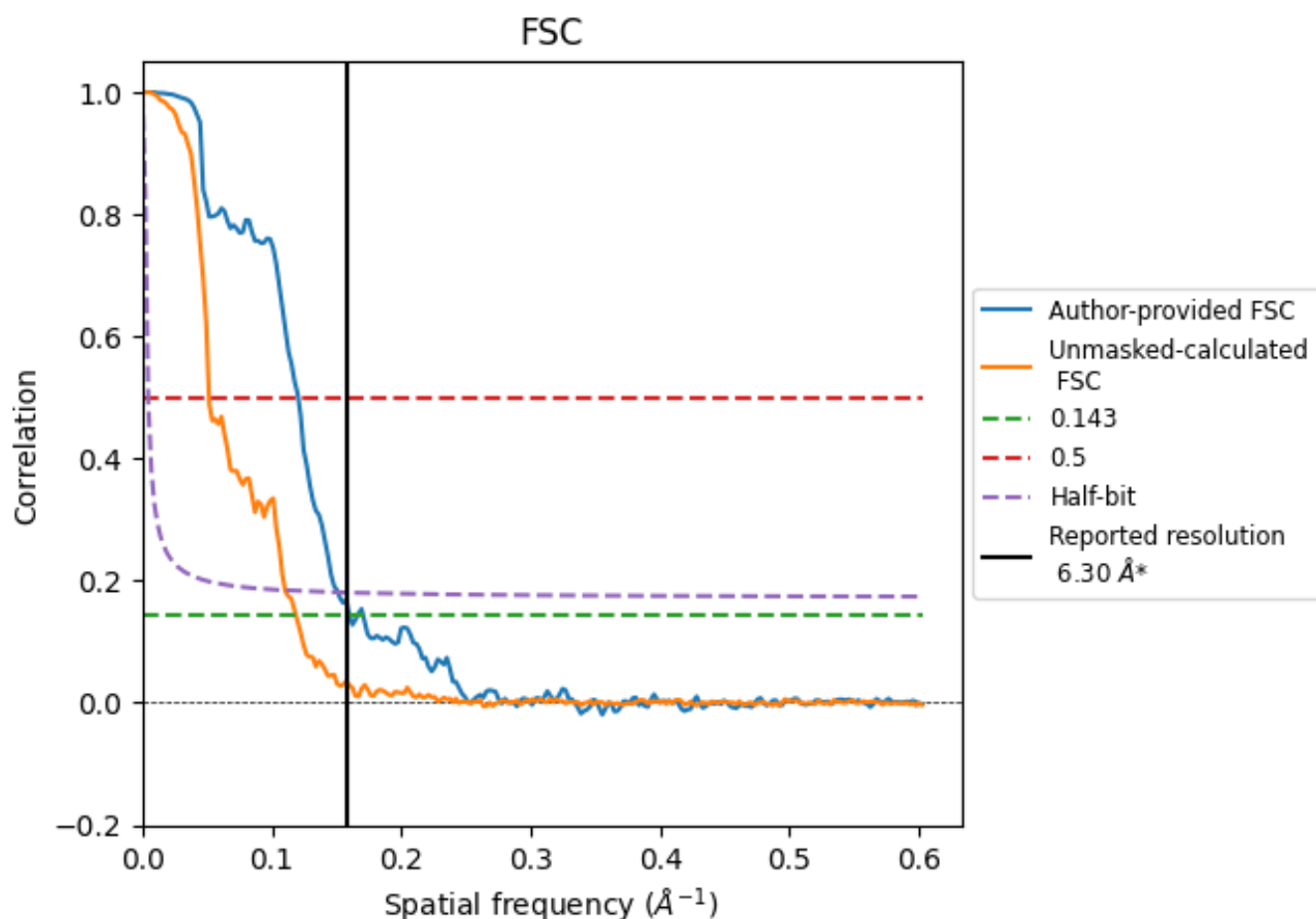


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

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 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

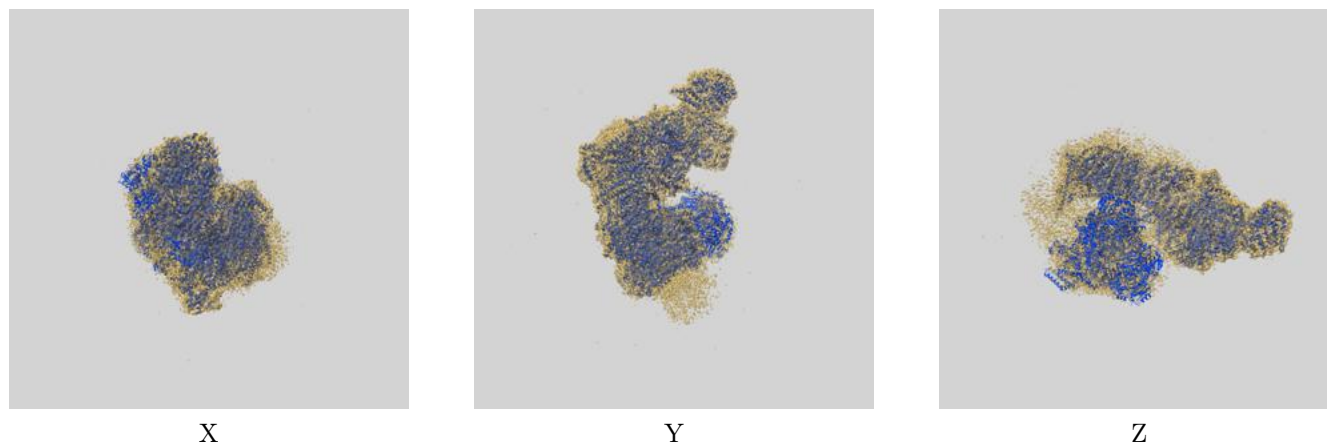
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.25	8.30	6.61
Unmasked-calculated*	8.42	19.38	9.06

*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 8.42 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

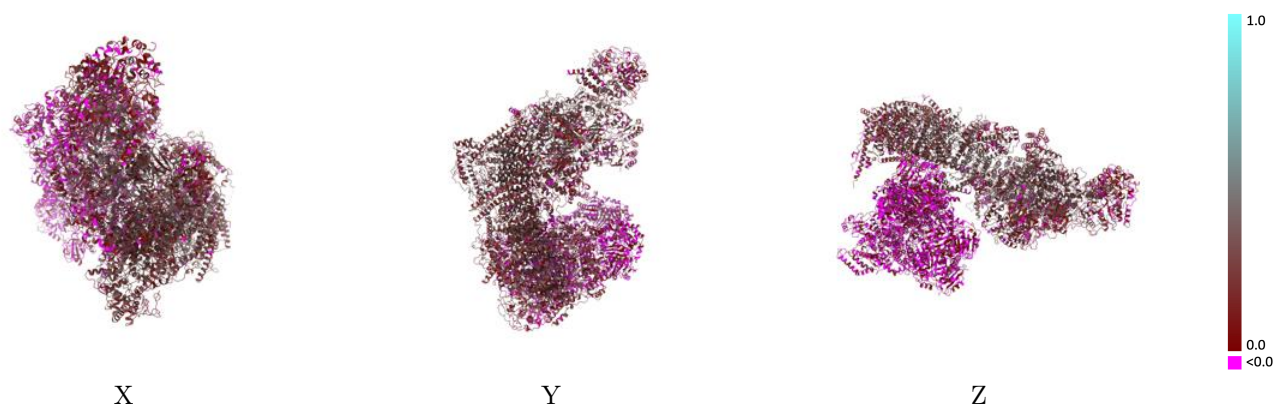
This section contains information regarding the fit between EMDB map EMD-35352 and PDB model 8IC2. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



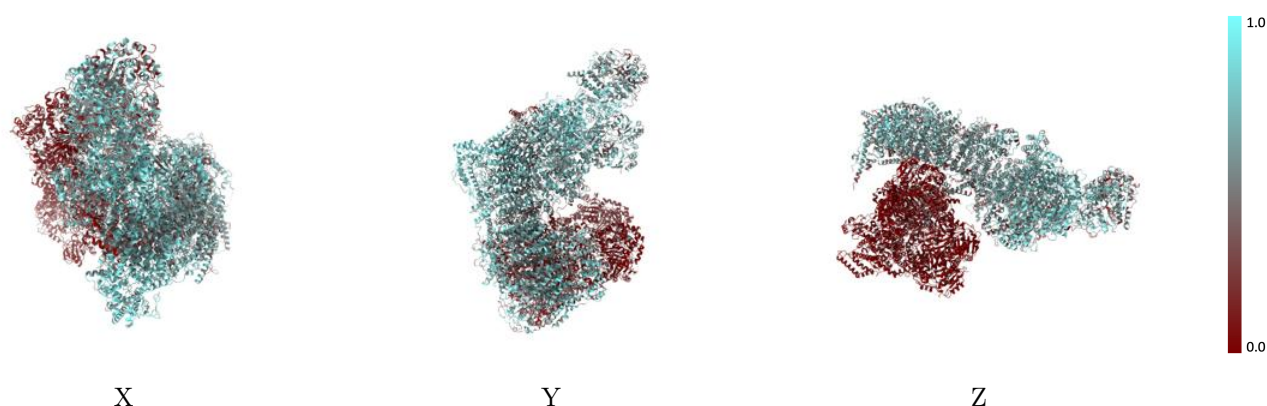
The images above show the 3D surface view of the map at the recommended contour level 0.0082 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



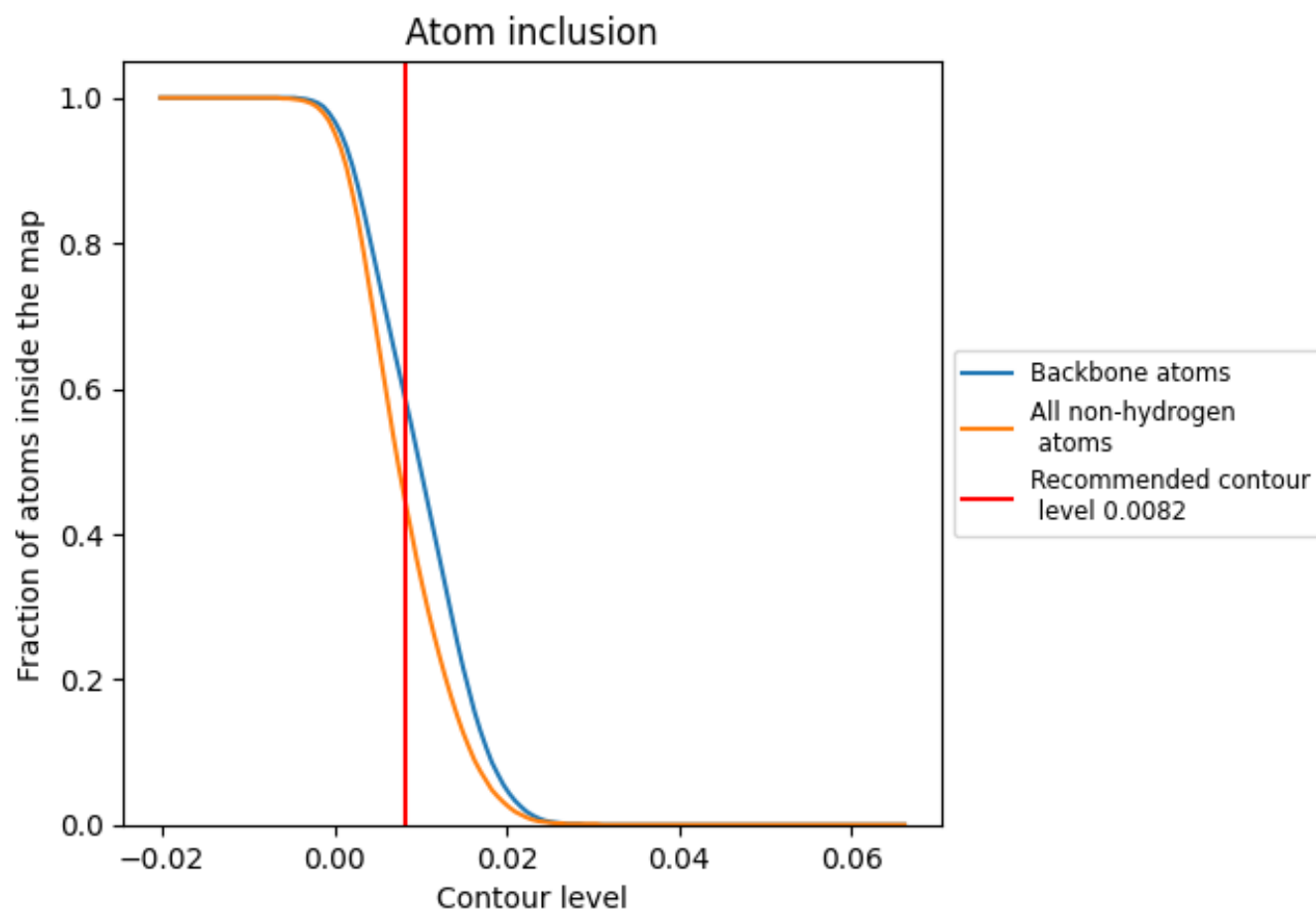
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0082).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 45% 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 (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4470	 0.1620
A	 0.6300	 0.2860
AA	 0.0700	 0.0200
AB	 0.0460	 0.0120
AC	 0.0610	 -0.0060
AD	 0.0420	 -0.0050
AE	 0.0500	 -0.0000
AF	 0.0580	 0.0020
AG	 0.0440	 -0.0140
AH	 0.0140	 0.0180
AI	 0.0780	 -0.0240
AJ	 0.0650	 -0.0270
AK	 0.0500	 -0.0080
Aa	 0.0790	 0.0060
Ab	 0.0970	 0.0020
Ac	 0.1120	 0.0070
Ad	 0.0490	 -0.0020
Ae	 0.0270	 0.0020
Af	 0.0760	 0.0280
Ag	 0.1020	 0.0200
Ah	 0.0230	 0.0210
Aj	 0.0370	 -0.0150
Ak	 0.0460	 -0.0170
B	 0.7370	 0.2950
C	 0.7190	 0.2680
D	 0.7110	 0.3040
E	 0.5840	 0.1820
F	 0.5730	 0.1700
G	 0.6660	 0.2170
H	 0.6640	 0.2950
I	 0.7580	 0.3010
J	 0.5800	 0.2550
K	 0.6600	 0.2980
L	 0.6060	 0.2500
M	 0.6240	 0.2910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N	 0.6810	 0.3080
O	 0.6070	 0.2140
P	 0.6080	 0.1960
Q	 0.6230	 0.2630
R	 0.4540	 0.1950
S	 0.6130	 0.1520
T	 0.4760	 0.1260
U	 0.6600	 0.2200
V	 0.6430	 0.1750
W	 0.6640	 0.2260
X	 0.7620	 0.2650
Y	 0.4750	 0.2170
Z	 0.7340	 0.2500
a	 0.7750	 0.2800
b	 0.7270	 0.2540
c	 0.5820	 0.2290
d	 0.6170	 0.2230
e	 0.7340	 0.2790
f	 0.6200	 0.2590
g	 0.6070	 0.2300
h	 0.6340	 0.2510
i	 0.6070	 0.2300
j	 0.6300	 0.1610
k	 0.6270	 0.2090
l	 0.6080	 0.2260
m	 0.5370	 0.2100
n	 0.6180	 0.2200
o	 0.5820	 0.1390
p	 0.6770	 0.2430
q	 0.2250	 0.1500
r	 0.4090	 0.1190
s	 0.3530	 0.0670