



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:09 PM UTC

PDB ID : 9BXV / pdb_00009bxv
EMDB ID : EMD-45013
Title : Respiratory supercomplex I III
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-22
Resolution : 2.90 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:

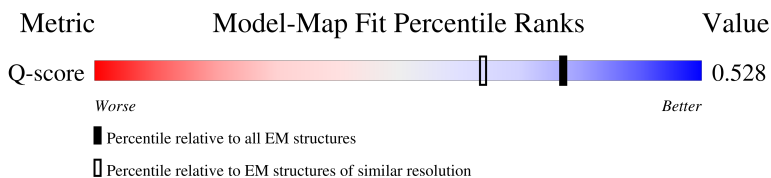
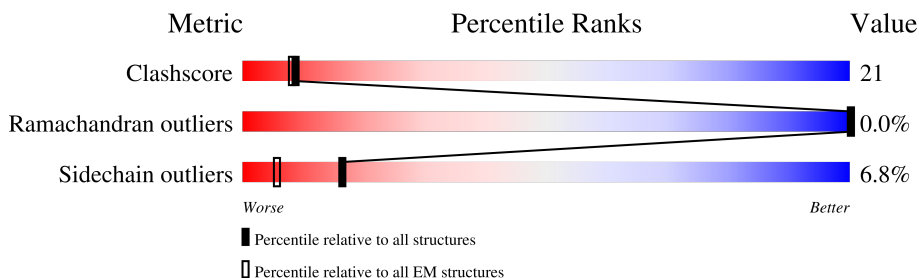
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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.



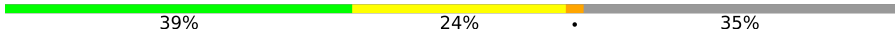
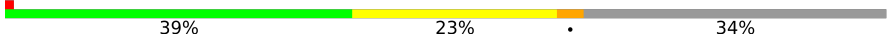
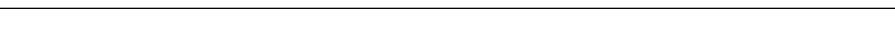
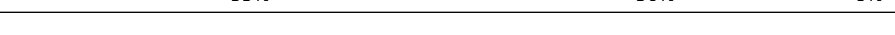
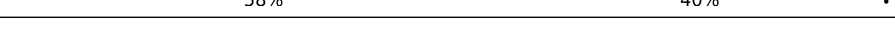
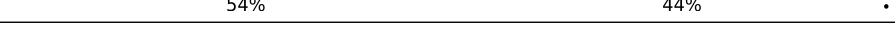
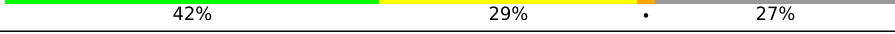
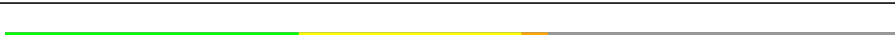
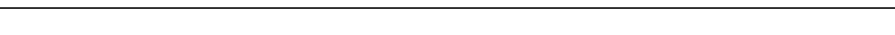
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	0	91	
1	Ab	91	
2	1	64	
2	Ac	64	

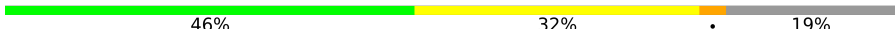
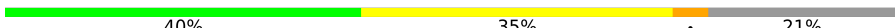
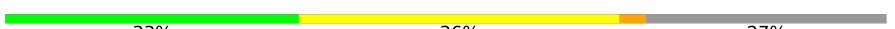
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	2	299	
3	4	299	
3	Ae	299	
3	Af	299	
4	3	56	
4	Ad	56	
5	6	453	
5	v	453	
6	7	379	
6	w	379	
7	8	326	
7	x	326	
8	9	111	
8	y	111	
9	a	189	
10	b	128	
11	c	186	
12	d	176	
13	e	154	
14	f	76	
15	g	122	
16	h	106	
17	i	347	
18	j	115	
19	k	98	

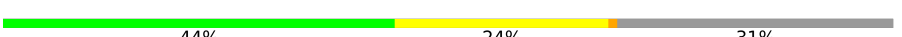
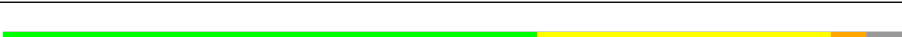
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	m	175	
21	n	58	
22	o	129	
23	p	221	
24	q	459	
25	r	318	
26	B	464	
27	C	469	
28	D	264	
29	E	249	
30	F	123	
31	H	212	
32	I	196	
33	J	175	
34	K	145	
35	L	372	
36	N	116	
37	O	156	
37	X	156	
38	P	99	
39	Q	154	
40	R	110	
41	S	70	
42	T	169	
43	U	357	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
44	V	141	
45	W	144	
46	Y	105	
47	Z	114	
48	l	606	
49	s	249	
50	t	137	
51	5	480	
51	u	480	
52	Aa	82	
52	z	82	
53	G	727	
54	M	113	

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	FES	2	301	-	-	X	-
55	FES	4	301	-	-	X	-
55	FES	E	301	-	-	X	-
59	SF4	H	301	-	-	X	-
59	SF4	H	302	-	-	X	-
59	SF4	I	201	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 98682 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 Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	68	Total	C	N	O	S	0	0
			557	338	100	114	5		
1	Ab	66	Total	C	N	O	S	0	0
			543	331	99	108	5		

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	60	Total	C	N	O	0	0
			493	322	87	84		
2	Ac	59	Total	C	N	O	0	0
			485	318	85	82		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	195	Total	C	N	O	S	0	0
			1513	953	264	289	7		
3	4	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
3	Ae	39	Total	C	N	O	S	0	0
			266	166	50	47	3		
3	Af	34	Total	C	N	O	S	0	0
			240	153	43	42	2		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	51	Total	C	N	O	S	0	0
			417	279	74	63	1		
4	Ad	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		
5	v	418	Total	C	N	O	S	0	0
			3140	1966	556	610	8		

- Molecule 6 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
6	w	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 7 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		
7	x	238	Total	C	N	O	S	0	0
			1896	1211	326	343	16		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	99	Total	C	N	O	S	0	0
			878	563	154	159	2		
8	y	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	108	Total	C	N	O	0	0
			900	591	156	153		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	153	Total	C	N	O	S	0	0
			1291	838	208	237	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	168	Total	C	N	O	S	0	0
			1417	890	258	261	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	99	Total	C	N	O	S	0	0
			826	530	137	155	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	46	Total	C	N	O	0	0
			391	259	67	65		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2711	1782	420	463	46		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	114	Total	C	N	O	S	0	0
			905	610	133	155	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	175	Total	C	N	O	S	0	0
			1338	897	190	238	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	56	Total	C	N	O	S	0	0
			475	308	87	79	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	459	Total	C	N	O	S	0	0
			3630	2410	572	609	39		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	430	Total	C	N	O	S	0	0
			3454	2207	593	630	24		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	208	Total	C	N	O	S	0	0
			1732	1121	297	312	2		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	94	Total	C	N	O	S	0	0
			727	444	136	144	3		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	H	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	I	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	118	Total	C	N	O	S	0	0
			962	608	173	178	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	144	Total	C	N	O	S	0	0
			1203	769	217	212	5		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	340	Total	C	N	O	S	0	0
			2735	1771	479	476	9		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	N	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 37 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	84	Total	C	N	O	S	0	0
			680	440	100	135	5		
37	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	83	Total	C	N	O	S	0	0
			669	419	125	123	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Q	112	Total	C	N	O	S	0	0
			954	610	176	163	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	T	82	Total	C	N	O	S	0	0
			638	414	109	114	1		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	318	Total	C	N	O	S	0	0
			2574	1638	437	489	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	W	140	Total	C	N	O	S	0	0
			1162	749	201	203	9		

- Molecule 46 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	62	Total	C	N	O	S	0	0
			531	352	88	90	1		

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	78	Total	C	N	O	S	0	0
			626	410	105	110	1		

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	l	603	Total	C	N	O	S	0	0
			4785	3174	741	819	51		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	119	Total	C	N	O	S	0	0
			1019	635	195	180	9		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
51	5	435	Total	C	N	O	S	0	0
			3374	2105	594	656	19		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	79	Total	C	N	O	S	0	0
			666	434	122	108	2		
52	Aa	78	Total	C	N	O	S	0	0
			662	432	121	107	2		

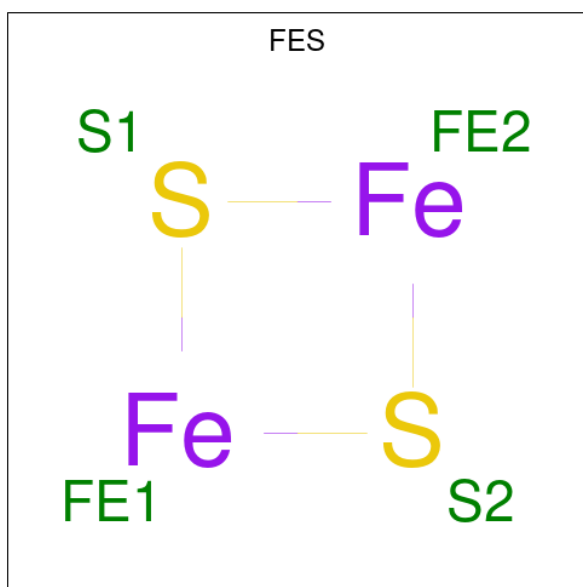
- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	G	684	Total	C	N	O	S	0	0
			5260	3298	917	1006	39		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

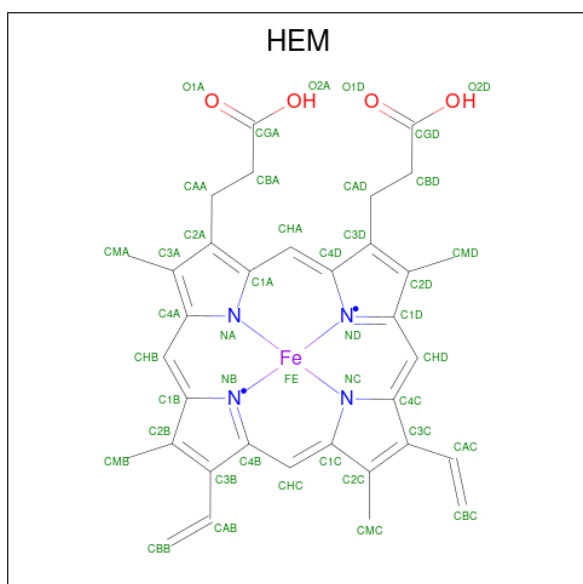
Mol	Chain	Residues	Atoms					AltConf	Trace
54	M	96	Total	C	N	O	S	0	0
			773	487	146	137	3		

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



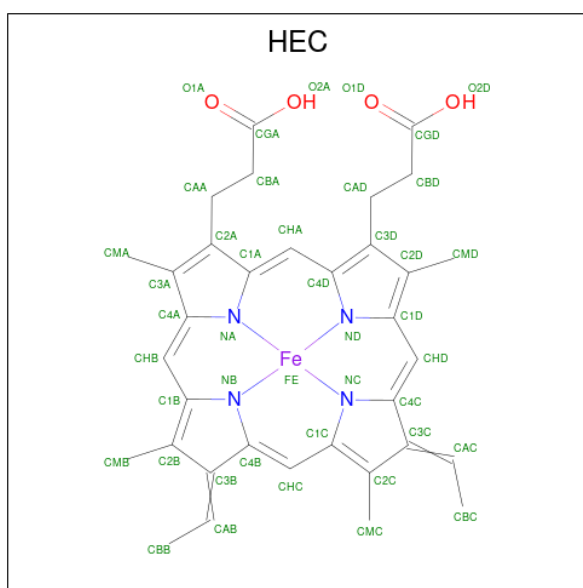
Mol	Chain	Residues	Atoms			AltConf
55	2	1	Total	Fe	S	0
			4	2	2	
55	4	1	Total	Fe	S	0
			4	2	2	
55	E	1	Total	Fe	S	0
			4	2	2	
55	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 56 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



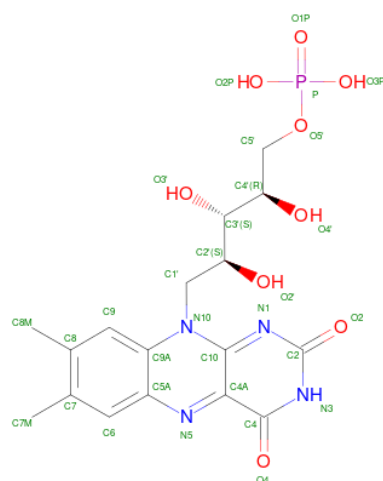
Mol	Chain	Residues	Atoms					AltConf
56	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	7	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
56	w	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 57 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



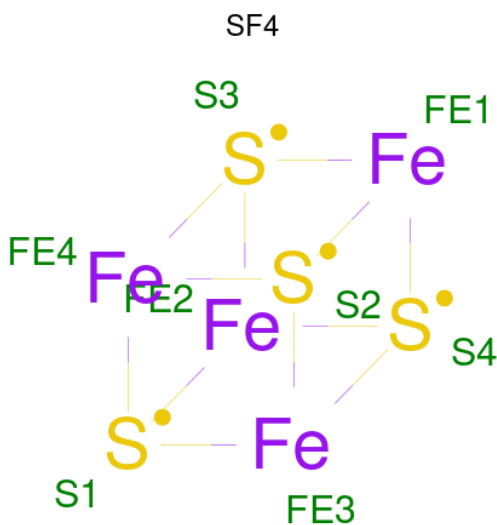
Mol	Chain	Residues	Atoms					AltConf
57	8	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
57	x	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



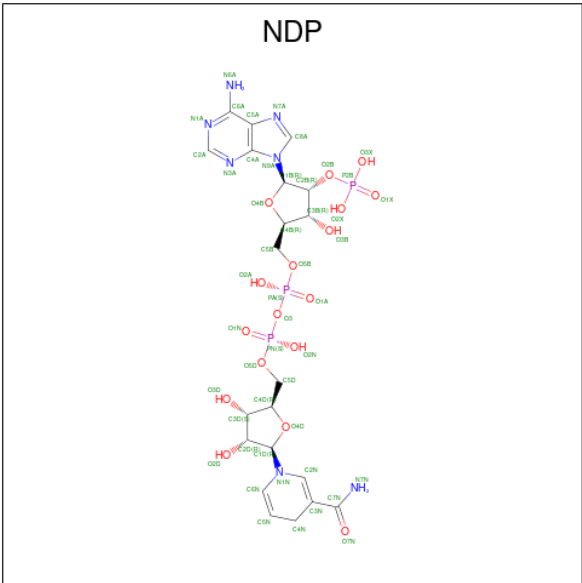
Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total 8	Fe 4	S 4	0
59	H	1	Total 8	Fe 4	S 4	0
59	H	1	Total 8	Fe 4	S 4	0

Continued on next page...

Continued from previous page...

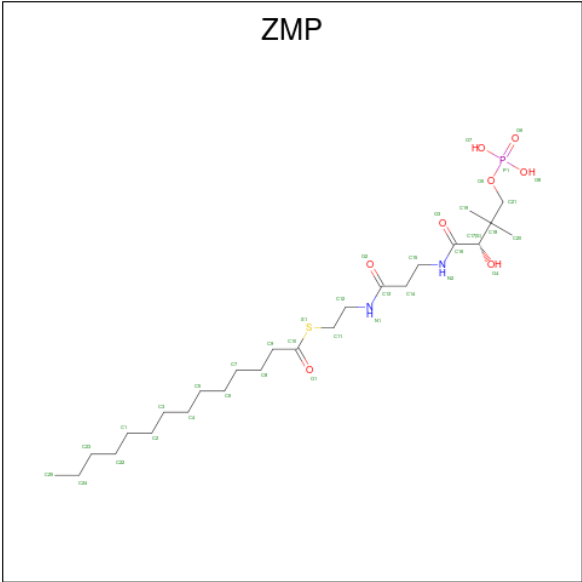
Mol	Chain	Residues	Atoms			AltConf
59	I	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 60 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 61 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

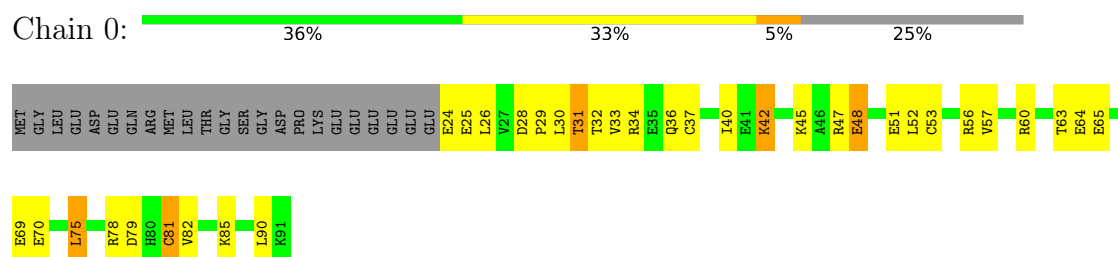


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
61	Q	1	30	18	2	8	1	1	0

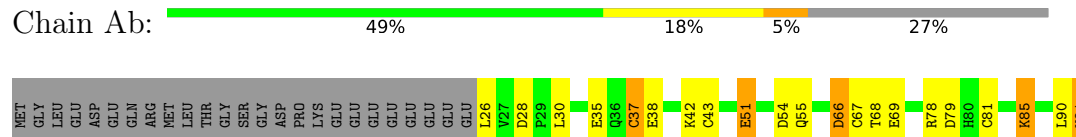
3 Residue-property plots

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.

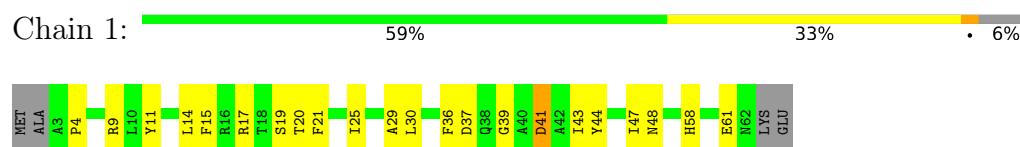
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



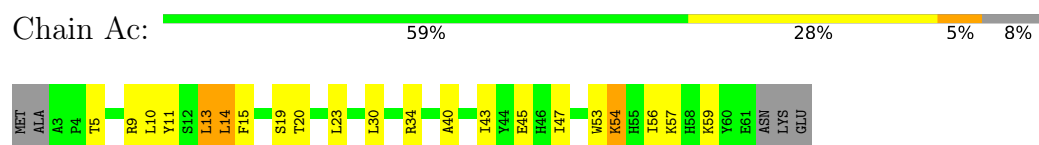
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



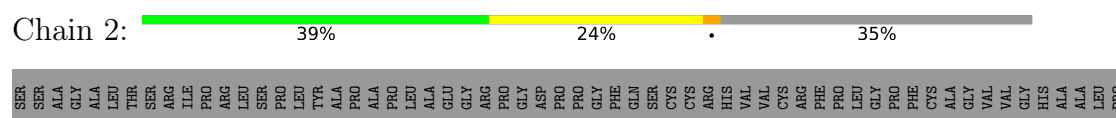
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

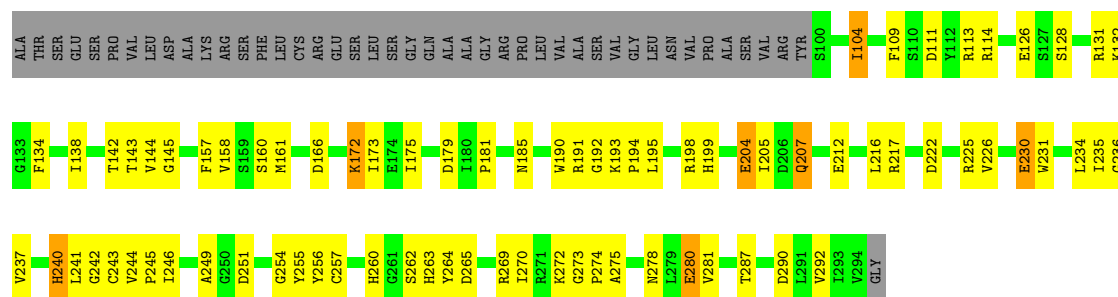


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

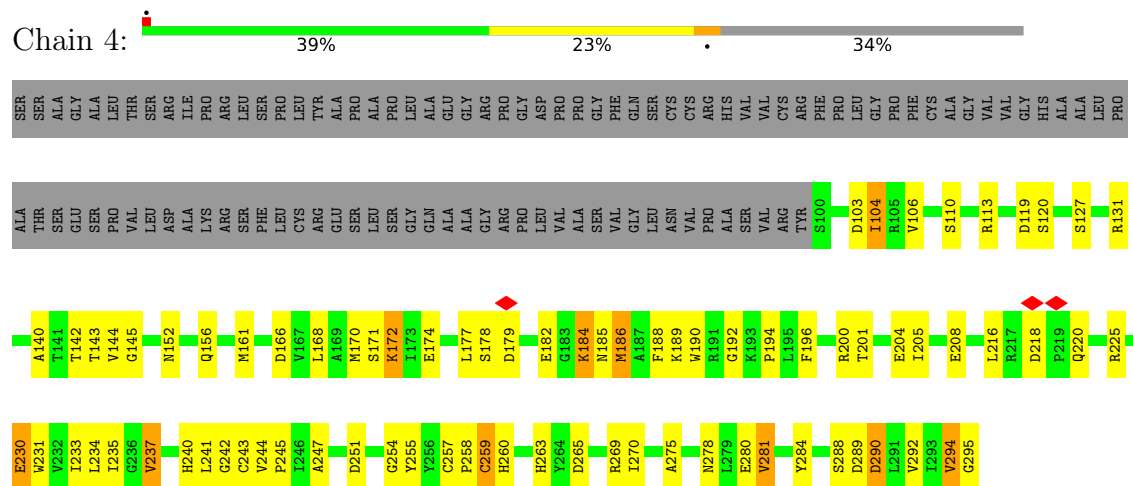


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

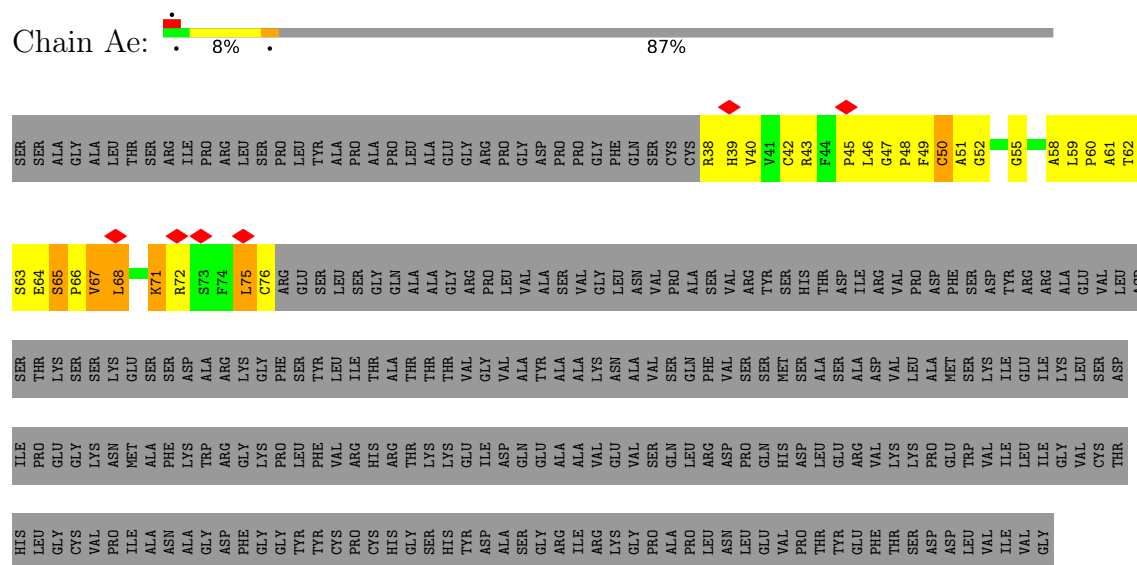




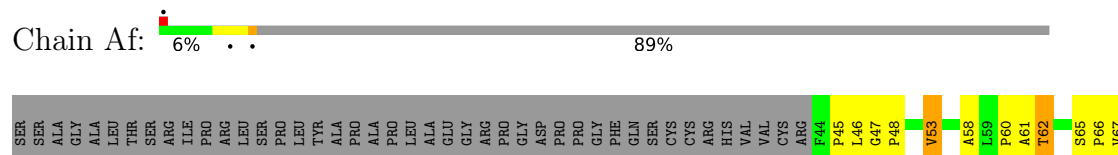
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

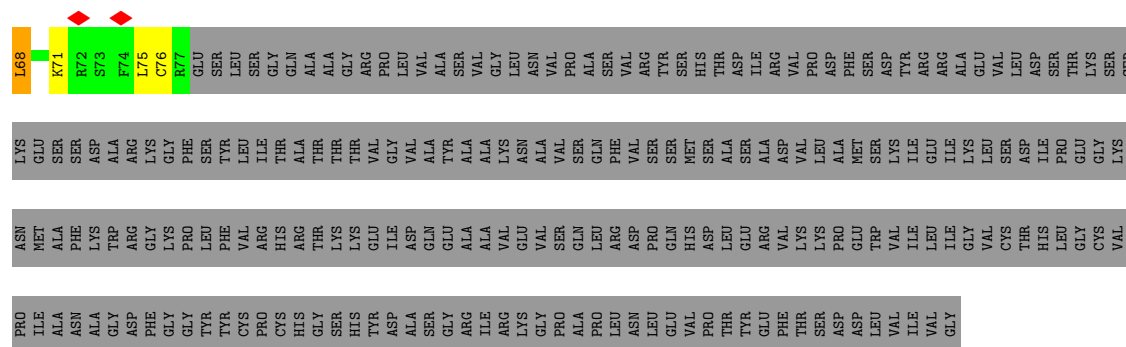


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1



- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1





- Molecule 4: Cytochrome b-c1 complex subunit 10

Chain 3: 68% 20% 9%



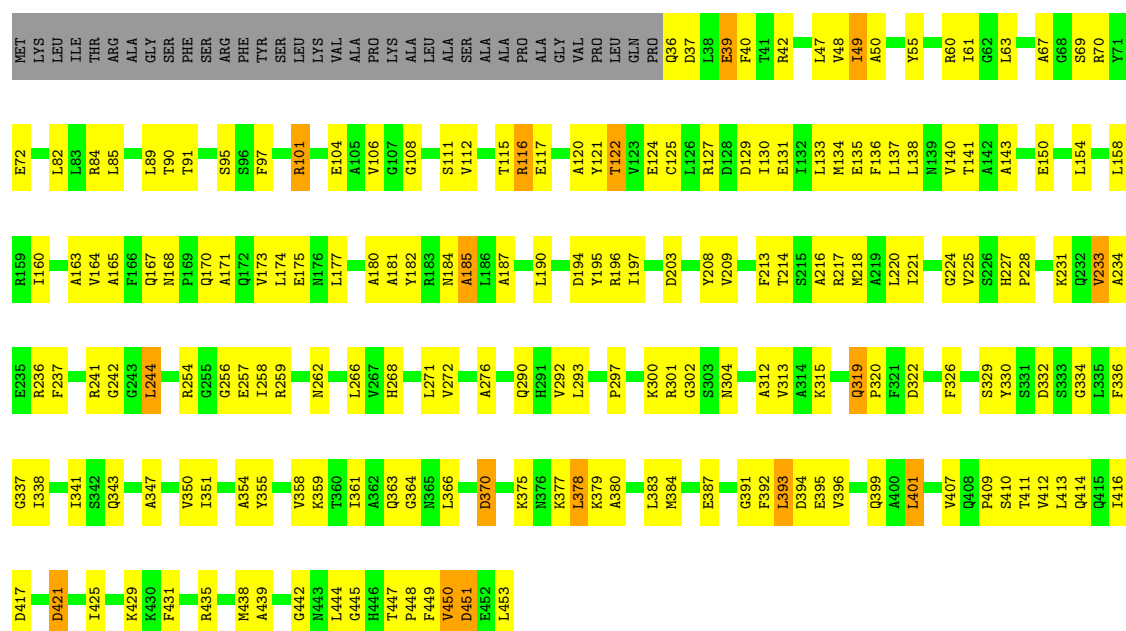
- Molecule 4: Cytochrome b-c1 complex subunit 10

Chain Ad: 68% 23% 9%



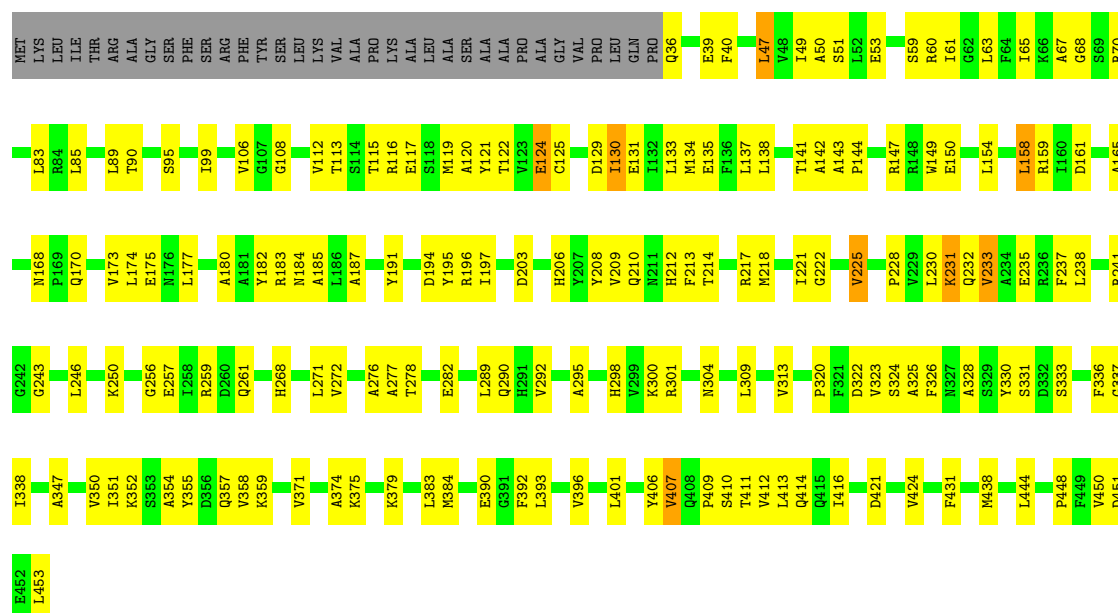
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6: 51% 38% 8%



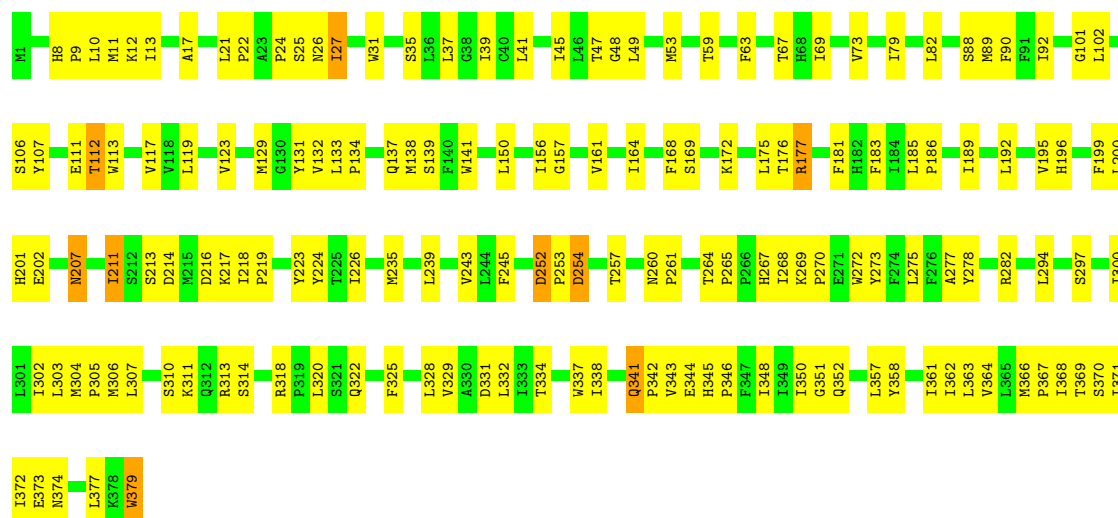
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain v:  55% 36% 8%



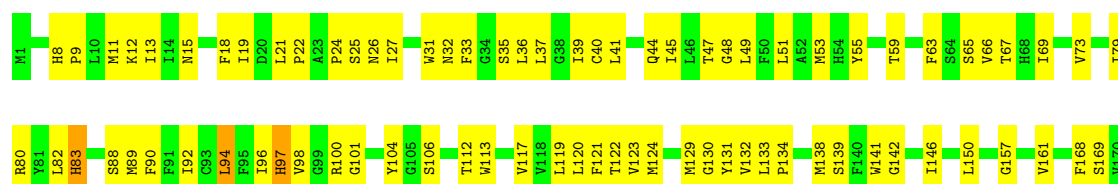
• Molecule 6: Cytochrome b

Chain 7:  58% 40% 2%



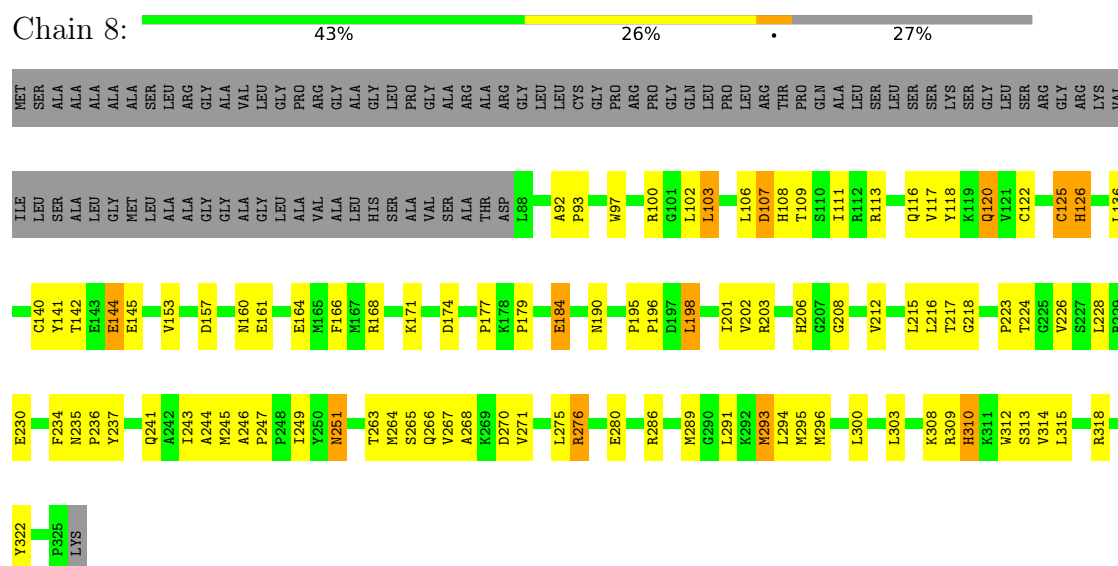
• Molecule 6: Cytochrome b

Chain w:  54% 44% 2%

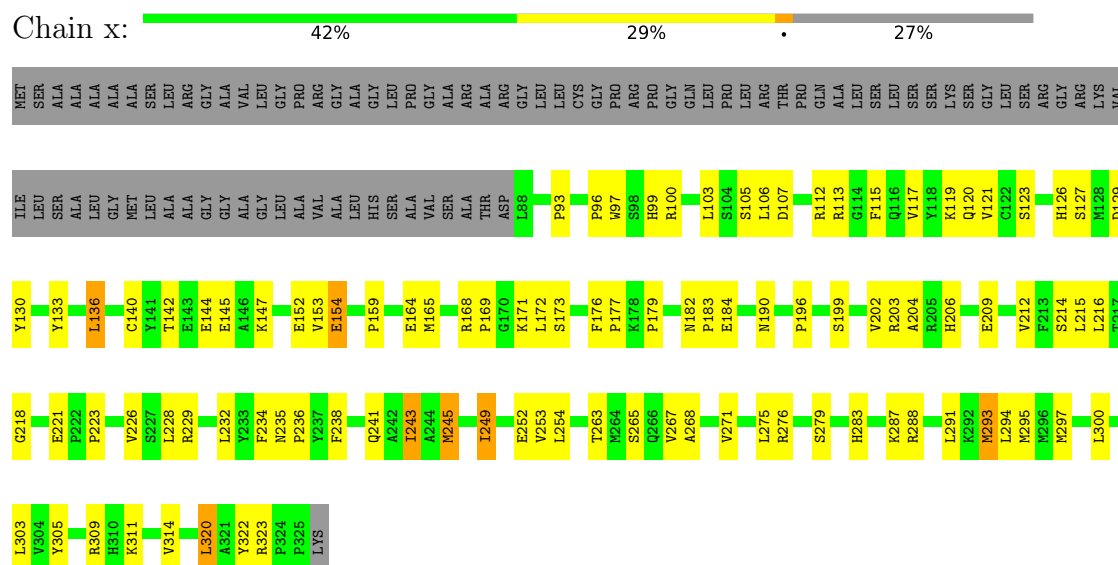




• Molecule 7: Cytochrome c1

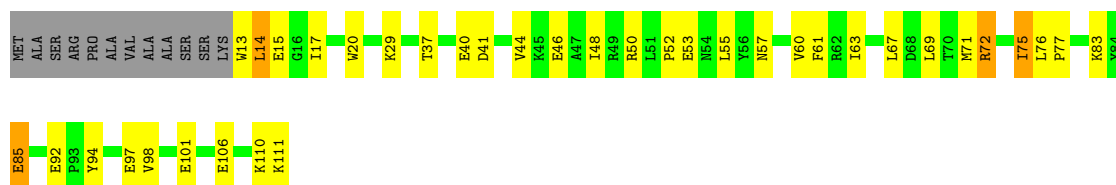


• Molecule 7: Cytochrome c1



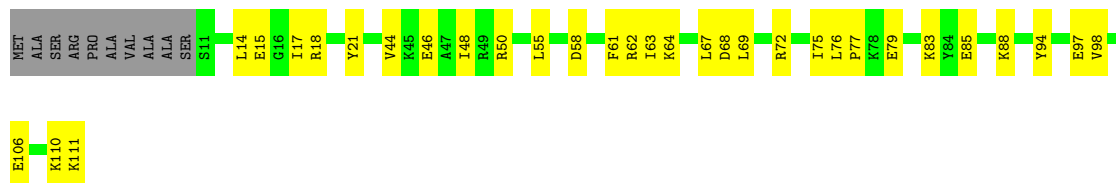
• Molecule 8: Cytochrome b-c1 complex subunit 7





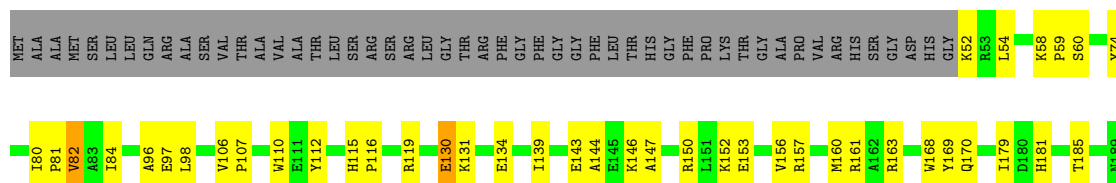
- Molecule 8: Cytochrome b-c1 complex subunit 7

Chain y:



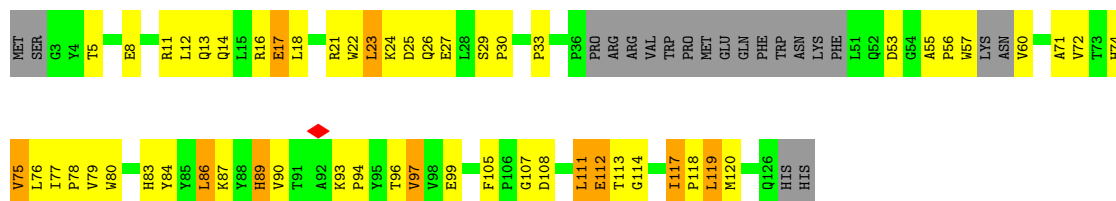
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:



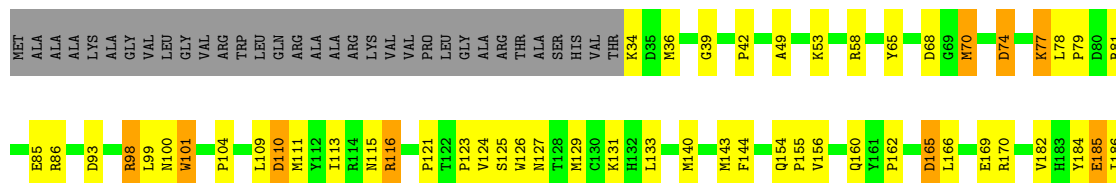
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:



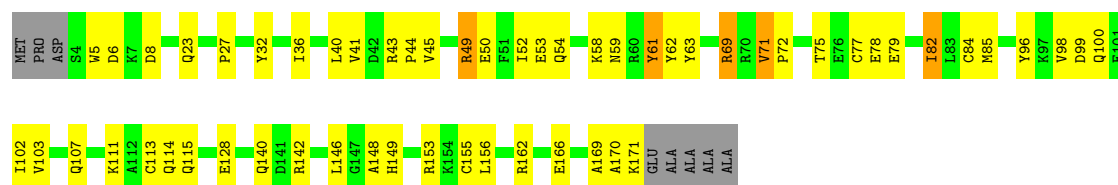
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:

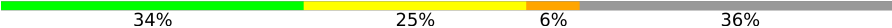


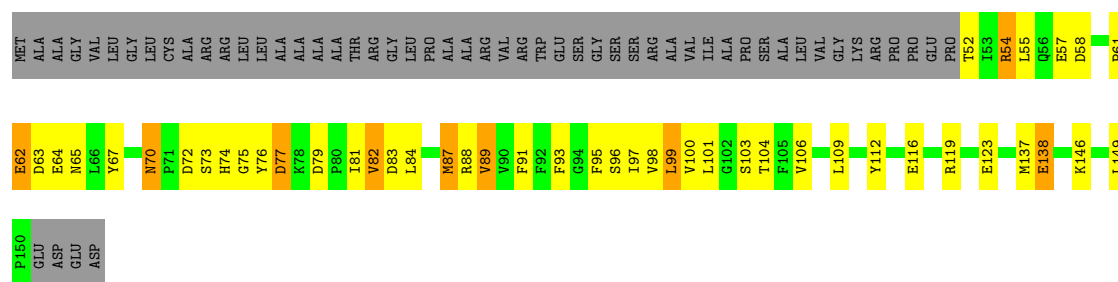
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 

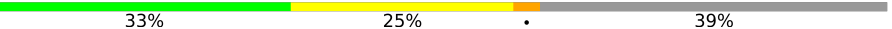


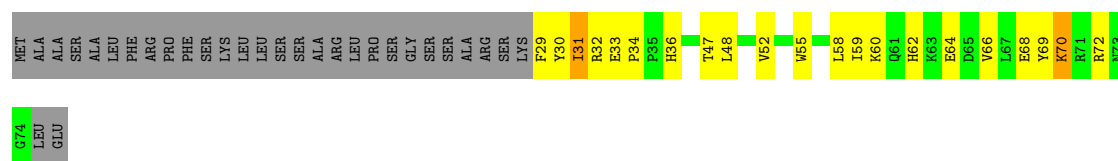
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 



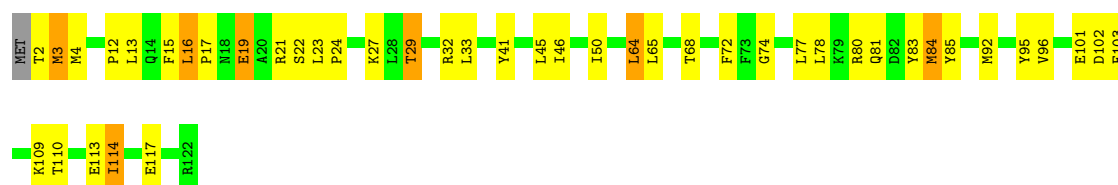
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

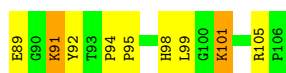
Chain g: 



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

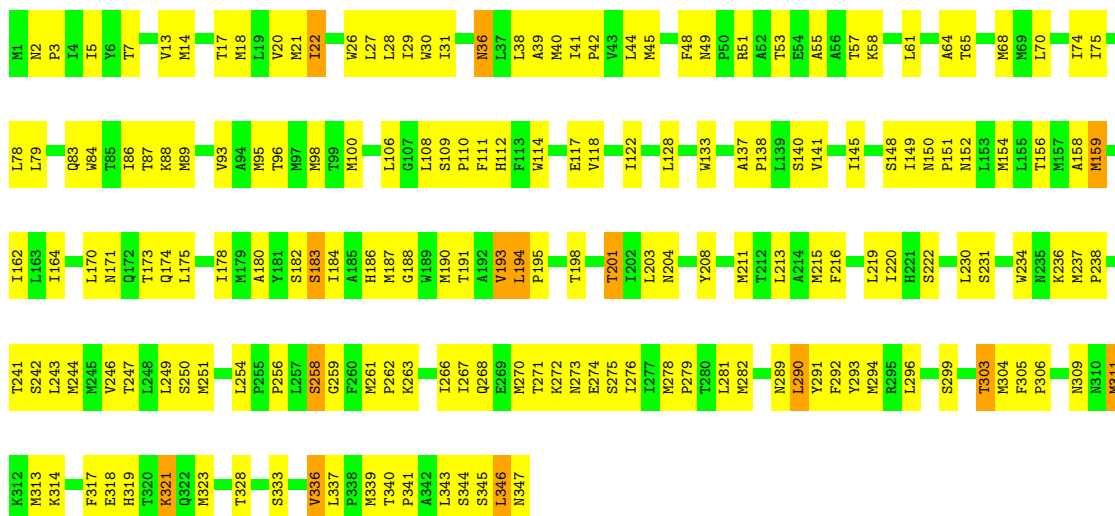
Chain h: 





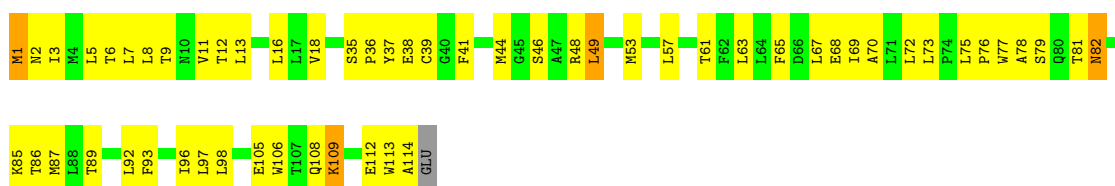
• Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i: 48% 48% .



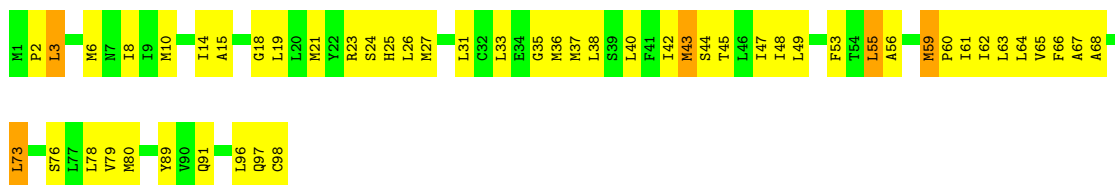
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j: 50% 46% . .



• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

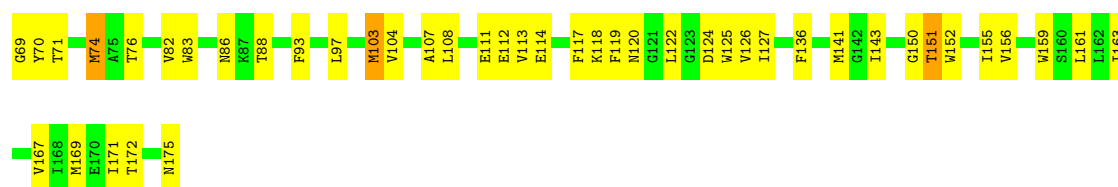
Chain k: 47% 48% 5%



• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

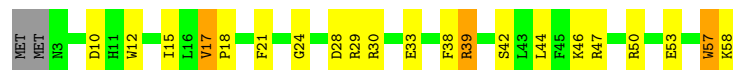
Chain m: 52% 44% .





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

Chain n: 60% 31% 5% .



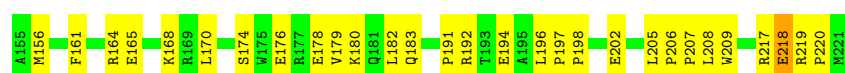
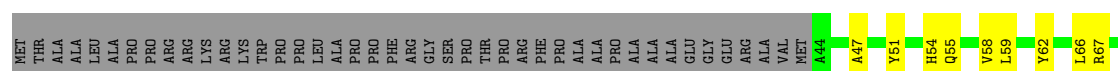
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 57% 40% ..



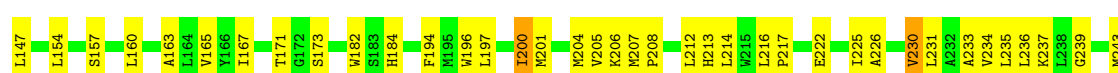
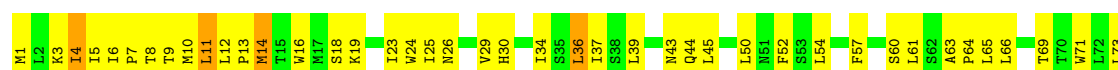
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

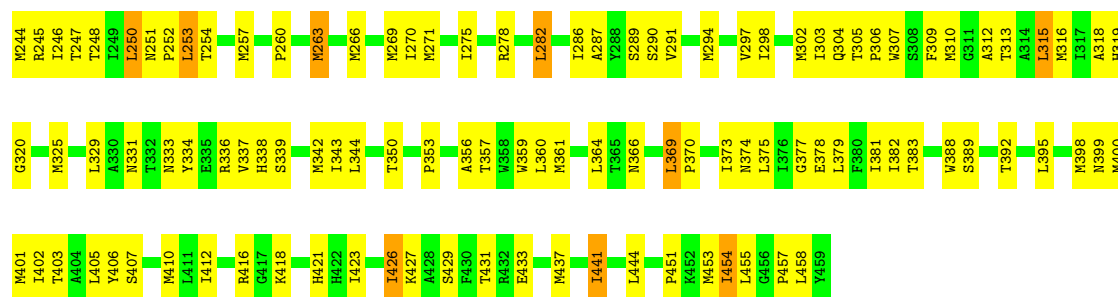
Chain p: 46% 32% . 19%



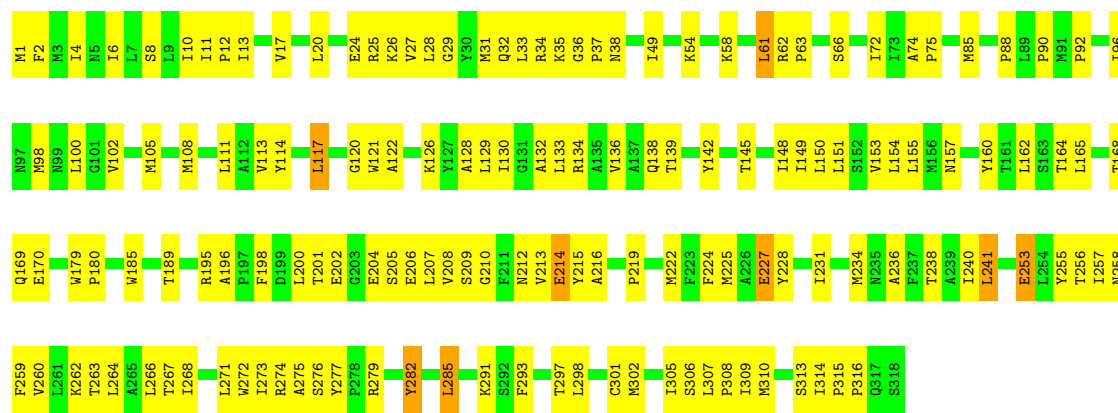
- Molecule 24: NADH-ubiquinone oxidoreductase chain 4

Chain q: 50% 47% .

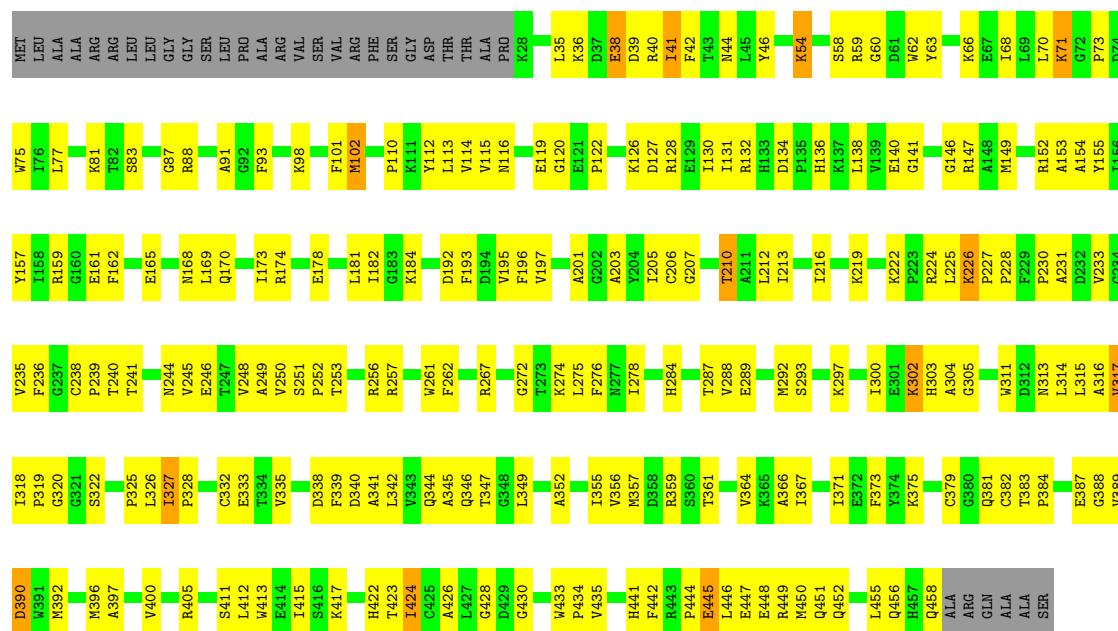




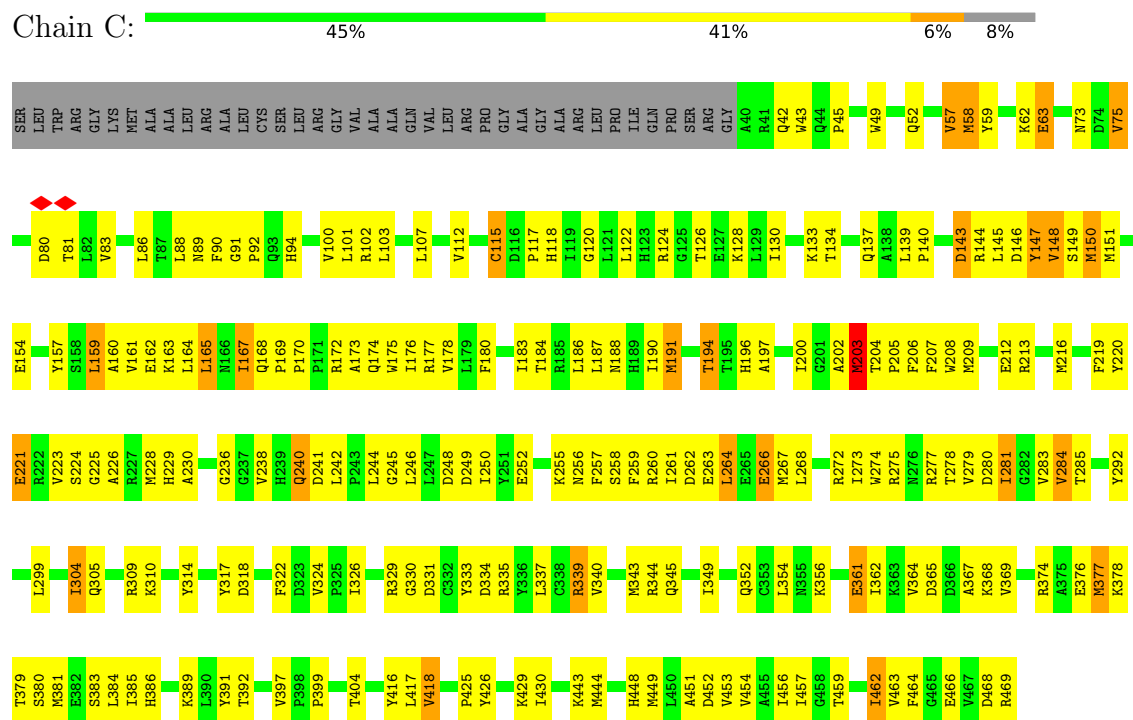
• Molecule 25: NADH-ubiquinone oxidoreductase chain 1



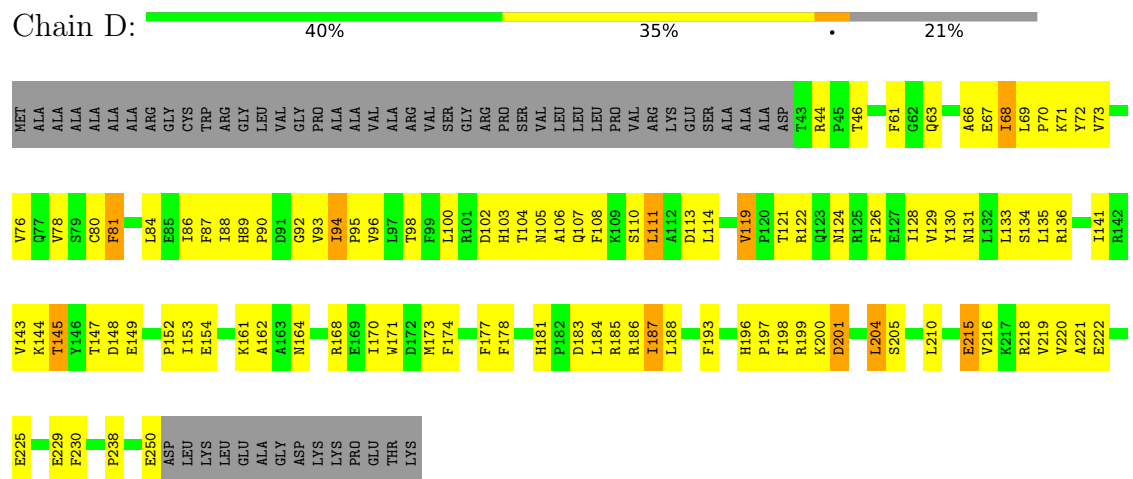
• Molecule 26: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



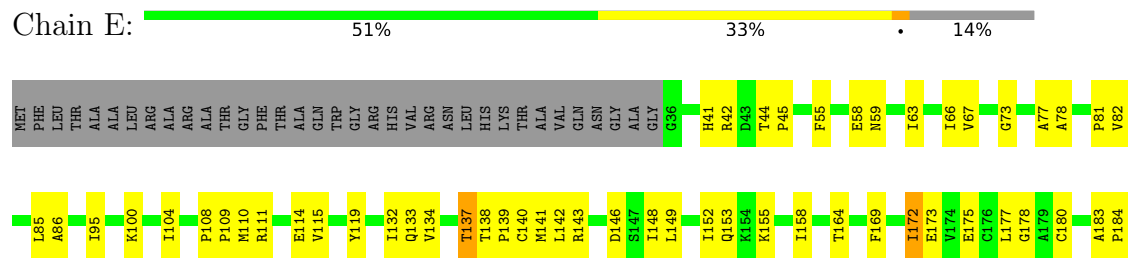
• Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

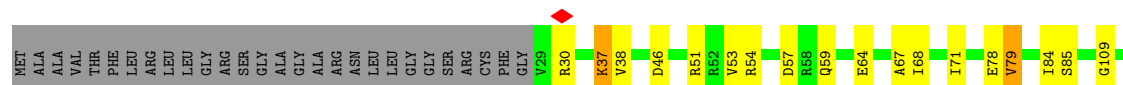


- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

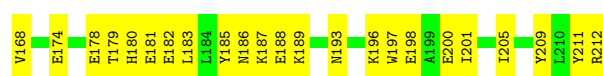
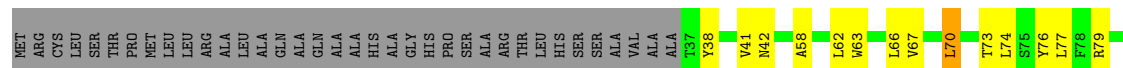




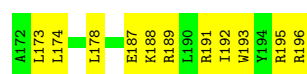
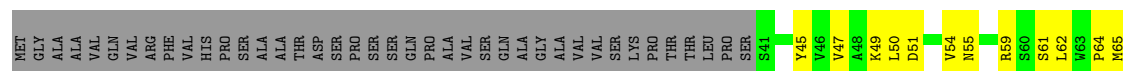
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



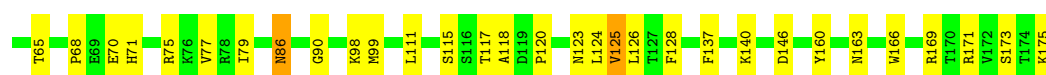
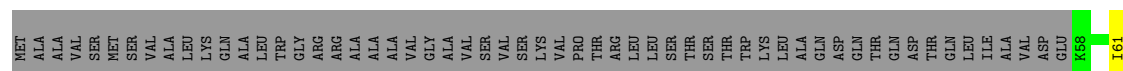
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

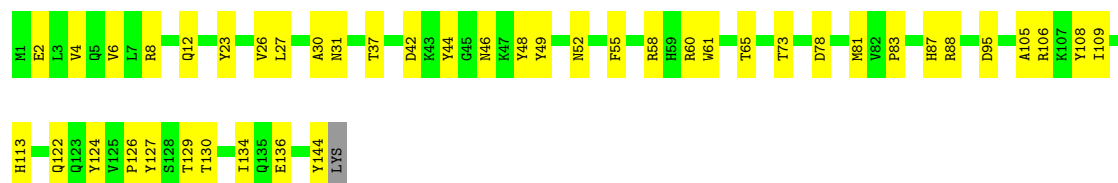


- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

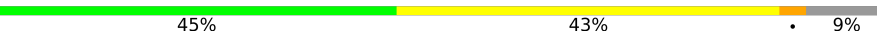


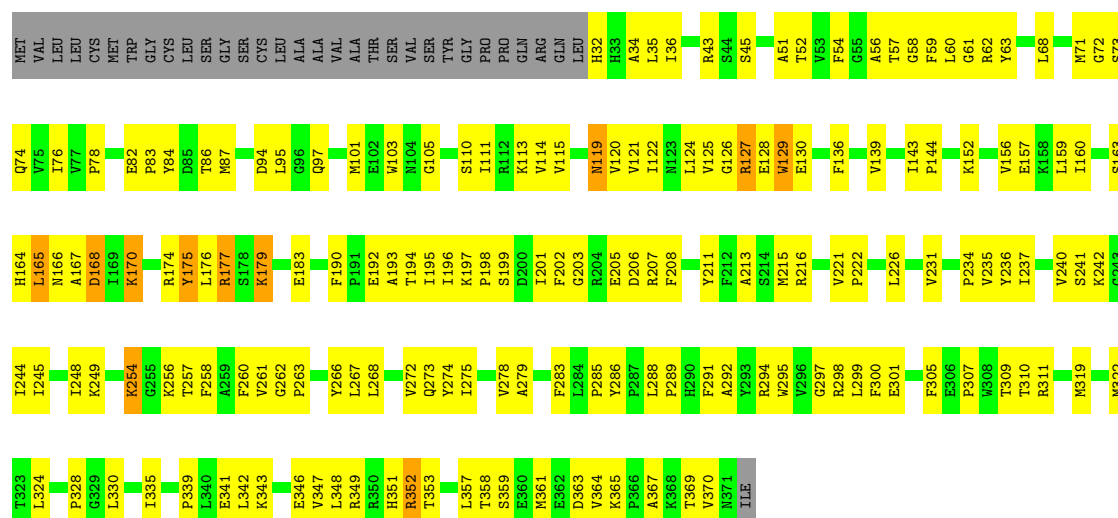
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain K: 



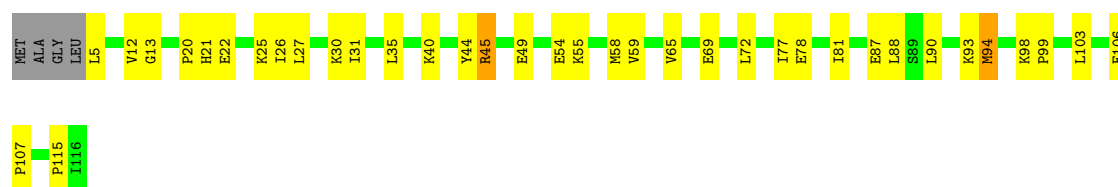
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 



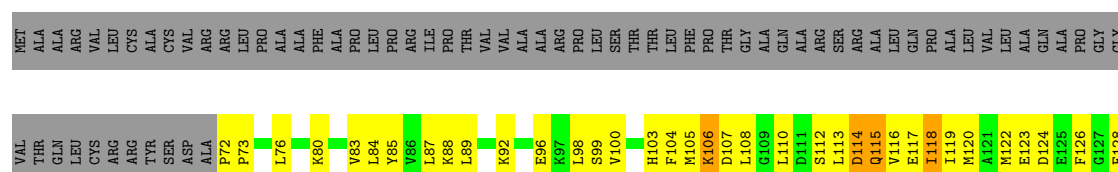
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

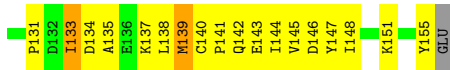
Chain N: 



- Molecule 37: Acyl carrier protein

Chain O: 





- Molecule 37: Acyl carrier protein

Chain X: 31% 22% 46%



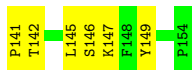
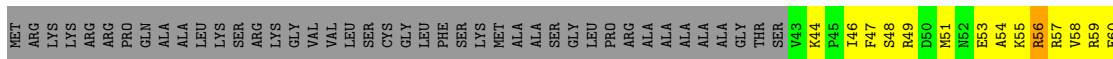
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 52% 30% 16%



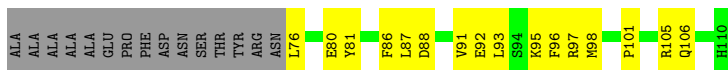
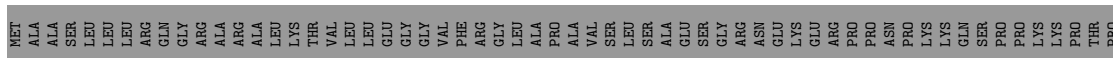
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 33% 36% 27%



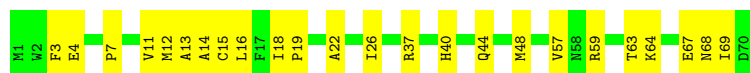
- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R: 17% 15% 68%



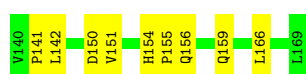
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  66% 34%



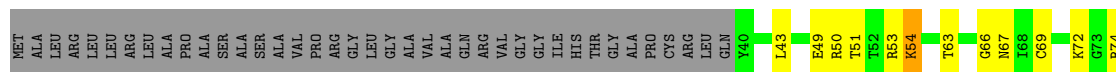
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T:  31% 18% 51%



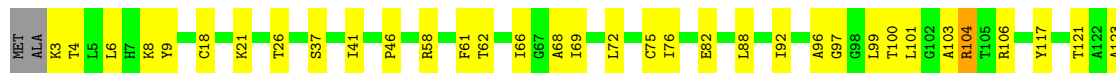
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U:  56% 30% 11%



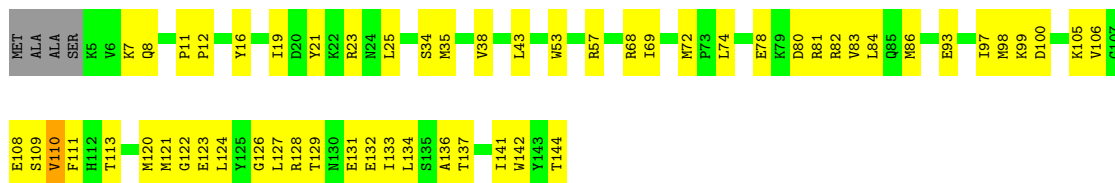
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  71% 26% 3%

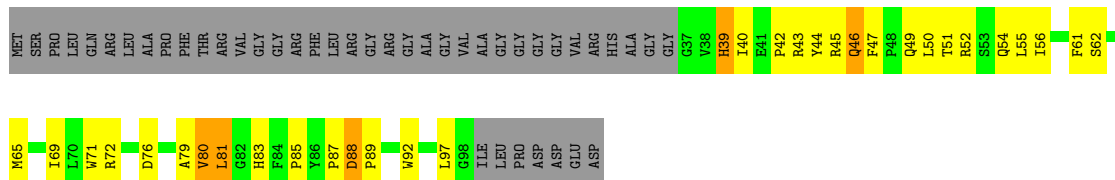
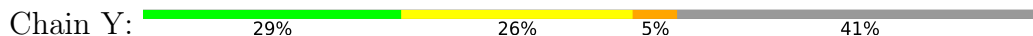


- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

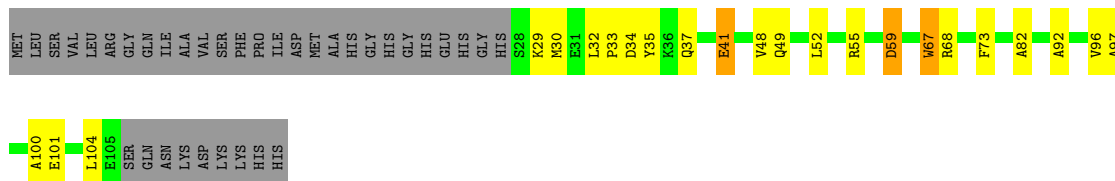
Chain W:  58% 38% 4%



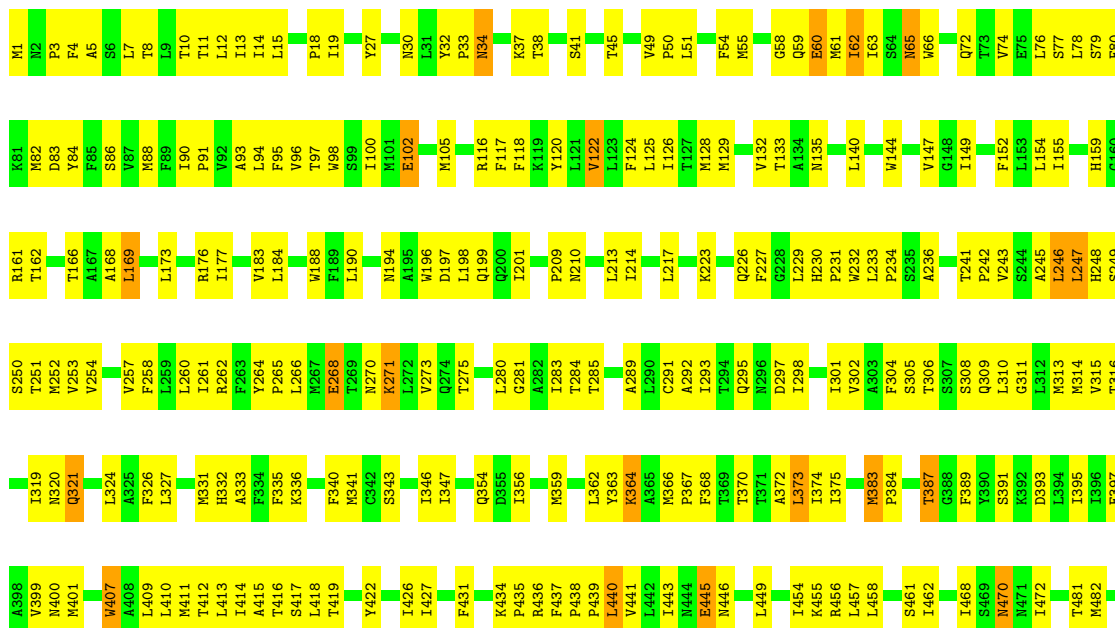
• Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

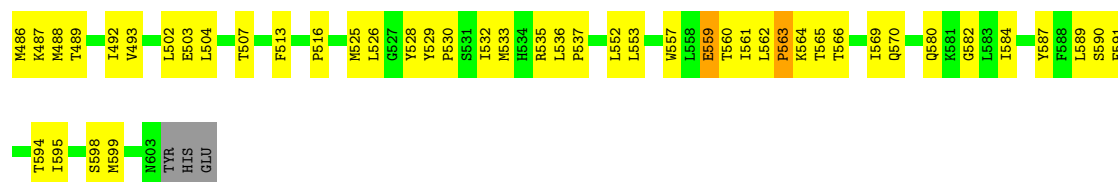


• Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



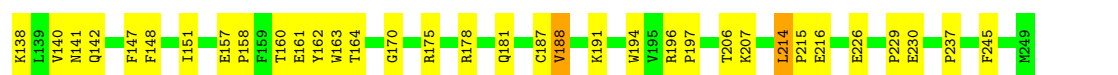
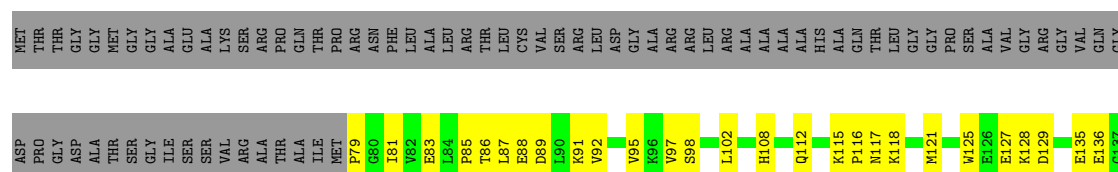
• Molecule 48: NADH-ubiquinone oxidoreductase chain 5





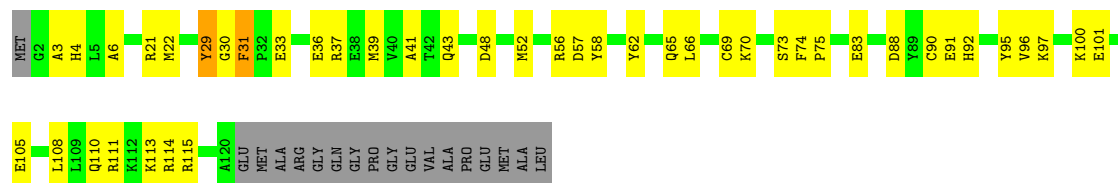
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain s: 44% 24% 31%



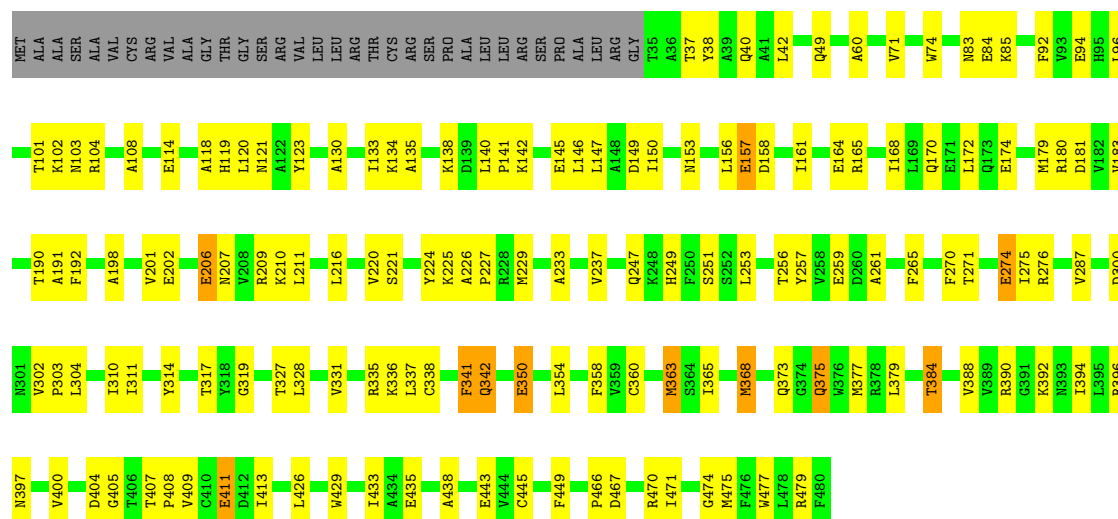
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t: 55% 31% 13%



- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain u: 62% 29% 7%



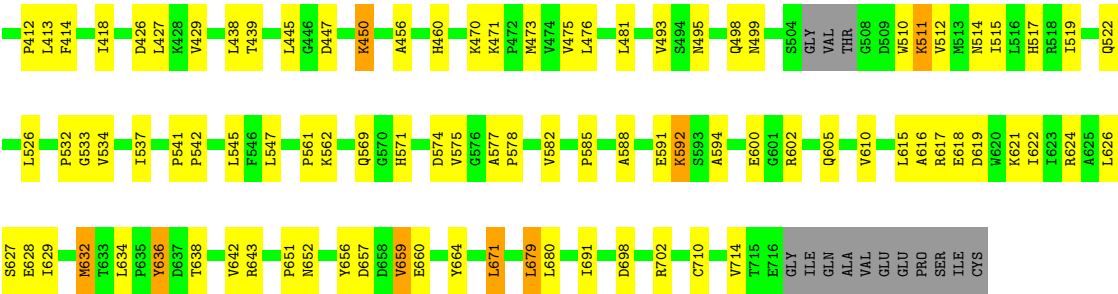
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

V400	N301	P204	MET
V405	P302	N207	ALA
P408	V306	L211	SER
V409	I310	S212	ALA
C410	D315	R213	VAL
E411	D318	L216	CYS
I412	G319	T217	VAL
I413	Y318	E218	ALA
G414	G319	Y219	GLY
R415	M324	V220	THR
L416	T327	Y224	GLY
L417	L328	K225	SER
L418	L328	A226	ARG
T419	V331	P227	VAL
L426	R335	R228	LEU
W429	K336	M229	LEU
I433	R337	A233	ARG
D437	C338	A234	CYS
A438	Q339	V237	SER
S439	F341	D244	PRO
V440	Y343	L245	LEU
V444	A349	G255	LEU
C445	E350	THR	GLY
F449	T351	TYR	THR
Y450	F358	VAL	ALA
D451	M363	GLU	ALA
G452	M368	ASP	ARG
C453	F371	ALA	GLY
A455	L372	VAL	THR
V456	R373	PRO	A36
I462	G374	E162	T37
E463	Q375	ALA	Y38
L465	W376	ALA	L42
P466	M377	PHI	L42
D467	R378	T266	E47
Y468	L379	R269	T48
I471	T384	E274	Q49
R472	V388	I275	L49
S473	V389	R276	A60
G474	R390	H277	S61
M475	G391	R278	
F476	K392	D279	T70
F480	N393	L282	W74
	I394	P283	I75
	R395	L284	T190
		P294	A191
		P298	F192
		N298	E92
		G299	N83
		P300	E94
			A198
			N57

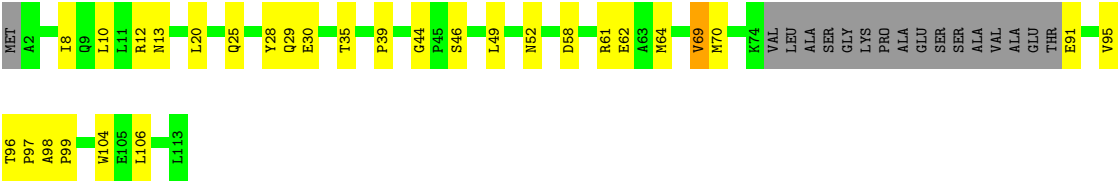
[illegible]

ME1	GLY	R3	E4	F5	L8	T9	R12	T15	T16	Y17	S18	L19	S20	P21	F22	E23	Q24	R25	A26	F27	P28	H29	Y30	F31	T32	L47	R48	V49	A50	P51	P52	V55	V59	Y60	T61	Q65	E68	R72	K73	E79	N80	ASP	YS
-----	-----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

[illegible]



● Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.222	Depositor
Minimum map value	-0.248	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, HEC, FMN, HEM, SF4, ZMP, FES

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	0	0.15	0/563	0.32	0/755
1	Ab	0.08	0/549	0.19	0/735
2	1	0.16	0/506	0.31	0/683
2	Ac	0.10	0/498	0.19	0/672
3	2	0.15	0/1546	0.29	0/2093
3	4	0.33	0/1551	0.47	0/2098
3	Ae	0.22	0/272	0.59	0/372
3	Af	0.23	0/246	0.45	0/335
4	3	0.15	0/433	0.31	0/593
4	Ad	0.11	0/437	0.22	0/598
5	6	0.22	0/3192	0.33	0/4322
5	v	0.13	0/3192	0.28	0/4322
6	7	0.18	0/3123	0.32	0/4269
6	w	0.29	0/3123	0.43	2/4269 (0.0%)
7	8	0.16	0/1954	0.32	0/2652
7	x	0.13	0/1954	0.24	0/2652
8	9	0.12	0/898	0.24	0/1204
8	y	0.13	0/913	0.24	0/1223
9	a	0.14	0/1184	0.31	0/1603
10	b	0.23	0/927	0.40	0/1264
11	c	0.13	0/1346	0.26	0/1840
12	d	0.12	0/1449	0.25	0/1953
13	e	0.14	0/849	0.30	0/1153
14	f	0.12	0/404	0.26	0/547
15	g	0.14	0/1031	0.25	0/1394
16	h	0.12	0/889	0.24	0/1190
17	i	0.15	0/2774	0.29	0/3768
18	j	0.15	0/929	0.32	0/1269
19	k	0.16	0/759	0.36	0/1029
20	m	0.16	0/1373	0.32	0/1860
21	n	0.23	0/487	0.39	0/659
22	o	0.15	0/1092	0.31	0/1481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	p	0.12	0/1590	0.27	0/2155
24	q	0.16	0/3721	0.31	0/5073
25	r	0.23	0/2581	0.41	0/3529
26	B	0.21	0/3393	0.36	0/4584
27	C	0.17	0/3547	0.34	1/4809 (0.0%)
28	D	0.17	0/1783	0.39	1/2428 (0.0%)
29	E	0.26	0/1698	0.41	0/2311
30	F	0.12	0/740	0.25	0/998
31	H	0.17	0/1443	0.33	0/1952
32	I	0.19	0/1279	0.30	0/1730
33	J	0.12	0/985	0.25	0/1329
34	K	0.12	0/1244	0.23	0/1693
35	L	0.30	0/2812	0.40	0/3812
36	N	0.36	0/929	0.52	0/1258
37	O	0.12	0/692	0.33	0/934
37	X	0.18	0/701	0.30	0/946
38	P	0.10	0/680	0.24	0/916
39	Q	0.13	0/978	0.27	0/1317
40	R	0.09	0/304	0.24	0/410
41	S	0.14	0/577	0.27	0/777
42	T	0.12	0/659	0.25	0/905
43	U	0.12	0/2634	0.25	0/3565
44	V	0.13	0/1037	0.28	0/1404
45	W	0.13	0/1193	0.27	0/1609
46	Y	0.14	0/555	0.33	0/760
47	Z	0.10	0/645	0.23	0/872
48	l	0.14	0/4914	0.30	0/6683
49	s	0.13	0/1436	0.29	0/1938
50	t	0.15	0/1043	0.30	0/1396
51	5	0.14	0/3442	0.27	0/4667
51	u	0.14	0/3531	0.27	0/4793
52	Aa	0.14	0/684	0.28	0/926
52	z	0.15	0/688	0.30	0/931
53	G	0.15	0/5347	0.28	0/7243
54	M	0.13	0/791	0.27	0/1069
All	All	0.18	0/100719	0.32	4/136579 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	6	0	1
6	7	0	1
7	8	0	1
25	r	0	1
27	C	0	1
35	L	0	1
36	N	0	1
51	u	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	104	THR	N-CA-C	-9.37	98.72	111.55
27	C	203	MET	N-CA-CB	-5.96	107.38	114.17
6	w	18	PHE	CA-C-N	-5.42	117.41	123.16
6	w	18	PHE	C-N-CA	-5.42	117.41	123.16

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	6	116	ARG	Sidechain
6	7	177	ARG	Sidechain
7	8	286	ARG	Sidechain
27	C	339	ARG	Sidechain
35	L	127	ARG	Sidechain
36	N	45	ARG	Sidechain
25	r	25	ARG	Sidechain
51	u	470	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	557	0	529	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ab	543	0	528	13	0
2	1	493	0	491	22	0
2	Ac	485	0	485	18	0
3	2	1513	0	1496	73	0
3	4	1518	0	1500	68	0
3	Ae	266	0	256	45	0
3	Af	240	0	240	58	0
4	3	417	0	414	14	0
4	Ad	421	0	418	13	0
5	6	3140	0	3121	155	0
5	v	3140	0	3121	147	0
6	7	3025	0	3090	149	0
6	w	3025	0	3090	163	0
7	8	1896	0	1845	86	0
7	x	1896	0	1843	94	0
8	9	878	0	870	32	0
8	y	893	0	888	21	0
9	a	1151	0	1164	46	0
10	b	900	0	903	52	0
11	c	1291	0	1185	64	0
12	d	1417	0	1393	52	0
13	e	826	0	789	41	0
14	f	391	0	392	18	0
15	g	1000	0	994	46	0
16	h	867	0	871	82	0
17	i	2711	0	2874	184	0
18	j	905	0	945	71	0
19	k	748	0	799	84	0
20	m	1338	0	1338	104	0
21	n	475	0	475	21	0
22	o	1062	0	1072	60	0
23	p	1534	0	1470	64	0
24	q	3630	0	3837	222	0
25	r	2508	0	2607	152	0
26	B	3318	0	3283	218	0
27	C	3454	0	3383	217	0
28	D	1732	0	1682	90	0
29	E	1658	0	1665	81	0
30	F	727	0	694	17	0
31	H	1412	0	1364	93	0
32	I	1248	0	1254	68	0
33	J	962	0	962	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	1203	0	1161	35	0
35	L	2735	0	2751	175	0
36	N	910	0	950	26	0
37	O	680	0	681	63	0
37	X	689	0	687	24	0
38	P	669	0	677	23	0
39	Q	954	0	960	61	0
40	R	295	0	279	17	0
41	S	562	0	557	21	0
42	T	638	0	637	23	0
43	U	2574	0	2532	88	0
44	V	1016	0	1022	31	0
45	W	1162	0	1156	64	0
46	Y	531	0	480	34	0
47	Z	626	0	607	19	0
48	l	4785	0	4935	276	0
49	s	1398	0	1374	53	0
50	t	1019	0	987	38	0
51	5	3374	0	3272	105	0
51	u	3459	0	3350	116	0
52	Aa	662	0	660	32	0
52	z	666	0	663	21	0
53	G	5260	0	5288	163	0
54	M	773	0	801	27	0
55	2	4	0	0	4	0
55	4	4	0	0	2	0
55	E	4	0	0	7	0
55	G	4	0	0	0	0
56	7	86	0	60	19	0
56	w	86	0	60	19	0
57	8	43	0	32	11	0
57	x	43	0	31	9	0
58	B	31	0	19	3	0
59	B	8	0	0	0	0
59	G	16	0	0	1	0
59	H	16	0	0	7	0
59	I	8	0	0	2	0
60	L	48	0	26	5	0
61	Q	30	0	30	1	0
All	All	98682	0	98345	4155	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 21.

All (4155) 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)
29:E:180:CYS:SG	55:E:301:FES:FE2	1.16	1.36
3:2:257:CYS:SG	55:2:301:FES:FE1	1.19	1.34
18:j:67:LEU:HD11	19:k:68:ALA:HB3	1.31	1.12
24:q:370:PRO:HB3	24:q:375:LEU:HD22	1.26	1.11
20:m:45:LEU:HD22	20:m:50:SER:HA	1.32	1.09
43:U:110:LEU:HD13	43:U:336:LEU:HD11	1.27	1.09
29:E:140:CYS:SG	55:E:301:FES:FE1	1.45	1.08
3:Af:45:PRO:HA	3:Af:66:PRO:HG3	1.35	1.08
7:x:216:LEU:HB3	7:x:249:ILE:HD11	1.29	1.07
53:G:64:CYS:HB3	53:G:75:CYS:HB3	1.37	1.04
27:C:183:ILE:HG23	27:C:216:MET:HE2	1.36	1.03
17:i:45:MET:HE1	20:m:171:ILE:HG23	1.42	1.02
22:o:17:THR:HB	23:p:110:GLU:HG2	1.42	1.02
26:B:41:ILE:HG22	26:B:253:THR:HG21	1.40	1.02
52:Aa:19:LEU:HD21	52:Aa:23:GLU:HB2	1.42	1.02
7:8:122:CYS:HB2	57:8:401:HEC:HAB	1.40	1.02
17:i:258:SER:HB2	17:i:336:VAL:HG12	1.39	1.01
37:O:140:CYS:HB3	37:O:143:GLU:HG3	1.39	1.00
51:u:120:LEU:HD13	51:u:133:ILE:HG12	1.44	1.00
20:m:55:MET:HA	20:m:55:MET:HE3	1.41	1.00
8:y:14:LEU:HD23	8:y:17:ILE:HD11	1.44	0.98
7:8:97:TRP:HB2	7:8:100:ARG:HG3	1.44	0.98
9:a:179:ILE:HG21	16:h:38:LYS:HG3	1.46	0.97
44:V:62:THR:HG22	44:V:104:ARG:HD3	1.44	0.96
13:e:54:ARG:HH21	17:i:306:PRO:HB3	1.30	0.95
3:2:245:PRO:HB2	3:2:255:TYR:HB3	1.49	0.94
56:7:402:HEM:HBC2	56:7:402:HEM:HMC2	1.48	0.94
46:Y:43:ARG:HB3	46:Y:46:GLN:HG2	1.49	0.94
17:i:41:ILE:HG21	19:k:73:LEU:HD21	1.49	0.93
3:2:257:CYS:HG	55:2:301:FES:FE1	0.70	0.93
5:6:170:GLN:HB3	3:Ae:67:VAL:HG22	1.46	0.93
26:B:318:ILE:HG12	26:B:357:MET:HE1	1.48	0.93
16:h:82:GLN:HG2	45:W:98:MET:HG2	1.50	0.93
27:C:367:ALA:HB3	53:G:149:ASP:HB2	1.49	0.93
6:w:89:MET:HE2	6:w:235:MET:HG3	1.48	0.93
3:Af:46:LEU:HG	3:Af:66:PRO:HB3	1.51	0.93
17:i:268:GLN:HA	24:q:165:VAL:HG11	1.50	0.92
20:m:125:TRP:HB2	45:W:137:THR:HG21	1.49	0.92
5:6:138:LEU:HD11	5:6:233:VAL:HG13	1.50	0.91
17:i:93:VAL:HG13	48:l:599:MET:HE1	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:313:MET:HE1	43:U:140:SER:HA	1.53	0.90
7:x:203:ARG:HG3	7:x:279:SER:HB3	1.51	0.90
2:Ac:11:TYR:HA	2:Ac:15:PHE:HB2	1.50	0.90
11:c:162:PRO:HB3	50:t:39:MET:HG3	1.53	0.90
26:B:364:VAL:HG12	26:B:400:VAL:HG12	1.52	0.90
24:q:370:PRO:HB3	24:q:375:LEU:CD2	2.01	0.90
6:7:53:MET:HB3	6:w:177:ARG:HD3	1.54	0.90
31:H:128:ILE:HG12	31:H:147:ILE:HG12	1.54	0.90
53:G:602:ARG:HB2	53:G:659:VAL:HG13	1.51	0.89
6:7:47:THR:HG23	6:7:79:ILE:HG23	1.54	0.89
56:7:401:HEM:HHC	56:7:401:HEM:HBB2	1.55	0.89
17:i:193:VAL:HG13	17:i:266:ILE:HG23	1.55	0.89
3:2:173:ILE:HD12	3:2:175:ILE:HD11	1.52	0.89
7:8:103:LEU:HD21	7:8:291:LEU:HB2	1.53	0.89
3:4:243:CYS:HA	6:w:264:THR:HG21	1.54	0.88
35:L:267:LEU:HG	35:L:370:VAL:HG21	1.56	0.88
19:k:31:LEU:HD21	20:m:67:VAL:HG11	1.56	0.88
28:D:218:ARG:HD2	39:Q:127:THR:HA	1.54	0.88
35:L:294:ARG:HG3	35:L:311:ARG:HG2	1.56	0.88
25:r:113:VAL:HG11	25:r:139:THR:HG21	1.56	0.88
6:w:338:ILE:HD11	6:w:350:ILE:HG22	1.55	0.88
36:N:106:GLU:HG3	36:N:107:PRO:HD2	1.55	0.88
5:v:295:ALA:HB1	3:Af:46:LEU:HD22	1.56	0.88
5:v:170:GLN:HB3	3:Af:67:VAL:HG21	1.56	0.87
35:L:278:VAL:HG12	35:L:364:VAL:HG21	1.54	0.87
7:8:125:CYS:CB	57:8:401:HEC:HBC2	2.04	0.87
6:w:300:ILE:HD11	6:w:363:LEU:HD21	1.56	0.87
5:v:231:LYS:O	5:v:235:GLU:HG2	1.73	0.86
24:q:251:ASN:HB2	24:q:252:PRO:HD3	1.56	0.86
37:O:138:LEU:HD23	37:O:144:ILE:HG12	1.55	0.86
20:m:3:MET:HE1	45:W:133:ILE:HG21	1.57	0.86
56:7:401:HEM:HHD	56:7:401:HEM:HBC2	1.56	0.86
6:w:94:LEU:O	6:w:98:VAL:HG23	1.76	0.86
22:o:109:ARG:HA	22:o:112:LYS:HE2	1.55	0.85
29:E:140:CYS:HG	55:E:301:FES:FE1	0.54	0.85
7:8:184:GLU:OE1	7:x:159:PRO:HB2	1.75	0.85
48:l:118:PHE:O	48:l:122:VAL:HG23	1.77	0.85
49:s:214:LEU:HD23	49:s:215:PRO:HD2	1.59	0.85
24:q:403:THR:HA	24:q:406:TYR:CE2	2.11	0.85
26:B:314:LEU:HD11	26:B:317:VAL:HG23	1.58	0.85
5:6:138:LEU:HD13	5:6:237:PHE:HB2	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:119:ASN:HD22	35:L:120:VAL:HG23	1.39	0.84
17:i:303:THR:HG22	27:C:45:PRO:HD3	1.59	0.84
24:q:306:PRO:HA	24:q:458:LEU:HD22	1.58	0.84
41:S:16:LEU:O	41:S:19:PRO:HD2	1.77	0.84
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.13	0.84
19:k:64:LEU:HD23	20:m:59:ILE:HD12	1.58	0.84
25:r:102:VAL:HG13	25:r:150:LEU:HD11	1.58	0.84
39:Q:46:ILE:HD13	39:Q:107:LEU:HD13	1.59	0.84
48:l:419:THR:HA	48:l:422:TYR:CE2	2.13	0.84
6:w:47:THR:HG23	6:w:79:ILE:HG23	1.59	0.84
35:L:231:VAL:HG22	35:L:267:LEU:HD23	1.58	0.84
53:G:387:LEU:HD12	53:G:514:ASN:HB3	1.60	0.84
24:q:25:ILE:O	24:q:29:VAL:HG23	1.78	0.84
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.60	0.83
3:Af:45:PRO:CA	3:Af:66:PRO:HG3	2.08	0.83
25:r:316:PRO:HG3	45:W:57:ARG:HB3	1.61	0.83
49:s:121:MET:HE2	49:s:121:MET:HA	1.59	0.83
5:6:55:TYR:HA	5:6:127:ARG:HH12	1.44	0.83
5:v:170:GLN:HB3	3:Af:67:VAL:CG2	2.08	0.83
18:j:44:MET:HA	39:Q:122:VAL:HG21	1.59	0.83
51:5:179:MET:HE1	51:5:282:LEU:HD13	1.61	0.83
39:Q:118:GLU:HB3	39:Q:124:LYS:HG3	1.61	0.83
27:C:285:THR:HG23	36:N:13:GLY:HA3	1.60	0.82
7:8:125:CYS:HB3	57:8:401:HEC:HBC2	1.60	0.81
37:O:114:ASP:O	37:O:118:ILE:HG23	1.79	0.81
41:S:69:ILE:HD13	49:s:148:PHE:HB3	1.63	0.81
5:v:70:ARG:O	5:v:185:ALA:HB1	1.80	0.81
6:w:132:VAL:HA	6:w:139:SER:HB3	1.62	0.81
6:7:102:LEU:HD22	6:7:304:MET:HE2	1.63	0.81
5:v:295:ALA:CB	3:Af:46:LEU:HD22	2.11	0.81
17:i:128:LEU:HD11	17:i:213:LEU:HD23	1.61	0.81
20:m:103:MET:HA	20:m:103:MET:HE3	1.62	0.81
5:v:228:PRO:O	5:v:232:GLN:HG3	1.80	0.81
48:l:391:SER:O	48:l:395:ILE:HG12	1.81	0.80
5:v:138:LEU:HD13	5:v:237:PHE:HB2	1.61	0.80
15:g:4:MET:HG3	17:i:347:ASN:HD21	1.46	0.80
24:q:73:LEU:HD22	24:q:103:GLN:OE1	1.81	0.80
56:w:402:HEM:HBC2	56:w:402:HEM:HMC1	1.62	0.80
26:B:371:ILE:CD1	26:B:396:MET:HG3	2.11	0.80
6:w:129:MET:HE1	6:w:185:LEU:HD12	1.64	0.80
6:7:132:VAL:HA	6:7:139:SER:HB3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:200:LYS:O	33:J:126:LEU:HD21	1.82	0.80
17:i:236:LYS:HG2	17:i:237:MET:HG3	1.64	0.80
26:B:41:ILE:HD12	26:B:250:VAL:HG12	1.62	0.79
27:C:73:ASN:HB2	43:U:195:VAL:HG13	1.65	0.79
7:8:228:LEU:HD11	7:8:234:PHE:HB2	1.64	0.79
44:V:69:ILE:HG13	44:V:100:THR:HG21	1.63	0.79
31:H:179:THR:OG1	31:H:182:GLU:HG3	1.83	0.79
39:Q:127:THR:O	39:Q:131:ARG:HG3	1.82	0.79
24:q:105:PHE:O	24:q:109:THR:HG23	1.81	0.79
17:i:68:MET:HG3	19:k:36:MET:HE3	1.63	0.78
51:u:229:MET:HE1	51:u:253:LEU:HD23	1.64	0.78
39:Q:114:MET:O	39:Q:117:GLU:HG2	1.84	0.78
48:l:5:ALA:HB2	48:l:61:MET:HE1	1.64	0.78
51:u:363:MET:HE3	52:z:6:GLY:HA3	1.65	0.78
19:k:89:TYR:HB3	19:k:91:GLN:OE1	1.83	0.78
48:l:356:ILE:HA	48:l:359:MET:HE2	1.65	0.78
24:q:208:PRO:HG3	24:q:216:LEU:HD13	1.64	0.78
25:r:185:TRP:HE1	25:r:238:THR:HG22	1.49	0.78
48:l:415:ALA:O	48:l:419:THR:HG23	1.82	0.78
44:V:4:THR:O	44:V:8:LYS:HG3	1.83	0.78
26:B:442:PHE:HB3	26:B:445:GLU:HG3	1.64	0.78
27:C:187:LEU:HD21	27:C:216:MET:HB2	1.64	0.78
35:L:183:GLU:HG3	35:L:195:ILE:HD13	1.64	0.78
48:l:15:LEU:O	48:l:18:PRO:HD2	1.84	0.78
6:w:253:PRO:HB3	7:x:203:ARG:O	1.83	0.78
7:x:322:TYR:HB2	8:y:61:PHE:CD1	2.19	0.78
3:2:270:ILE:HD13	3:2:275:ALA:HB3	1.64	0.78
13:e:79:ASP:HB2	13:e:82:VAL:CG1	2.14	0.78
13:e:106:VAL:HG13	24:q:453:MET:HE3	1.67	0.78
14:f:31:ILE:HD12	14:f:32:ARG:H	1.48	0.78
5:6:391:GLY:HA2	5:6:394:ASP:OD2	1.83	0.77
7:8:244:ALA:HB3	57:8:401:HEC:HBD2	1.66	0.77
12:d:71:VAL:HG22	12:d:72:PRO:HD2	1.64	0.77
28:D:220:VAL:HG21	39:Q:136:THR:HG21	1.66	0.77
35:L:163:SER:O	35:L:197:LYS:HA	1.84	0.77
37:O:100:VAL:HG12	37:O:142:GLN:HB2	1.65	0.77
37:O:143:GLU:HA	37:O:146:ASP:OD2	1.83	0.77
52:Aa:12:ARG:HD2	51:5:279:ASP:OD1	1.84	0.77
21:n:57:TRP:CE3	21:n:57:TRP:HA	2.19	0.77
43:U:88:PHE:HB2	43:U:161:LEU:HD23	1.66	0.77
48:l:7:LEU:O	48:l:11:THR:HG23	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:112:THR:HG22	6:7:196:HIS:CE1	2.20	0.77
25:r:26:LYS:HA	25:r:36:GLY:HA3	1.66	0.77
26:B:174:ARG:HA	40:R:93:LEU:HD21	1.66	0.77
7:8:122:CYS:CB	57:8:401:HEC:HAB	2.14	0.77
32:I:81:ALA:HB1	32:I:82:PRO:HD2	1.65	0.77
43:U:148:ALA:HB1	43:U:159:VAL:HG11	1.67	0.77
17:i:337:LEU:O	17:i:340:THR:HG23	1.84	0.77
46:Y:54:GLN:HE21	48:l:446:ASN:HB2	1.49	0.77
37:O:92:LYS:HD3	37:O:114:ASP:OD2	1.84	0.77
42:T:155:PRO:HD3	49:s:206:THR:HG21	1.65	0.77
7:8:153:VAL:HG21	7:8:177:PRO:HG2	1.67	0.77
26:B:396:MET:O	26:B:400:VAL:HG13	1.85	0.77
27:C:457:ILE:HG23	27:C:462:ILE:HD11	1.67	0.77
3:4:110:SER:HA	3:4:113:ARG:HD2	1.67	0.76
18:j:46:SER:OG	18:j:49:LEU:HD13	1.84	0.76
5:v:295:ALA:O	3:Af:46:LEU:HD13	1.83	0.76
26:B:68:ILE:HG23	26:B:75:TRP:HZ3	1.50	0.76
26:B:288:VAL:HG21	26:B:303:HIS:HB3	1.66	0.76
5:6:259:ARG:HB3	5:6:444:LEU:CD1	2.14	0.76
53:G:50:LEU:O	53:G:54:GLU:HG2	1.85	0.76
18:j:67:LEU:CD1	19:k:68:ALA:HB3	2.13	0.76
57:x:401:HEC:HMC1	57:x:401:HEC:HBC3	1.68	0.76
29:E:143:ARG:O	29:E:184:PRO:HG3	1.85	0.76
17:i:65:THR:HG22	19:k:19:LEU:HD21	1.68	0.76
11:c:133:LEU:HD23	48:l:532:ILE:CD1	2.15	0.76
27:C:205:PRO:HB3	27:C:264:LEU:HD12	1.68	0.76
53:G:64:CYS:SG	53:G:72:ALA:HB3	2.25	0.76
5:6:216:ALA:HB3	5:6:244:LEU:H	1.50	0.76
10:b:55:ALA:HB1	10:b:60:VAL:HG23	1.68	0.76
17:i:14:MET:O	17:i:18:MET:HG2	1.86	0.76
20:m:28:TYR:HA	20:m:31:LEU:HG	1.67	0.75
36:N:21:HIS:O	36:N:25:LYS:HG3	1.86	0.75
5:v:407:VAL:HG23	5:v:411:THR:HB	1.66	0.75
3:2:243:CYS:SG	6:7:264:THR:HG21	2.27	0.75
48:l:65:ASN:HD21	48:l:78:LEU:HB3	1.51	0.75
34:K:95:ASP:H	54:M:35:THR:HG23	1.52	0.75
38:P:38:GLU:HG3	38:P:39:LYS:HG2	1.67	0.75
51:5:170:GLN:O	51:5:174:GLU:HG3	1.86	0.75
51:5:319:GLY:HA3	3:Ae:58:ALA:HB3	1.67	0.75
53:G:341:ILE:HD11	53:G:537:ILE:HG13	1.68	0.75
32:I:74:VAL:HA	32:I:77:MET:HE2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:332:HIS:HA	48:l:335:PHE:CZ	2.21	0.75
22:o:17:THR:HB	23:p:110:GLU:CG	2.17	0.75
26:B:319:PRO:HG3	26:B:347:THR:HB	1.67	0.75
27:C:248:ASP:O	27:C:252:GLU:HG2	1.86	0.75
32:I:116:ALA:O	32:I:120:VAL:HG23	1.86	0.75
42:T:142:LEU:HD11	42:T:151:VAL:HG11	1.68	0.75
6:w:265:PRO:HG2	6:w:268:ILE:HG13	1.68	0.75
20:m:52:LEU:O	20:m:56:VAL:HG23	1.87	0.75
25:r:264:LEU:O	25:r:268:ILE:HG12	1.86	0.75
51:u:120:LEU:HD13	51:u:133:ILE:CG1	2.17	0.75
3:Ae:49:PHE:O	3:Ae:51:ALA:N	2.20	0.75
6:7:337:TRP:HH2	6:7:350:ILE:HD13	1.52	0.75
31:H:150:THR:HG23	32:I:139:GLY:HA3	1.68	0.75
7:x:228:LEU:HD11	7:x:234:PHE:HB2	1.69	0.75
49:s:160:THR:HA	49:s:163:TRP:CD1	2.22	0.74
6:w:318:ARG:O	6:w:322:GLN:HG3	1.87	0.74
38:P:42:VAL:HG12	38:P:46:LYS:HE2	1.68	0.74
48:l:49:VAL:HB	48:l:50:PRO:HD3	1.70	0.74
48:l:302:VAL:O	48:l:306:THR:HG23	1.88	0.74
24:q:269:MET:HG3	24:q:270:ILE:HD12	1.67	0.74
24:q:370:PRO:CB	24:q:375:LEU:HD22	2.14	0.74
30:F:71:ILE:HD11	30:F:115:GLY:HA3	1.69	0.74
6:7:9:PRO:O	6:7:13:ILE:HG12	1.87	0.74
18:j:63:LEU:CD2	20:m:63:GLY:HA2	2.17	0.74
22:o:30:ARG:NH1	51:u:259:GLU:O	2.20	0.74
24:q:263:MET:HA	24:q:263:MET:HE3	1.69	0.74
25:r:2:PHE:CE2	25:r:6:ILE:HD11	2.22	0.74
25:r:32:GLN:HG2	27:C:204:THR:HG23	1.69	0.74
35:L:78:PRO:HB2	35:L:103:TRP:CD1	2.23	0.74
10:b:74:HIS:O	10:b:78:PRO:HG2	1.87	0.74
16:h:77:SER:HB3	20:m:122:LEU:HD11	1.69	0.74
48:l:566:THR:O	48:l:570:GLN:HG2	1.88	0.74
2:l:19:SER:HB2	4:3:23:MET:HB3	1.69	0.74
9:a:131:LYS:HA	21:n:58:LYS:HA	1.70	0.74
20:m:3:MET:HE1	45:W:133:ILE:CG2	2.17	0.74
37:O:104:PHE:HB3	37:O:110:LEU:HD21	1.69	0.74
45:W:120:MET:HG2	45:W:123:GLU:HG3	1.69	0.74
24:q:306:PRO:HA	24:q:458:LEU:CD2	2.18	0.74
6:7:141:TRP:CD1	6:7:265:PRO:HD3	2.22	0.74
24:q:325:MET:HE2	24:q:329:LEU:HD11	1.69	0.74
26:B:210:THR:HB	26:B:224:ARG:H	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:247:THR:HB	24:q:304:GLN:HE21	1.53	0.73
53:G:698:ASP:O	53:G:702:ARG:HG3	1.88	0.73
5:6:170:GLN:CB	3:Ae:67:VAL:HG22	2.18	0.73
17:i:117:GLU:O	19:k:96:LEU:HD13	1.88	0.73
48:l:414:ILE:O	48:l:418:LEU:HG	1.88	0.73
56:w:401:HEM:HMC2	56:w:401:HEM:HBC2	1.70	0.73
8:y:69:LEU:HD11	8:y:76:LEU:HD13	1.70	0.73
35:L:139:VAL:HA	35:L:143:ILE:HD12	1.70	0.73
42:T:90:ILE:H	42:T:90:ILE:HD12	1.53	0.73
17:i:313:MET:HE2	43:U:143:LEU:HD22	1.71	0.73
21:n:57:TRP:HA	21:n:57:TRP:HE3	1.52	0.73
35:L:288:LEU:HD12	35:L:289:PRO:HD2	1.68	0.73
43:U:224:GLY:HA2	43:U:229:MET:HE3	1.71	0.73
51:5:207:ASN:O	51:5:211:LEU:HG	1.88	0.73
51:u:141:PRO:O	51:u:145:GLU:HG3	1.89	0.73
6:w:278:TYR:CE2	6:w:282:ARG:HD3	2.24	0.73
3:Ae:46:LEU:CB	3:Ae:66:PRO:HB3	2.19	0.73
24:q:400:MET:HE1	48:l:183:VAL:HG21	1.70	0.73
3:2:109:PHE:O	3:2:113:ARG:HG3	1.88	0.73
3:2:173:ILE:HD13	3:2:190:TRP:HB2	1.71	0.73
3:4:263:HIS:O	3:4:270:ILE:HD12	1.89	0.73
6:7:338:ILE:HD13	6:7:351:GLY:HA2	1.69	0.73
11:c:133:LEU:HD23	48:l:532:ILE:HD11	1.71	0.73
32:I:98:ARG:HA	32:I:125:PRO:HD3	1.70	0.73
48:l:88:MET:O	48:l:91:PRO:HD2	1.89	0.73
11:c:140:MET:CE	48:l:283:ILE:HA	2.18	0.73
3:2:185:ASN:HB2	3:2:198:ARG:HE	1.54	0.72
16:h:75:ARG:NH1	45:W:108:GLU:O	2.22	0.72
26:B:371:ILE:HD13	26:B:396:MET:HG3	1.71	0.72
3:4:177:LEU:N	3:4:290:ASP:O	2.22	0.72
9:a:130:GLU:O	9:a:134:GLU:HG2	1.90	0.72
17:i:96:THR:O	17:i:100:MET:HG2	1.86	0.72
20:m:9:LEU:O	20:m:39:VAL:HG11	1.88	0.72
8:9:44:VAL:O	8:9:48:ILE:HG12	1.89	0.72
17:i:270:MET:HE1	17:i:278:MET:HG2	1.71	0.72
35:L:254:LYS:HD2	35:L:254:LYS:O	1.90	0.72
38:P:18:GLU:HG3	38:P:68:ARG:HB3	1.72	0.72
53:G:575:VAL:O	53:G:578:PRO:HD2	1.88	0.72
53:G:624:ARG:NH1	53:G:628:GLU:HB2	2.04	0.72
26:B:184:LYS:HE3	40:R:98:MET:HB3	1.70	0.72
11:c:162:PRO:CB	50:t:39:MET:HG3	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:142:ARG:HD2	13:e:138:GLU:O	1.88	0.72
13:e:89:VAL:CG1	24:q:29:VAL:HG22	2.19	0.72
25:r:90:PRO:HD2	25:r:240:ILE:HD13	1.71	0.72
35:L:114:VAL:HG13	35:L:115:VAL:HG13	1.72	0.72
35:L:206:ASP:OD2	35:L:208:PHE:HB3	1.88	0.72
53:G:627:SER:HB3	53:G:632:MET:O	1.89	0.72
8:9:69:LEU:HD11	8:9:76:LEU:HD13	1.72	0.72
48:l:321:GLN:HG2	48:l:324:LEU:HD12	1.72	0.72
51:u:101:THR:HB	51:u:153:ASN:O	1.90	0.72
51:5:405:GLY:C	51:5:408:PRO:HD2	2.14	0.72
53:G:602:ARG:HB2	53:G:659:VAL:CG1	2.19	0.72
27:C:361:GLU:HG2	54:M:44:GLY:HA2	1.72	0.72
6:w:55:TYR:HA	6:w:65:SER:OG	1.90	0.72
17:i:65:THR:HG22	19:k:19:LEU:CD2	2.19	0.71
24:q:76:MET:HE3	24:q:99:LEU:HD22	1.71	0.71
26:B:316:ALA:HA	26:B:327:ILE:O	1.90	0.71
7:8:126:HIS:ND1	7:8:198:LEU:HG	2.04	0.71
26:B:71:LYS:HG2	26:B:75:TRP:CD2	2.24	0.71
31:H:76:TYR:HA	31:H:79:ARG:HD3	1.71	0.71
6:w:47:THR:HG23	6:w:79:ILE:CG2	2.20	0.71
6:7:119:LEU:HD21	6:7:192:LEU:HB2	1.71	0.71
48:l:65:ASN:H	48:l:65:ASN:HD22	1.38	0.71
2:1:30:LEU:HD21	4:3:48:ILE:HG13	1.72	0.71
3:4:216:LEU:HD13	3:4:269:ARG:HD2	1.70	0.71
24:q:416:ARG:HG2	48:l:159:HIS:HB3	1.71	0.71
25:r:102:VAL:CG1	25:r:150:LEU:HD11	2.20	0.71
51:u:225:LYS:O	51:u:229:MET:HG3	1.90	0.71
5:v:355:TYR:O	5:v:359:LYS:HG3	1.89	0.71
3:Ae:43:ARG:O	3:Ae:45:PRO:HD3	1.90	0.71
5:6:387:GLU:OE2	51:5:405:GLY:HA2	1.90	0.71
8:9:57:ASN:HA	8:9:60:VAL:HG22	1.72	0.71
25:r:236:ALA:HA	25:r:263:THR:HG22	1.71	0.71
35:L:122:ILE:HD11	35:L:248:ILE:HD11	1.72	0.71
6:w:51:LEU:HD12	6:w:83:HIS:HD2	1.55	0.71
22:o:18:LEU:HD11	23:p:114:TRP:CG	2.26	0.71
25:r:102:VAL:CG1	25:r:150:LEU:HD21	2.21	0.71
51:u:180:ARG:O	51:u:183:VAL:HG12	1.90	0.71
52:Aa:19:LEU:HD23	52:Aa:20:SER:N	2.05	0.71
10:b:13:GLN:O	10:b:17:GLU:HG3	1.89	0.71
5:v:131:GLU:O	5:v:135:GLU:HG2	1.91	0.71
53:G:89:VAL:HB	53:G:94:MET:HG3	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:39:GLY:O	2:1:43:ILE:HG12	1.91	0.71
6:7:24:PRO:HB2	6:7:27:ILE:HG22	1.73	0.71
17:i:112:HIS:HB2	17:i:184:ILE:HD13	1.72	0.71
29:E:66:ILE:HD13	29:E:81:PRO:HB2	1.73	0.71
31:H:150:THR:CG2	32:I:139:GLY:HA3	2.21	0.71
7:x:153:VAL:HG21	7:x:177:PRO:HG3	1.71	0.71
7:8:243:ILE:HG13	7:8:245:MET:H	1.56	0.70
32:I:64:PRO:HD3	32:I:91:VAL:HG13	1.71	0.70
6:7:223:TYR:O	6:7:226:ILE:HG22	1.91	0.70
22:o:25:ILE:HG23	51:u:261:ALA:HA	1.73	0.70
24:q:226:ALA:O	24:q:230:VAL:HG22	1.91	0.70
26:B:426:ALA:HB3	58:B:501:FMN:HM81	1.72	0.70
32:I:62:LEU:O	32:I:91:VAL:HA	1.91	0.70
36:N:27:LEU:O	36:N:31:ILE:HG13	1.91	0.70
24:q:71:TRP:O	24:q:74:PRO:HD2	1.91	0.70
41:S:4:GLU:O	41:S:7:PRO:HD2	1.90	0.70
35:L:170:LYS:H	35:L:170:LYS:HD3	1.56	0.70
52:Aa:8:LEU:HB2	51:5:463:GLU:OE2	1.91	0.70
26:B:174:ARG:O	26:B:178:GLU:HG2	1.92	0.70
48:l:562:LEU:HB2	48:l:563:PRO:HD3	1.73	0.70
5:v:85:LEU:HD12	5:v:158:LEU:HD12	1.71	0.70
26:B:276:PHE:CD1	26:B:352:ALA:HB1	2.27	0.70
51:u:229:MET:CE	51:u:253:LEU:HD23	2.21	0.70
17:i:42:PRO:HG3	20:m:167:VAL:HG22	1.73	0.70
18:j:85:LYS:O	18:j:89:THR:HG23	1.91	0.70
20:m:55:MET:HA	20:m:55:MET:CE	2.21	0.70
27:C:137:GLN:O	27:C:140:PRO:HD2	1.91	0.70
49:s:160:THR:HA	49:s:163:TRP:NE1	2.05	0.70
5:6:174:LEU:HD11	3:Ae:67:VAL:HG23	1.73	0.70
51:5:70:THR:HB	51:5:410:CYS:SG	2.32	0.70
56:7:402:HEM:HMB2	56:7:402:HEM:HBB2	1.74	0.70
52:Aa:73:LYS:NZ	1:Ab:66:ASP:H	1.89	0.70
12:d:23:GLN:HE21	50:t:73:SER:HB3	1.56	0.70
27:C:381:MET:HE3	27:C:381:MET:HA	1.74	0.70
35:L:111:ILE:O	35:L:115:VAL:HG22	1.92	0.70
37:O:113:LEU:O	37:O:117:GLU:HG3	1.91	0.70
43:U:263:ARG:HD3	43:U:264:GLU:N	2.07	0.70
48:l:341:MET:HE2	48:l:457:LEU:HD12	1.74	0.70
48:l:373:LEU:HD22	48:l:431:PHE:CE2	2.26	0.70
5:v:138:LEU:HD12	5:v:233:VAL:HG22	1.71	0.70
3:4:184:LYS:NZ	3:4:184:LYS:HB3	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:344:GLU:O	6:7:348:ILE:HG13	1.92	0.69
20:m:45:LEU:CD2	20:m:50:SER:HA	2.18	0.69
43:U:72:LYS:HE3	43:U:163:ARG:HG3	1.73	0.69
4:3:14:ALA:O	4:3:18:ILE:HG13	1.92	0.69
37:O:133:ILE:H	37:O:133:ILE:HD13	1.57	0.69
45:W:34:SER:O	45:W:38:VAL:HG23	1.92	0.69
56:w:402:HEM:HBB2	56:w:402:HEM:HMB2	1.73	0.69
5:v:63:LEU:HD23	5:v:141:THR:HG21	1.74	0.69
10:b:89:HIS:CD2	10:b:96:THR:HB	2.27	0.69
17:i:31:ILE:HG23	19:k:66:PHE:CZ	2.26	0.69
25:r:253:GLU:O	25:r:257:ILE:HG13	1.91	0.69
26:B:162:PHE:CZ	29:E:178:GLY:HA3	2.27	0.69
28:D:204:LEU:HD12	28:D:205:SER:H	1.57	0.69
3:4:142:THR:OG1	7:8:303:LEU:HB3	1.93	0.69
22:o:91:ALA:O	22:o:95:ILE:HG13	1.91	0.69
25:r:34:ARG:HG2	32:I:82:PRO:HA	1.74	0.69
27:C:90:PHE:O	27:C:94:HIS:HB2	1.93	0.69
28:D:66:ALA:HA	28:D:73:VAL:HG21	1.74	0.69
29:E:188:ILE:HG22	29:E:189:ASN:H	1.55	0.69
43:U:352:LYS:HD3	43:U:353:TRP:HD1	1.57	0.69
7:x:127:SER:HB2	7:x:179:PRO:HD2	1.74	0.69
17:i:2:ASN:HB3	17:i:5:ILE:HD13	1.75	0.69
17:i:149:ILE:HD13	17:i:154:MET:HE3	1.75	0.69
25:r:102:VAL:HG11	25:r:150:LEU:HD21	1.74	0.69
35:L:202:PHE:HA	35:L:206:ASP:OD2	1.92	0.69
46:Y:51:THR:CG2	46:Y:54:GLN:HG3	2.23	0.69
53:G:541:PRO:HB2	53:G:561:PRO:HD3	1.73	0.69
3:Af:65:SER:HB3	3:Af:66:PRO:CD	2.22	0.69
26:B:319:PRO:HB3	26:B:327:ILE:HD11	1.73	0.69
31:H:101:HIS:H	31:H:149:MET:HE1	1.56	0.69
39:Q:141:PRO:HB2	39:Q:146:SER:OG	1.92	0.69
42:T:128:ILE:O	42:T:132:ARG:HG3	1.92	0.69
37:X:115:GLN:O	37:X:118:ILE:HG13	1.93	0.69
7:x:133:TYR:HA	7:x:136:LEU:HD12	1.74	0.69
9:a:179:ILE:HD11	16:h:41:ILE:HB	1.73	0.69
20:m:3:MET:HE3	20:m:125:TRP:CD1	2.27	0.69
24:q:63:ALA:HB3	24:q:64:PRO:HD3	1.75	0.69
26:B:397:ALA:O	26:B:400:VAL:HG22	1.93	0.69
25:r:234:MET:O	25:r:238:THR:HG23	1.93	0.68
26:B:292:MET:HE1	26:B:349:LEU:HD22	1.75	0.68
18:j:48:ARG:NH2	25:r:121:TRP:O	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:63:LEU:HD11	20:m:66:VAL:HG21	1.74	0.68
11:c:110:ASP:OD1	11:c:110:ASP:N	2.26	0.68
28:D:103:HIS:CE1	28:D:105:ASN:HA	2.29	0.68
46:Y:54:GLN:NE2	48:l:446:ASN:HB2	2.08	0.68
48:l:559:GLU:O	48:l:563:PRO:HD2	1.93	0.68
11:c:140:MET:HE1	48:l:283:ILE:HA	1.75	0.68
24:q:122:PHE:CE1	24:q:206:LYS:HE3	2.29	0.68
25:r:165:LEU:HD23	25:r:241:LEU:HA	1.73	0.68
26:B:46:TYR:CE1	29:E:226:GLU:HA	2.28	0.68
28:D:80:CYS:SG	54:M:64:MET:HG3	2.34	0.68
48:l:162:THR:O	48:l:166:THR:HG23	1.94	0.68
27:C:180:PHE:CZ	27:C:223:VAL:HG11	2.28	0.68
28:D:102:ASP:HB2	36:N:90:LEU:HD22	1.74	0.68
29:E:110:MET:O	29:E:114:GLU:HG3	1.92	0.68
39:Q:63:ARG:O	39:Q:67:ARG:HG2	1.93	0.68
24:q:93:LYS:O	24:q:97:THR:HG23	1.93	0.68
32:l:187:GLU:HB3	35:L:82:GLU:OE2	1.93	0.68
16:h:50:ILE:O	16:h:54:LYS:NZ	2.26	0.68
22:o:83:THR:HB	22:o:84:PRO:HD2	1.76	0.68
27:C:229:HIS:HD2	32:l:167:PRO:HD3	1.58	0.68
35:L:283:PHE:CZ	35:L:285:PRO:HG3	2.28	0.68
48:l:383:MET:SD	48:l:384:PRO:HD2	2.34	0.68
53:G:69:LEU:HD11	53:G:225:ILE:HD13	1.75	0.68
5:6:171:ALA:O	5:6:175:GLU:HG2	1.94	0.68
6:7:338:ILE:HD11	6:7:350:ILE:HG22	1.74	0.68
18:j:39:CYS:O	27:C:92:PRO:HD2	1.94	0.68
6:w:173:ALA:O	6:w:177:ARG:HG2	1.94	0.68
12:d:149:HIS:CE1	24:q:248:THR:HG22	2.29	0.68
24:q:76:MET:SD	24:q:230:VAL:HG13	2.33	0.68
27:C:236:GLY:O	27:C:364:VAL:HG23	1.94	0.68
37:X:89:LEU:HD11	47:Z:35:TYR:HB2	1.74	0.68
48:l:76:LEU:HD21	48:l:196:TRP:HE3	1.59	0.68
48:l:291:CYS:O	48:l:295:GLN:HG2	1.94	0.68
18:j:70:ALA:HB2	20:m:59:ILE:HD11	1.76	0.68
24:q:266:MET:O	24:q:269:MET:HG2	1.92	0.68
26:B:444:PRO:O	26:B:448:GLU:HG3	1.94	0.68
27:C:381:MET:HE2	27:C:385:ILE:HG13	1.76	0.68
51:u:317:THR:HG21	3:Af:53:VAL:HG22	1.75	0.68
10:b:29:SER:HB2	10:b:30:PRO:HD2	1.76	0.67
24:q:57:PHE:CD1	24:q:113:THR:HG22	2.29	0.67
24:q:94:LEU:O	24:q:98:MET:HG2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:195:ARG:HD3	25:r:231:ILE:HD11	1.75	0.67
36:N:78:GLU:O	36:N:81:ILE:HG12	1.93	0.67
39:Q:142:THR:HA	39:Q:147:LYS:HE3	1.76	0.67
6:w:343:VAL:HG12	6:w:348:ILE:HD11	1.76	0.67
17:i:170:LEU:HD22	17:i:291:TYR:HD2	1.59	0.67
19:k:33:LEU:HD23	19:k:36:MET:CE	2.23	0.67
28:D:76:VAL:HG22	54:M:70:MET:HB3	1.75	0.67
48:l:306:THR:HG22	48:l:336:LYS:HG2	1.76	0.67
49:s:138:LYS:O	49:s:142:GLN:HG3	1.93	0.67
3:4:220:GLN:HE21	3:4:278:ASN:HD22	1.39	0.67
25:r:92:PRO:HB3	25:r:255:TYR:CD1	2.29	0.67
26:B:314:LEU:CD1	26:B:317:VAL:HG23	2.24	0.67
27:C:203:MET:O	27:C:203:MET:HG2	1.94	0.67
53:G:183:ILE:HG23	53:G:195:LEU:O	1.95	0.67
53:G:338:VAL:HG23	53:G:363:SER:HB2	1.76	0.67
17:i:304:MET:O	27:C:45:PRO:HD2	1.94	0.67
20:m:17:PHE:HA	20:m:20:PHE:CE2	2.29	0.67
24:q:361:MET:HB2	24:q:441:ILE:HD11	1.76	0.67
25:r:301:CYS:O	25:r:305:ILE:HG13	1.95	0.67
48:l:10:THR:HA	48:l:13:ILE:HG22	1.76	0.67
49:s:121:MET:O	49:s:125:TRP:HD1	1.77	0.67
3:4:120:SER:HA	51:5:269:ARG:HE	1.58	0.67
5:6:297:PRO:HB3	5:6:304:ASN:HD21	1.59	0.67
11:c:155:PRO:HD3	50:t:4:HIS:CE1	2.30	0.67
25:r:179:TRP:HE1	45:W:43:LEU:HG	1.59	0.67
32:I:70:ALA:HB3	32:I:107:GLY:CA	2.25	0.67
48:l:97:THR:HG22	48:l:246:LEU:HD21	1.76	0.67
48:l:155:ILE:HD12	48:l:236:ALA:O	1.95	0.67
1:0:90:LEU:HD11	7:x:265:SER:HB3	1.77	0.67
5:6:111:SER:HB3	3:Ae:59:LEU:HG	1.76	0.67
22:o:112:LYS:NZ	24:q:388:TRP:O	2.27	0.67
25:r:157:ASN:HA	25:r:168:THR:HG21	1.77	0.67
26:B:213:ILE:HG23	26:B:235:VAL:HA	1.77	0.67
6:w:131:TYR:O	6:w:134:PRO:HD2	1.94	0.67
6:7:368:ILE:O	6:7:372:ILE:HG13	1.94	0.67
12:d:107:GLN:O	12:d:111:LYS:HG3	1.95	0.67
48:l:246:LEU:HB3	48:l:247:LEU:HD23	1.75	0.67
48:l:346:ILE:HG12	48:l:366:MET:HE1	1.77	0.67
48:l:536:LEU:HB3	48:l:537:PRO:HD3	1.75	0.67
6:w:89:MET:CE	6:w:235:MET:HG3	2.25	0.67
17:i:193:VAL:CG1	17:i:266:ILE:HG23	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:28:LEU:CD2	25:r:275:ALA:HB2	2.25	0.67
36:N:106:GLU:CG	36:N:107:PRO:HD2	2.24	0.67
37:O:104:PHE:CD2	37:O:139:MET:HA	2.30	0.67
3:2:257:CYS:SG	55:2:301:FES:S2	2.91	0.67
5:6:214:THR:HB	5:6:242:GLY:O	1.95	0.67
6:7:131:TYR:O	6:7:134:PRO:HD2	1.94	0.67
27:C:258:SER:O	27:C:261:ILE:HG22	1.95	0.67
29:E:169:PHE:HE2	29:E:209:LYS:HG3	1.60	0.67
46:Y:65:MET:HE2	48:l:375:ILE:HG12	1.77	0.67
13:e:82:VAL:HG23	24:q:25:ILE:HD11	1.75	0.67
27:C:160:ALA:HA	27:C:404:THR:HG21	1.75	0.67
28:D:168:ARG:NH2	28:D:187:ILE:HG23	2.09	0.67
48:l:481:THR:HB	50:t:92:HIS:HD2	1.60	0.67
52:z:65:GLN:O	52:z:69:LYS:HG3	1.94	0.67
5:6:297:PRO:HG3	3:Ae:71:LYS:HB2	1.75	0.66
6:7:278:TYR:CE2	6:7:282:ARG:HD3	2.31	0.66
24:q:16:TRP:NE1	24:q:97:THR:HG21	2.10	0.66
24:q:65:LEU:O	24:q:69:THR:HG23	1.94	0.66
48:l:373:LEU:HD22	48:l:431:PHE:HE2	1.59	0.66
51:u:373:GLN:HE22	51:u:471:ILE:HG23	1.60	0.66
54:M:98:ALA:HB1	54:M:99:PRO:HD2	1.77	0.66
17:i:61:LEU:O	17:i:65:THR:HG23	1.94	0.66
48:l:533:MET:O	48:l:537:PRO:HD2	1.94	0.66
51:u:317:THR:HB	3:Af:53:VAL:CG1	2.24	0.66
51:5:158:ASP:O	51:5:162:GLU:HG2	1.95	0.66
16:h:71:LYS:HE2	45:W:110:VAL:HG13	1.77	0.66
26:B:157:TYR:HB2	26:B:212:LEU:HD21	1.77	0.66
32:I:86:MET:HE1	32:I:93:PHE:CD2	2.31	0.66
43:U:85:LEU:HD22	43:U:158:GLY:HA3	1.76	0.66
2:1:11:TYR:HA	2:1:15:PHE:HB2	1.77	0.66
6:7:63:PHE:O	6:7:67:THR:HG23	1.95	0.66
12:d:79:GLU:HG2	15:g:109:LYS:O	1.95	0.66
25:r:11:ILE:HB	25:r:12:PRO:HD3	1.76	0.66
6:w:26:ASN:ND2	6:w:208:PRO:HD2	2.11	0.66
6:w:88:SER:O	6:w:92:ILE:HG13	1.96	0.66
7:x:322:TYR:HB2	8:y:61:PHE:CG	2.30	0.66
24:q:398:MET:O	24:q:402:ILE:HG13	1.95	0.66
46:Y:47:PHE:HE1	48:l:364:LYS:HD3	1.60	0.66
51:u:336:LYS:HE2	51:u:336:LYS:HA	1.76	0.66
7:x:112:ARG:HB2	7:x:140:CYS:HB2	1.76	0.66
2:Ac:54:LYS:HD3	2:Ac:54:LYS:H	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:44:SER:CB	19:k:59:MET:HE3	2.25	0.66
24:q:401:MET:HA	48:l:176:ARG:HG2	1.77	0.66
26:B:38:GLU:HA	29:E:239:LYS:HE3	1.77	0.66
7:x:159:PRO:HG3	7:x:165:MET:CE	2.26	0.66
5:6:319:GLN:HB3	5:6:320:PRO:HD2	1.78	0.66
10:b:76:LEU:O	10:b:79:VAL:HG12	1.95	0.66
19:k:18:GLY:O	20:m:23:LYS:NZ	2.25	0.66
22:o:6:TYR:OH	22:o:12:ALA:HB1	1.94	0.66
3:2:225:ARG:HG3	3:2:281:VAL:HG21	1.76	0.66
8:9:13:TRP:CG	8:9:14:LEU:H	2.12	0.66
13:e:97:ILE:O	13:e:101:LEU:HB2	1.96	0.66
17:i:95:MET:HE2	17:i:149:ILE:HA	1.78	0.66
24:q:109:THR:HG22	24:q:121:LEU:CB	2.26	0.66
37:O:103:HIS:O	37:O:107:ASP:HB2	1.96	0.66
37:O:110:LEU:HB2	37:O:114:ASP:HB3	1.78	0.66
52:Aa:73:LYS:HZ1	1:Ab:66:ASP:H	1.42	0.66
53:G:624:ARG:HH12	53:G:628:GLU:HB2	1.58	0.66
5:6:399:GLN:HG2	3:Ae:39:HIS:HD2	1.61	0.66
21:n:12:TRP:O	21:n:15:ILE:HG22	1.95	0.66
51:u:165:ARG:HD3	51:u:209:ARG:HA	1.78	0.66
3:2:173:ILE:HG23	3:2:190:TRP:HD1	1.61	0.66
3:4:184:LYS:HB3	3:4:184:LYS:HZ3	1.59	0.66
23:p:81:TYR:HB2	47:Z:48:VAL:HG13	1.78	0.66
26:B:159:ARG:HG3	26:B:161:GLU:OE1	1.96	0.66
26:B:382:CYS:SG	26:B:423:THR:HA	2.36	0.66
51:5:377:MET:HE1	51:5:450:TYR:CD2	2.31	0.66
7:8:293:MET:HG3	7:8:294:LEU:N	2.10	0.65
26:B:162:PHE:HZ	29:E:178:GLY:HA3	1.59	0.65
28:D:69:LEU:O	28:D:73:VAL:HG22	1.96	0.65
5:v:290:GLN:OE1	3:Af:46:LEU:HD23	1.96	0.65
13:e:93:PHE:O	13:e:98:VAL:HG23	1.97	0.65
27:C:374:ARG:HA	27:C:377:MET:HG2	1.78	0.65
45:W:23:ARG:HG3	45:W:25:LEU:HD13	1.76	0.65
6:w:63:PHE:O	6:w:67:THR:HG23	1.96	0.65
52:Aa:19:LEU:CD2	52:Aa:23:GLU:HB2	2.21	0.65
9:a:146:LYS:O	9:a:150:ARG:HG3	1.95	0.65
18:j:63:LEU:HD21	20:m:63:GLY:HA2	1.77	0.65
35:L:60:LEU:HD23	35:L:124:LEU:HD23	1.78	0.65
5:6:138:LEU:CD1	5:6:233:VAL:HG13	2.26	0.65
27:C:200:ILE:HD11	27:C:274:TRP:NE1	2.10	0.65
27:C:452:ASP:O	27:C:456:ILE:HG13	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:245:ILE:O	35:L:249:LYS:HG3	1.97	0.65
6:7:239:LEU:O	6:7:243:VAL:HG23	1.95	0.65
19:k:27:MET:HE2	20:m:67:VAL:HG13	1.79	0.65
26:B:452:GLN:O	26:B:456:GLN:HG3	1.96	0.65
31:H:118:LEU:HD23	31:H:119:CYS:N	2.12	0.65
34:K:2:GLU:O	34:K:6:VAL:HG23	1.96	0.65
11:c:49:ALA:O	11:c:53:LYS:HD3	1.97	0.65
14:f:68:GLU:HG2	15:g:21:ARG:HE	1.61	0.65
18:j:112:GLU:OE1	18:j:112:GLU:N	2.30	0.65
19:k:8:ILE:HD13	19:k:42:ILE:HG22	1.78	0.65
24:q:74:PRO:O	24:q:78:MET:HG3	1.97	0.65
52:z:49:VAL:O	52:z:52:PRO:HD2	1.96	0.65
53:G:219:SER:O	53:G:222:ILE:HG12	1.97	0.65
5:6:302:GLY:O	3:Ae:71:LYS:HE3	1.97	0.65
13:e:81:ILE:HD12	13:e:81:ILE:H	1.61	0.65
22:o:108:ASP:O	22:o:112:LYS:HG3	1.95	0.65
27:C:368:LYS:HG2	27:C:386:HIS:CE1	2.32	0.65
35:L:279:ALA:O	35:L:352:ARG:HG3	1.97	0.65
37:O:104:PHE:HD1	37:O:108:LEU:HD12	1.62	0.65
45:W:12:PRO:HD3	45:W:16:TYR:CZ	2.31	0.65
4:Ad:14:ALA:O	4:Ad:18:ILE:HG13	1.96	0.65
24:q:139:GLN:HB2	24:q:222:GLU:OE1	1.97	0.65
46:Y:44:TYR:CD2	46:Y:45:ARG:HG3	2.31	0.65
51:u:224:TYR:O	51:u:225:LYS:HD2	1.95	0.65
8:y:44:VAL:O	8:y:48:ILE:HG12	1.96	0.65
3:2:234:LEU:HD23	3:2:281:VAL:HG22	1.77	0.65
5:6:449:PHE:CZ	5:v:183:ARG:HB2	2.32	0.65
35:L:143:ILE:HB	35:L:144:PRO:HD3	1.78	0.65
7:x:216:LEU:HB3	7:x:249:ILE:CD1	2.17	0.65
6:7:245:PHE:HE2	7:8:102:LEU:HB3	1.62	0.65
17:i:79:LEU:HD23	19:k:47:ILE:HG12	1.79	0.65
17:i:89:MET:HB2	17:i:95:MET:HG2	1.76	0.65
29:E:132:ILE:HD11	29:E:169:PHE:HB3	1.79	0.65
37:X:90:TYR:OH	37:X:92:LYS:HD3	1.97	0.65
48:l:88:MET:HE2	48:l:326:PHE:CE2	2.32	0.65
51:5:156:LEU:O	51:5:213:ARG:NH1	2.30	0.65
53:G:339:ALA:HB1	53:G:537:ILE:HD12	1.79	0.65
53:G:710:CYS:O	53:G:714:VAL:HG12	1.97	0.65
3:4:270:ILE:HD13	3:4:275:ALA:HB3	1.79	0.64
5:6:174:LEU:CD1	3:Ae:67:VAL:HG23	2.27	0.64
8:9:94:TYR:O	8:9:98:VAL:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:134:GLU:HB3	21:n:38:PHE:O	1.97	0.64
16:h:101:LYS:HA	16:h:101:LYS:HE3	1.77	0.64
48:l:289:ALA:O	48:l:293:ILE:HG13	1.98	0.64
51:u:174:GLU:OE2	3:Af:76:CYS:HA	1.98	0.64
5:v:113:THR:HA	3:Af:61:ALA:O	1.97	0.64
5:6:61:ILE:HD11	5:6:225:VAL:HG11	1.79	0.64
6:7:264:THR:HG23	6:7:265:PRO:HD2	1.78	0.64
6:7:282:ARG:CZ	6:7:343:VAL:HG22	2.27	0.64
24:q:302:MET:HE2	24:q:302:MET:HA	1.78	0.64
27:C:283:VAL:HA	27:C:330:GLY:O	1.96	0.64
3:4:234:LEU:HD23	3:4:281:VAL:HG13	1.80	0.64
17:i:38:LEU:HD23	19:k:73:LEU:HD12	1.77	0.64
26:B:447:GLU:O	26:B:451:GLN:HG3	1.96	0.64
38:P:42:VAL:O	38:P:46:LYS:HG3	1.98	0.64
48:l:97:THR:HG21	48:l:125:LEU:HD13	1.79	0.64
5:v:276:ALA:HB2	5:v:282:GLU:HB3	1.77	0.64
3:4:192:GLY:HA3	6:w:169:SER:OG	1.96	0.64
5:6:449:PHE:CE1	5:v:183:ARG:HB2	2.33	0.64
6:7:270:PRO:HD2	6:7:275:LEU:HD23	1.78	0.64
11:c:123:PRO:HA	23:p:117:GLN:NE2	2.12	0.64
14:f:60:LYS:O	14:f:64:GLU:HG3	1.98	0.64
20:m:26:PRO:HB2	20:m:71:THR:HG21	1.78	0.64
35:L:203:GLY:H	35:L:206:ASP:HB2	1.62	0.64
42:T:106:ALA:O	42:T:110:ILE:HG13	1.97	0.64
45:W:93:GLU:O	45:W:97:ILE:HG13	1.97	0.64
48:l:468:ILE:O	48:l:472:ILE:HG23	1.97	0.64
51:u:145:GLU:HG2	51:u:249:HIS:CE1	2.33	0.64
5:v:295:ALA:CA	3:Af:46:LEU:HD22	2.27	0.64
6:w:141:TRP:CD1	6:w:265:PRO:HD3	2.32	0.64
53:G:495:ASN:HA	53:G:498:GLN:HG2	1.78	0.64
8:9:14:LEU:HD23	8:9:17:ILE:HD11	1.80	0.64
13:e:91:PHE:HA	13:e:95:PHE:HD2	1.62	0.64
24:q:108:MET:HB3	24:q:121:LEU:HD13	1.80	0.64
24:q:312:ALA:O	24:q:316:MET:HG3	1.98	0.64
35:L:298:ARG:HB2	35:L:311:ARG:HD2	1.78	0.64
48:l:270:ASN:OD1	48:l:273:VAL:HG23	1.97	0.64
48:l:375:ILE:HD12	48:l:458:LEU:HD22	1.79	0.64
49:s:92:VAL:HG21	49:s:138:LYS:HG2	1.79	0.64
51:5:300:ASP:O	51:5:303:PRO:HD2	1.98	0.64
15:g:12:PRO:HD3	16:h:8:LYS:NZ	2.12	0.64
27:C:194:THR:OG1	27:C:206:PHE:HA	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:186:ARG:NH2	28:D:193:PHE:O	2.30	0.64
6:w:25:SER:HB3	6:w:218:ILE:HG23	1.79	0.64
6:w:119:LEU:HD21	6:w:192:LEU:HB2	1.79	0.64
9:a:169:TYR:OH	44:V:141:VAL:HG21	1.97	0.64
10:b:87:LYS:HE3	12:d:49:ARG:CG	2.28	0.64
11:c:140:MET:HG3	48:l:407:TRP:CZ3	2.33	0.64
25:r:58:LYS:NZ	32:I:125:PRO:HG2	2.13	0.64
26:B:225:LEU:HB3	26:B:227:PRO:HD2	1.80	0.64
42:T:141:PRO:HG3	49:s:118:LYS:HD2	1.78	0.64
6:w:138:MET:HE2	6:w:254:ASP:HB2	1.80	0.64
52:z:76:ALA:HA	52:z:79:GLU:HG2	1.79	0.64
11:c:113:ILE:HD11	11:c:116:ARG:HG3	1.79	0.64
26:B:317:VAL:HG22	26:B:356:VAL:HA	1.80	0.64
34:K:52:ASN:HB3	54:M:29:GLN:NE2	2.12	0.64
48:l:251:THR:O	48:l:254:VAL:HG22	1.98	0.64
6:w:89:MET:HE2	6:w:235:MET:CG	2.23	0.64
51:5:335:ARG:HB2	51:5:337:LEU:HG	1.80	0.64
19:k:37:MET:SD	19:k:67:ALA:HB2	2.38	0.64
31:H:119:CYS:HB3	31:H:158:CYS:HB3	1.80	0.64
47:Z:34:ASP:O	47:Z:37:GLN:HG2	1.98	0.64
48:l:88:MET:HE2	48:l:326:PHE:HE2	1.62	0.64
3:2:172:LYS:O	3:2:172:LYS:HD3	1.98	0.64
7:8:93:PRO:HG2	1:Ab:79:ASP:HB3	1.78	0.64
16:h:82:GLN:O	16:h:86:LEU:HD13	1.98	0.64
27:C:101:LEU:HB2	27:C:464:PHE:CZ	2.33	0.64
31:H:205:ILE:O	31:H:209:TYR:HB3	1.98	0.64
35:L:283:PHE:CE2	35:L:285:PRO:HG3	2.33	0.64
37:O:84:LEU:HB3	37:O:88:LYS:NZ	2.13	0.64
3:2:270:ILE:HG22	3:2:278:ASN:OD1	1.97	0.63
5:6:177:LEU:HD11	5:6:272:VAL:HG22	1.79	0.63
17:i:238:PRO:O	17:i:241:THR:HG22	1.97	0.63
26:B:184:LYS:HE3	40:R:98:MET:CB	2.28	0.63
27:C:377:MET:HE3	27:C:384:LEU:HD13	1.80	0.63
37:O:104:PHE:HB3	37:O:110:LEU:HD11	1.78	0.63
43:U:206:VAL:HB	43:U:257:VAL:HG22	1.78	0.63
37:X:143:GLU:HA	37:X:146:ASP:OD2	1.98	0.63
48:l:298:ILE:O	48:l:302:VAL:HG23	1.98	0.63
6:w:303:LEU:HB3	6:w:306:MET:HE2	1.79	0.63
7:8:271:VAL:O	7:8:275:LEU:HG	1.98	0.63
10:b:72:VAL:HA	10:b:76:LEU:HB2	1.80	0.63
12:d:71:VAL:HG22	12:d:72:PRO:CD	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:119:ARG:O	13:e:123:GLU:HG3	1.98	0.63
17:i:106:LEU:HG	17:i:138:PRO:HB2	1.80	0.63
24:q:325:MET:SD	24:q:441:ILE:HG13	2.39	0.63
34:K:134:ILE:HD13	53:G:298:LYS:HA	1.80	0.63
6:w:117:VAL:HG11	6:w:302:ILE:HD11	1.80	0.63
7:8:122:CYS:HB2	57:8:401:HEC:CAB	2.23	0.63
57:8:401:HEC:HHD	57:8:401:HEC:HBC3	1.79	0.63
11:c:184:TYR:HD1	50:t:36:GLU:HA	1.64	0.63
18:j:72:LEU:O	25:r:151:LEU:HD11	1.98	0.63
25:r:216:ALA:O	25:r:219:PRO:HD2	1.98	0.63
6:7:341:GLN:HG3	6:7:342:PRO:HD2	1.80	0.63
7:8:103:LEU:HD11	7:8:291:LEU:HD13	1.80	0.63
26:B:88:ARG:HB2	26:B:244:ASN:HD22	1.62	0.63
32:I:189:ARG:HG3	35:L:82:GLU:CD	2.23	0.63
34:K:60:ARG:HH22	34:K:95:ASP:HA	1.63	0.63
8:9:14:LEU:O	8:9:17:ILE:HG12	1.97	0.63
10:b:11:ARG:NH1	23:p:196:LEU:HB2	2.14	0.63
23:p:72:TRP:CZ2	48:l:516:PRO:HB3	2.33	0.63
24:q:108:MET:CB	24:q:121:LEU:HD13	2.28	0.63
24:q:109:THR:HG22	24:q:121:LEU:HB2	1.80	0.63
26:B:340:ASP:O	26:B:344:GLN:HG2	1.98	0.63
27:C:165:LEU:HD13	27:C:397:VAL:HG22	1.79	0.63
30:F:79:VAL:O	30:F:121:PRO:HD3	1.98	0.63
33:J:86:ASN:HB3	53:G:224:ASP:OD1	1.98	0.63
35:L:278:VAL:O	35:L:352:ARG:HD2	1.98	0.63
36:N:94:MET:HE3	36:N:99:PRO:HG2	1.81	0.63
6:w:186:PRO:O	6:w:190:THR:HG23	1.99	0.63
53:G:307:ILE:HD13	53:G:582:VAL:HG22	1.79	0.63
26:B:71:LYS:HG2	26:B:75:TRP:CG	2.33	0.63
26:B:316:ALA:HB2	26:B:442:PHE:CZ	2.32	0.63
27:C:228:MET:HG3	32:I:167:PRO:HG3	1.80	0.63
38:P:35:ASP:HA	38:P:38:GLU:HG2	1.81	0.63
48:l:86:SER:HB3	48:l:133:THR:HG22	1.81	0.63
53:G:59:GLN:HG2	53:G:62:ARG:HH12	1.63	0.63
2:1:30:LEU:CD2	4:3:48:ILE:HG13	2.28	0.63
3:4:104:ILE:HG13	3:4:104:ILE:O	1.98	0.63
26:B:141:GLY:HA2	26:B:252:PRO:HD3	1.80	0.63
26:B:276:PHE:HD1	26:B:352:ALA:HB1	1.63	0.63
6:w:94:LEU:HD21	56:w:401:HEM:HAB	1.81	0.63
7:x:127:SER:HB2	7:x:179:PRO:CD	2.29	0.63
37:O:116:VAL:O	37:O:120:MET:HG3	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:437:PHE:HB2	48:l:438:PRO:HD2	1.80	0.63
51:5:120:LEU:HD13	51:5:133:ILE:HG12	1.80	0.63
3:2:192:GLY:HA3	6:7:169:SER:OG	1.98	0.63
5:6:127:ARG:HH21	5:6:224:GLY:HA2	1.63	0.63
43:U:297:ARG:HA	43:U:300:VAL:HG22	1.81	0.63
5:v:295:ALA:HB1	3:Af:46:LEU:CD2	2.27	0.63
5:v:324:SER:HB3	3:Af:68:LEU:HG	1.80	0.63
6:7:245:PHE:CE2	7:8:102:LEU:HB3	2.34	0.62
29:E:186:VAL:HG22	29:E:196:LEU:HD12	1.81	0.62
31:H:118:LEU:HD23	31:H:119:CYS:SG	2.39	0.62
7:8:203:ARG:CZ	7:8:280:GLU:HG2	2.28	0.62
17:i:128:LEU:HD11	17:i:213:LEU:HA	1.80	0.62
35:L:113:LYS:HG3	35:L:114:VAL:N	2.13	0.62
43:U:256:GLU:HG3	43:U:278:LEU:HD22	1.80	0.62
44:V:123:ALA:O	44:V:127:MET:HG3	1.99	0.62
3:2:241:LEU:HD12	3:2:260:HIS:CE1	2.34	0.62
27:C:147:TYR:HB3	32:I:71:CYS:HB3	1.82	0.62
28:D:61:PHE:CZ	28:D:106:ALA:HB2	2.34	0.62
35:L:301:GLU:CD	35:L:310:THR:HG23	2.24	0.62
43:U:256:GLU:OE2	43:U:280:CYS:HB2	1.99	0.62
37:X:119:ILE:HG21	37:X:135:ALA:HB1	1.82	0.62
46:Y:51:THR:HG22	46:Y:54:GLN:HG3	1.81	0.62
17:i:128:LEU:HD13	17:i:216:PHE:HB2	1.80	0.62
20:m:127:ILE:HA	45:W:120:MET:CE	2.29	0.62
25:r:105:MET:HE2	25:r:162:LEU:HD11	1.80	0.62
52:Aa:19:LEU:HD21	52:Aa:23:GLU:CB	2.26	0.62
5:6:412:VAL:O	5:6:416:ILE:HG12	1.98	0.62
28:D:173:MET:O	28:D:196:HIS:HB3	1.99	0.62
35:L:222:PRO:HB3	35:L:286:TYR:OH	1.99	0.62
48:l:147:VAL:CG1	48:l:252:MET:HG3	2.28	0.62
49:s:188:VAL:HG13	49:s:194:TRP:HB2	1.81	0.62
51:5:190:THR:HB	51:5:275:ILE:HG13	1.82	0.62
3:4:106:VAL:CG2	51:5:275:ILE:HD11	2.29	0.62
11:c:156:VAL:HG11	50:t:95:TYR:CZ	2.35	0.62
18:j:73:LEU:O	18:j:76:PRO:HD2	2.00	0.62
24:q:318:ALA:HB2	24:q:373:ILE:HG13	1.81	0.62
24:q:433:GLU:O	24:q:437:MET:HG2	1.99	0.62
32:I:45:TYR:O	32:I:49:LYS:HG2	1.99	0.62
48:l:226:GLN:OE1	48:l:284:THR:HG21	1.99	0.62
53:G:271:MET:HE2	53:G:271:MET:HA	1.81	0.62
3:4:245:PRO:HB2	3:4:255:TYR:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:97:VAL:HG13	48:l:61:MET:HE3	1.82	0.62
11:c:185:GLU:OE1	50:t:37:ARG:HA	2.00	0.62
20:m:39:VAL:O	20:m:43:ILE:HG13	1.99	0.62
26:B:120:GLY:HA2	26:B:159:ARG:HH21	1.64	0.62
27:C:448:HIS:HB3	27:C:452:ASP:HB2	1.82	0.62
35:L:101:MET:CE	35:L:114:VAL:HA	2.30	0.62
51:5:388:VAL:O	51:5:392:LYS:HG3	2.00	0.62
10:b:93:LYS:HB3	10:b:96:THR:CG2	2.29	0.62
25:r:58:LYS:HZ3	32:l:125:PRO:HG2	1.64	0.62
25:r:307:LEU:HD12	25:r:310:MET:HE3	1.81	0.62
33:J:68:PRO:HG2	33:J:71:HIS:ND1	2.15	0.62
48:l:309:GLN:O	48:l:313:MET:HG3	1.99	0.62
6:7:367:PRO:O	6:7:371:ILE:HG13	2.00	0.62
11:c:154:GLN:NE2	48:l:400:ASN:O	2.32	0.62
17:i:68:MET:HE1	19:k:37:MET:SD	2.40	0.62
23:p:72:TRP:CH2	48:l:516:PRO:HB3	2.35	0.62
25:r:61:LEU:O	25:r:61:LEU:HD13	1.99	0.62
7:x:215:LEU:HG	7:x:235:ASN:ND2	2.13	0.62
6:7:26:ASN:HD21	6:7:207:ASN:HB2	1.64	0.62
33:J:61:ILE:O	33:J:65:THR:HG23	1.99	0.62
53:G:323:LEU:HB3	53:G:629:ILE:HD12	1.81	0.62
27:C:329:ARG:HB2	27:C:331:ASP:OD1	1.99	0.61
48:l:27:TYR:OH	48:l:116:ARG:HG2	2.00	0.61
48:l:341:MET:CE	48:l:457:LEU:HD12	2.30	0.61
3:Af:45:PRO:HA	3:Af:66:PRO:CG	2.22	0.61
3:2:204:GLU:O	3:2:207:GLN:HG3	2.00	0.61
21:n:17:VAL:HG11	24:q:30:HIS:CG	2.35	0.61
28:D:110:SER:OG	28:D:133:LEU:HB3	1.99	0.61
3:2:245:PRO:HB2	3:2:255:TYR:CB	2.27	0.61
9:a:179:ILE:HD11	16:h:41:ILE:CG2	2.31	0.61
28:D:128:ILE:HB	28:D:145:THR:HG23	1.81	0.61
38:P:18:GLU:OE2	38:P:20:ARG:HD3	2.00	0.61
3:Ae:65:SER:HB2	3:Ae:66:PRO:HD2	1.82	0.61
5:6:63:LEU:HD23	5:6:141:THR:HG21	1.83	0.61
56:7:402:HEM:HBA1	56:7:402:HEM:HHA	1.81	0.61
18:j:87:MET:HE1	25:r:309:ILE:HD11	1.82	0.61
24:q:1:MET:HE2	24:q:111:THR:HG21	1.82	0.61
26:B:128:ARG:HG2	26:B:132:ARG:NH1	2.15	0.61
27:C:128:LYS:HB2	28:D:198:PHE:CE1	2.35	0.61
27:C:212:GLU:O	27:C:216:MET:HG3	2.00	0.61
37:O:104:PHE:HD2	37:O:139:MET:HA	1.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:225:LYS:O	51:5:229:MET:HG3	2.01	0.61
5:6:266:LEU:HD22	3:Ae:72:ARG:NH2	2.15	0.61
5:6:312:ALA:O	5:6:315:LYS:HG2	2.00	0.61
6:7:264:THR:HG23	6:7:268:ILE:HD11	1.82	0.61
6:7:337:TRP:CZ3	6:7:350:ILE:HG21	2.36	0.61
20:m:93:PHE:CE2	20:m:97:LEU:HD11	2.35	0.61
21:n:39:ARG:HD3	21:n:58:LYS:H	1.64	0.61
25:r:28:LEU:HD22	25:r:275:ALA:HB2	1.82	0.61
31:H:63:TRP:HB3	31:H:66:LEU:HD12	1.83	0.61
7:x:216:LEU:CB	7:x:249:ILE:HD11	2.17	0.61
53:G:257:VAL:HG11	53:G:413:LEU:HB2	1.81	0.61
28:D:185:ARG:HA	39:Q:114:MET:HE3	1.83	0.61
30:F:37:LYS:H	30:F:37:LYS:HD3	1.63	0.61
51:u:207:ASN:O	51:u:211:LEU:HG	1.99	0.61
10:b:93:LYS:HD2	10:b:94:PRO:HD2	1.82	0.61
10:b:94:PRO:HB3	12:d:5:TRP:CG	2.35	0.61
17:i:294:MET:CE	24:q:130:LEU:HD21	2.30	0.61
18:j:70:ALA:CB	20:m:59:ILE:HD11	2.30	0.61
24:q:16:TRP:HE1	24:q:97:THR:HG21	1.65	0.61
24:q:157:SER:O	24:q:160:LEU:HB3	2.01	0.61
25:r:34:ARG:HD3	27:C:207:PHE:CD1	2.35	0.61
26:B:35:LEU:HD23	26:B:40:ARG:HG2	1.82	0.61
34:K:52:ASN:HB3	54:M:29:GLN:HE22	1.66	0.61
48:l:419:THR:HA	48:l:422:TYR:CZ	2.35	0.61
7:x:314:VAL:CG2	52:z:21:PRO:HG3	2.31	0.61
6:7:318:ARG:O	6:7:322:GLN:HG3	2.01	0.61
8:9:13:TRP:CD1	8:9:14:LEU:H	2.19	0.61
15:g:15:PHE:O	15:g:80:ARG:HD2	2.00	0.61
17:i:3:PRO:O	17:i:7:THR:HG23	2.00	0.61
17:i:173:THR:HG22	27:C:58:MET:HE2	1.83	0.61
26:B:210:THR:HG21	26:B:224:ARG:HB2	1.82	0.61
27:C:240:GLN:HB3	31:H:96:ARG:NH2	2.16	0.61
32:I:67:PHE:CZ	32:I:113:MET:HE2	2.36	0.61
35:L:43:ARG:HG2	35:L:94:ASP:HB2	1.81	0.61
48:l:147:VAL:HG11	48:l:252:MET:HG3	1.82	0.61
51:5:164:GLU:O	51:5:168:ILE:HG13	2.01	0.61
7:8:217:THR:HA	7:8:264:MET:HE2	1.83	0.61
16:h:26:PRO:HD3	19:k:55:LEU:HD13	1.82	0.61
20:m:27:ILE:HD12	20:m:71:THR:HG21	1.83	0.61
23:p:170:LEU:HG	23:p:205:LEU:HD11	1.83	0.61
26:B:300:ILE:O	26:B:304:ALA:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:275:ARG:O	27:C:279:VAL:HB	1.99	0.61
35:L:330:LEU:HB3	35:L:335:ILE:HG23	1.83	0.61
47:Z:32:LEU:HD12	47:Z:32:LEU:H	1.65	0.61
6:w:277:ALA:HB1	6:w:294:LEU:HG	1.81	0.61
7:x:320:LEU:HD12	7:x:320:LEU:O	2.01	0.61
3:2:249:ALA:HB3	3:2:256:TYR:HB3	1.82	0.61
10:b:87:LYS:HE3	12:d:49:ARG:HG3	1.83	0.61
24:q:10:MET:O	24:q:13:PRO:HD2	2.00	0.61
27:C:62:LYS:HG3	27:C:63:GLU:N	2.15	0.61
27:C:352:GLN:O	27:C:356:LYS:HG2	2.01	0.61
31:H:158:CYS:HA	31:H:161:ALA:HB3	1.83	0.61
6:w:157:GLY:O	6:w:161:VAL:HG23	2.00	0.61
3:4:171:SER:HB2	6:w:168:PHE:CZ	2.36	0.60
6:7:137:GLN:HB2	6:7:257:THR:HG23	1.81	0.60
13:e:89:VAL:HG13	24:q:29:VAL:HG22	1.82	0.60
31:H:119:CYS:HB2	59:H:302:SF4:S3	2.41	0.60
34:K:48:TYR:OH	34:K:83:PRO:HD2	2.00	0.60
39:Q:145:LEU:HG	39:Q:149:TYR:CE2	2.36	0.60
48:l:368:PHE:CZ	48:l:455:LYS:HG3	2.36	0.60
5:v:290:GLN:HG3	5:v:325:ALA:HB3	1.83	0.60
1:Ab:28:ASP:OD2	1:Ab:30:LEU:HB3	2.01	0.60
51:5:142:LYS:O	51:5:146:LEU:HG	2.01	0.60
24:q:5:ILE:O	24:q:9:THR:HG23	2.01	0.60
26:B:278:ILE:HG21	26:B:304:ALA:HB2	1.83	0.60
5:v:159:ARG:NH1	5:v:197:ILE:HG21	2.17	0.60
7:x:113:ARG:O	7:x:117:VAL:HG23	2.02	0.60
10:b:33:PRO:HD2	23:p:156:MET:O	2.02	0.60
5:v:347:ALA:O	5:v:351:ILE:HG13	2.01	0.60
51:5:445:CYS:O	51:5:449:PHE:HB2	2.00	0.60
1:0:47:ARG:O	1:0:51:GLU:HG2	2.02	0.60
10:b:56:PRO:O	10:b:57:TRP:HB2	2.02	0.60
23:p:88:ALA:O	23:p:92:GLU:HG3	2.02	0.60
25:r:17:VAL:HG13	25:r:228:TYR:HB2	1.83	0.60
1:Ab:51:GLU:O	1:Ab:55:GLN:HG3	2.01	0.60
2:1:17:ARG:HG2	2:1:20:THR:OG1	2.02	0.60
5:6:177:LEU:HD21	5:6:272:VAL:HG11	1.83	0.60
11:c:121:PRO:HB3	22:o:13:THR:O	2.01	0.60
11:c:154:GLN:CD	48:l:401:MET:HA	2.26	0.60
26:B:327:ILE:HG23	26:B:347:THR:CG2	2.30	0.60
27:C:139:LEU:HD23	27:C:157:TYR:HD2	1.66	0.60
33:J:86:ASN:HB3	53:G:224:ASP:CG	2.27	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Q:51:MET:HG3	39:Q:55:LYS:HE2	1.83	0.60
5:v:209:VAL:O	5:v:213:PHE:HB2	2.02	0.60
3:2:237:VAL:HG13	3:2:242:GLY:HA2	1.83	0.60
3:4:225:ARG:NH2	3:4:278:ASN:HB3	2.16	0.60
6:7:59:THR:HG23	6:7:172:LYS:HA	1.81	0.60
6:7:303:LEU:HD22	6:7:306:MET:HE1	1.84	0.60
10:b:89:HIS:CE1	10:b:90:VAL:HG23	2.36	0.60
25:r:206:GLU:OE1	27:C:451:ALA:HB2	2.02	0.60
35:L:152:LYS:HG2	35:L:190:PHE:CD2	2.36	0.60
44:V:18:CYS:SG	44:V:75:CYS:HB3	2.41	0.60
48:l:79:SER:OG	48:l:135:ASN:HB3	2.01	0.60
48:l:245:ALA:HB2	48:l:340:PHE:HB3	1.82	0.60
49:s:92:VAL:CG2	49:s:138:LYS:HG2	2.32	0.60
6:w:101:GLY:HA2	6:w:106:SER:HB2	1.84	0.60
3:2:104:ILE:CG2	7:x:323:ARG:HE	2.14	0.60
5:6:322:ASP:HB2	3:Ae:72:ARG:HG3	1.84	0.60
17:i:31:ILE:HD11	19:k:62:ILE:HG21	1.82	0.60
20:m:30:GLY:O	20:m:34:ILE:HG13	2.01	0.60
25:r:37:PRO:HA	32:I:88:ARG:HA	1.84	0.60
26:B:327:ILE:HG23	26:B:347:THR:HG21	1.84	0.60
5:v:412:VAL:O	5:v:416:ILE:HG12	2.02	0.60
4:Ad:8:PRO:O	4:Ad:12:GLU:HG3	2.02	0.60
53:G:341:ILE:HG12	53:G:545:LEU:HD11	1.83	0.60
16:h:81:ARG:HD2	20:m:111:GLU:HG3	1.84	0.60
23:p:142:PRO:HG2	23:p:145:CYS:SG	2.41	0.60
25:r:49:ILE:H	25:r:49:ILE:HD12	1.67	0.60
25:r:293:PHE:O	25:r:297:THR:HG23	2.01	0.60
26:B:110:PRO:O	26:B:238:CYS:HB3	2.02	0.60
43:U:258:LEU:HD21	43:U:278:LEU:HD21	1.84	0.60
48:l:93:ALA:O	48:l:97:THR:HG23	2.01	0.60
48:l:210:ASN:O	48:l:214:ILE:HG13	2.02	0.60
51:u:317:THR:HB	3:Af:53:VAL:HG13	1.83	0.60
6:w:97:HIS:CE1	6:w:100:ARG:HH22	2.19	0.60
6:w:294:LEU:O	6:w:294:LEU:HD23	2.02	0.60
6:w:357:LEU:O	6:w:361:ILE:HG13	2.01	0.60
7:x:96:PRO:HA	7:x:100:ARG:HE	1.65	0.60
2:1:36:PHE:HZ	7:x:295:MET:HB2	1.65	0.60
3:2:104:ILE:HD12	3:2:104:ILE:O	2.02	0.60
6:7:362:ILE:HA	6:7:366:MET:HE3	1.83	0.60
16:h:94:PRO:CG	16:h:99:LEU:HD21	2.31	0.60
20:m:127:ILE:HA	45:W:120:MET:HE2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:167:PRO:HB3	59:I:201:SF4:S2	2.41	0.60
2:1:25:ILE:HD13	3:2:143:THR:HG21	1.83	0.60
6:7:8:HIS:ND1	6:7:11:MET:HG2	2.17	0.60
17:i:258:SER:O	17:i:261:MET:HG2	2.02	0.60
25:r:27:VAL:HG12	25:r:31:MET:HE2	1.84	0.60
25:r:88:PRO:HB3	25:r:98:MET:HE3	1.83	0.60
27:C:374:ARG:O	27:C:377:MET:HG3	2.02	0.60
27:C:456:ILE:O	27:C:459:THR:HG22	2.02	0.60
48:l:264:TYR:CD2	48:l:265:PRO:HD3	2.37	0.60
5:v:407:VAL:CG2	5:v:411:THR:HB	2.31	0.60
6:7:303:LEU:HD22	6:7:306:MET:CE	2.32	0.59
20:m:125:TRP:HH2	45:W:126:GLY:HA2	1.67	0.59
35:L:339:PRO:HG2	35:L:342:LEU:HG	1.84	0.59
37:O:115:GLN:O	37:O:118:ILE:HG13	2.01	0.59
51:u:164:GLU:O	51:u:168:ILE:HG13	2.02	0.59
5:v:358:VAL:HG11	5:v:431:PHE:CD2	2.37	0.59
8:y:63:ILE:O	8:y:67:LEU:HG	2.02	0.59
53:G:69:LEU:HD11	53:G:225:ILE:CD1	2.31	0.59
15:g:64:LEU:O	15:g:68:THR:HG23	2.02	0.59
26:B:422:HIS:O	53:G:76:ARG:HD3	2.02	0.59
51:u:396:ARG:O	51:u:400:VAL:HG22	2.02	0.59
3:4:172:LYS:HB2	3:4:172:LYS:HZ3	1.66	0.59
56:7:402:HEM:HBC2	56:7:402:HEM:CMC	2.30	0.59
11:c:39:GLY:O	11:c:74:ASP:HB2	2.03	0.59
17:i:30:TRP:CZ2	19:k:37:MET:HE1	2.37	0.59
17:i:171:ASN:ND2	27:C:58:MET:O	2.34	0.59
18:j:77:TRP:HH2	25:r:100:LEU:HD21	1.65	0.59
20:m:86:ASN:ND2	20:m:88:THR:OG1	2.36	0.59
26:B:382:CYS:SG	26:B:384:PRO:HD2	2.42	0.59
27:C:229:HIS:CD2	32:I:167:PRO:HD3	2.37	0.59
28:D:76:VAL:HG23	54:M:69:VAL:HB	1.85	0.59
28:D:126:PHE:HZ	28:D:199:ARG:HE	1.50	0.59
30:F:51:ARG:O	30:F:54:ARG:HG2	2.01	0.59
48:l:316:THR:HG21	48:l:395:ILE:HD12	1.84	0.59
48:l:489:THR:O	48:l:493:VAL:HG23	2.02	0.59
51:u:373:GLN:NE2	51:u:471:ILE:HG23	2.16	0.59
18:j:38:GLU:HG3	27:C:89:ASN:HB2	1.84	0.59
28:D:129:VAL:HG22	28:D:144:LYS:HD2	1.84	0.59
31:H:38:TYR:CE2	54:M:106:LEU:HD13	2.37	0.59
37:O:105:MET:HG2	37:O:139:MET:HG2	1.84	0.59
48:l:34:ASN:OD1	48:l:34:ASN:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:319:ILE:HG13	48:l:399:VAL:HG22	1.82	0.59
6:w:123:VAL:HG22	6:w:189:ILE:HD13	1.84	0.59
53:G:349:GLU:O	53:G:352:VAL:HG12	2.02	0.59
6:7:364:VAL:O	6:7:367:PRO:HD2	2.03	0.59
17:i:256:PRO:HD3	24:q:124:ALA:HB1	1.85	0.59
17:i:340:THR:N	17:i:341:PRO:HD2	2.18	0.59
18:j:44:MET:HG3	39:Q:122:VAL:HG23	1.84	0.59
20:m:151:THR:O	20:m:155:ILE:HG13	2.02	0.59
24:q:92:LYS:O	24:q:96:ILE:HG13	2.02	0.59
28:D:135:LEU:H	28:D:135:LEU:HD12	1.68	0.59
51:u:96:LEU:HD11	51:u:156:LEU:HD23	1.83	0.59
51:u:407:THR:HB	51:u:408:PRO:HD3	1.84	0.59
12:d:75:THR:OG1	13:e:146:LYS:HD2	2.02	0.59
16:h:60:PHE:O	16:h:64:VAL:HG23	2.03	0.59
17:i:106:LEU:HD22	17:i:187:MET:HE2	1.85	0.59
24:q:231:LEU:O	24:q:236:LEU:HG	2.03	0.59
27:C:268:LEU:HD22	27:C:274:TRP:CD1	2.38	0.59
30:F:68:ILE:O	30:F:71:ILE:HG22	2.03	0.59
5:v:39:GLU:O	5:v:50:ALA:HA	2.03	0.59
5:v:313:VAL:HG11	5:v:350:VAL:HG13	1.85	0.59
3:Ae:48:PRO:HA	3:Ae:65:SER:C	2.27	0.59
6:7:361:ILE:HG22	6:7:366:MET:HE2	1.85	0.59
12:d:27:PRO:HB2	12:d:32:TYR:HE2	1.68	0.59
18:j:61:THR:HG21	18:j:105:GLU:CD	2.28	0.59
25:r:72:ILE:O	25:r:75:PRO:HD2	2.03	0.59
25:r:273:ILE:HG23	25:r:277:TYR:HD2	1.68	0.59
26:B:114:VAL:HG11	26:B:212:LEU:HD22	1.85	0.59
35:L:319:MET:CE	35:L:322:MET:HE3	2.32	0.59
48:l:37:LYS:HD2	48:l:105:MET:HE1	1.85	0.59
48:l:250:SER:HB2	48:l:333:ALA:HA	1.83	0.59
6:w:32:ASN:HD21	6:w:227:LYS:HG2	1.66	0.59
11:c:93:ASP:HB2	11:c:100:ASN:HA	1.85	0.59
16:h:85:LYS:O	16:h:89:GLU:HG2	2.03	0.59
18:j:44:MET:HE3	39:Q:122:VAL:HB	1.84	0.59
24:q:454:ILE:HD13	24:q:454:ILE:H	1.67	0.59
29:E:246:GLN:HB3	29:E:249:LEU:HD23	1.85	0.59
37:O:138:LEU:CD2	37:O:144:ILE:HG12	2.29	0.59
42:T:142:LEU:HD12	42:T:142:LEU:O	2.03	0.59
7:x:229:ARG:HB2	7:x:232:LEU:HD12	1.85	0.59
21:n:50:ARG:HG2	21:n:53:GLU:OE1	2.02	0.59
24:q:423:ILE:HG22	24:q:426:ILE:HD12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:V:88:LEU:O	44:V:92:ILE:HG13	2.03	0.59
7:x:159:PRO:HG3	7:x:165:MET:SD	2.42	0.59
3:2:270:ILE:CD1	3:2:275:ALA:HB3	2.33	0.59
12:d:69:ARG:NH2	21:n:46:LYS:O	2.35	0.59
24:q:379:LEU:O	24:q:383:THR:HG23	2.01	0.59
36:N:77:ILE:O	36:N:81:ILE:HG23	2.03	0.59
38:P:18:GLU:CD	38:P:20:ARG:HD3	2.26	0.59
6:w:66:VAL:CG1	6:w:80:ARG:HE	2.15	0.59
52:Aa:26:ALA:C	52:Aa:28:PRO:HD3	2.27	0.59
13:e:79:ASP:HB2	13:e:82:VAL:HG12	1.84	0.58
19:k:2:PRO:HG3	20:m:127:ILE:HD13	1.85	0.58
20:m:26:PRO:HB2	20:m:71:THR:CG2	2.33	0.58
24:q:76:MET:CE	24:q:99:LEU:HD22	2.33	0.58
25:r:96:ILE:HG23	45:W:144:THR:HB	1.85	0.58
25:r:273:ILE:HG23	25:r:277:TYR:CD2	2.37	0.58
48:l:117:PHE:CZ	48:l:243:VAL:HG23	2.38	0.58
49:s:214:LEU:HD23	49:s:215:PRO:CD	2.31	0.58
7:x:97:TRP:HB2	7:x:100:ARG:HG3	1.83	0.58
51:5:338:CYS:SG	51:5:358:PHE:HB2	2.43	0.58
9:a:130:GLU:OE1	9:a:131:LYS:N	2.36	0.58
10:b:55:ALA:CB	10:b:60:VAL:HG23	2.33	0.58
17:i:84:TRP:HH2	19:k:59:MET:HE2	1.68	0.58
18:j:77:TRP:CH2	25:r:100:LEU:HD21	2.38	0.58
24:q:1:MET:SD	24:q:111:THR:HG21	2.43	0.58
26:B:313:ASN:O	26:B:359:ARG:HG3	2.02	0.58
35:L:213:ALA:O	35:L:216:ARG:HG2	2.02	0.58
39:Q:91:GLU:HG2	39:Q:95:LYS:NZ	2.17	0.58
49:s:162:TYR:CZ	49:s:181:GLN:HB2	2.38	0.58
6:7:186:PRO:HG2	56:7:401:HEM:HMC3	1.86	0.58
15:g:17:PRO:HG2	15:g:83:TYR:CZ	2.38	0.58
16:h:89:GLU:HB3	16:h:91:LYS:HE3	1.85	0.58
20:m:107:ALA:HB2	20:m:113:VAL:HG11	1.85	0.58
26:B:71:LYS:HB2	26:B:71:LYS:NZ	2.18	0.58
26:B:154:ALA:HB2	26:B:193:PHE:HZ	1.67	0.58
27:C:241:ASP:OD2	45:W:8:GLN:NE2	2.37	0.58
42:T:126:TYR:O	42:T:130:ILE:HG13	2.02	0.58
48:l:74:VAL:HG21	48:l:190:LEU:HD11	1.85	0.58
50:t:92:HIS:O	50:t:96:VAL:HG23	2.03	0.58
6:w:139:SER:H	6:w:255:ASN:HD21	1.50	0.58
51:5:294:PRO:HB2	51:5:298:ASN:HB3	1.85	0.58
53:G:50:LEU:HD21	53:G:62:ARG:HH21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:49:ILE:O	5:6:49:ILE:HG12	2.02	0.58
6:7:119:LEU:HD21	6:7:192:LEU:CB	2.34	0.58
11:c:115:ASN:HA	48:l:166:THR:CG2	2.34	0.58
12:d:96:TYR:O	12:d:100:GLN:HG3	2.03	0.58
18:j:53:MET:HE1	20:m:69:GLY:HA3	1.86	0.58
19:k:59:MET:HG3	19:k:60:PRO:HD3	1.86	0.58
24:q:122:PHE:CE1	24:q:206:LYS:HG3	2.39	0.58
26:B:116:ASN:ND2	26:B:207:GLY:O	2.37	0.58
49:s:187:CYS:SG	49:s:188:VAL:N	2.76	0.58
3:2:263:HIS:O	3:2:270:ILE:HD12	2.03	0.58
25:r:185:TRP:O	25:r:189:THR:HG23	2.04	0.58
26:B:249:ALA:O	26:B:252:PRO:HD2	2.03	0.58
28:D:171:TRP:HE1	39:Q:114:MET:HE1	1.69	0.58
31:H:38:TYR:O	54:M:106:LEU:HD12	2.04	0.58
32:I:55:ASN:O	32:I:59:ARG:HG2	2.03	0.58
35:L:167:ALA:HA	35:L:176:LEU:HB3	1.85	0.58
38:P:92:GLU:HG2	38:P:93:ASN:N	2.18	0.58
44:V:58:ARG:O	44:V:62:THR:HG23	2.03	0.58
7:x:305:TYR:O	7:x:309:ARG:HG2	2.03	0.58
8:y:94:TYR:O	8:y:98:VAL:HG23	2.03	0.58
3:4:161:MET:HE3	6:w:177:ARG:HD2	1.85	0.58
5:6:394:ASP:OD1	5:6:395:GLU:N	2.36	0.58
8:9:52:PRO:HD2	8:9:55:LEU:HD12	1.85	0.58
11:c:65:TYR:CE2	11:c:77:LYS:HG2	2.37	0.58
11:c:78:LEU:HB3	11:c:79:PRO:HD2	1.86	0.58
13:e:89:VAL:HG11	24:q:29:VAL:HG22	1.85	0.58
16:h:68:LEU:HD21	17:i:79:LEU:HD13	1.85	0.58
17:i:29:ILE:HD12	17:i:86:ILE:HG12	1.85	0.58
19:k:33:LEU:HD23	19:k:36:MET:HE2	1.83	0.58
27:C:449:MET:O	27:C:453:VAL:HG23	2.04	0.58
28:D:215:GLU:HG3	35:L:63:TYR:CD2	2.39	0.58
35:L:346:GLU:HG2	39:Q:79:ASP:OD2	2.03	0.58
48:l:503:GLU:O	48:l:507:THR:HG23	2.03	0.58
5:v:195:TYR:CE2	5:v:196:ARG:HG2	2.38	0.58
8:y:106:GLU:O	8:y:110:LYS:HG3	2.03	0.58
24:q:122:PHE:HE1	24:q:206:LYS:HG3	1.67	0.58
26:B:140:GLU:HG3	26:B:252:PRO:HG3	1.85	0.58
26:B:161:GLU:HB3	29:E:192:TYR:OH	2.04	0.58
27:C:284:VAL:HG22	27:C:335:ARG:HH21	1.69	0.58
28:D:181:HIS:HD2	28:D:183:ASP:H	1.50	0.58
48:l:389:PHE:O	48:l:393:ASP:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:168:ARG:HG3	7:x:169:PRO:HD2	1.84	0.58
5:6:138:LEU:CD1	5:6:237:PHE:HB2	2.34	0.58
16:h:71:LYS:HB3	45:W:110:VAL:CG2	2.34	0.58
24:q:10:MET:C	24:q:13:PRO:HD2	2.28	0.58
24:q:251:ASN:CB	24:q:252:PRO:HD3	2.31	0.58
25:r:2:PHE:O	25:r:6:ILE:HG13	2.03	0.58
35:L:121:VAL:HG23	35:L:156:VAL:HG11	1.86	0.58
37:X:89:LEU:CD1	47:Z:35:TYR:HB2	2.34	0.58
5:v:108:GLY:HA3	5:v:133:LEU:HD21	1.86	0.58
6:w:27:ILE:HG12	6:w:224:TYR:CZ	2.39	0.58
57:x:401:HEC:HMB3	57:x:401:HEC:HBB2	1.86	0.58
3:Af:46:LEU:HD12	3:Af:47:GLY:N	2.19	0.58
6:7:264:THR:CG2	6:7:265:PRO:HD2	2.34	0.58
22:o:94:GLY:HA2	48:l:553:LEU:HD21	1.85	0.58
26:B:325:PRO:HG3	26:B:433:TRP:HB3	1.84	0.58
27:C:225:GLY:HA3	31:H:96:ARG:O	2.04	0.58
48:l:368:PHE:HZ	48:l:455:LYS:HG3	1.68	0.58
1:0:57:VAL:HG22	1:0:65:GLU:HG3	1.86	0.58
5:6:131:GLU:O	5:6:135:GLU:HG2	2.04	0.58
6:7:300:ILE:HD12	6:7:303:LEU:HD12	1.86	0.58
8:9:57:ASN:HA	8:9:60:VAL:CG2	2.34	0.58
18:j:2:ASN:HB3	25:r:96:ILE:HD11	1.85	0.58
23:p:118:HIS:O	23:p:121:PRO:HD3	2.04	0.58
24:q:207:MET:HE1	24:q:297:VAL:CG1	2.34	0.58
24:q:208:PRO:HD3	24:q:236:LEU:HD22	1.86	0.58
25:r:63:PRO:HB2	25:r:66:SER:HB3	1.85	0.58
26:B:302:LYS:HD2	26:B:303:HIS:NE2	2.19	0.58
27:C:133:LYS:HE2	31:H:124:PRO:O	2.04	0.58
35:L:289:PRO:HB2	35:L:291:PHE:CE1	2.39	0.58
5:6:117:GLU:OE2	5:6:330:TYR:HB3	2.04	0.57
22:o:5:LYS:HB2	22:o:5:LYS:NZ	2.20	0.57
32:I:70:ALA:HB3	32:I:107:GLY:HA3	1.86	0.57
35:L:275:ILE:HG23	35:L:348:LEU:CD1	2.34	0.57
45:W:68:ARG:O	45:W:72:MET:HG3	2.03	0.57
48:l:253:VAL:HB	48:l:310:LEU:HD11	1.86	0.57
51:u:157:GLU:O	51:u:161:ILE:HG13	2.04	0.57
17:i:112:HIS:NE2	17:i:164:ILE:HG21	2.19	0.57
29:E:239:LYS:N	29:E:239:LYS:HE2	2.19	0.57
5:v:36:GLN:HG3	5:v:53:GLU:HB3	1.86	0.57
53:G:179:CYS:O	53:G:180:THR:OG1	2.22	0.57
6:7:101:GLY:HA2	6:7:106:SER:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:223:TYR:HB3	7:8:312:TRP:CE2	2.38	0.57
11:c:140:MET:SD	48:l:283:ILE:HG23	2.44	0.57
19:k:44:SER:HB2	19:k:59:MET:HE3	1.86	0.57
23:p:218:GLU:OE1	23:p:219:ARG:NH1	2.37	0.57
24:q:116:ILE:HG21	49:s:245:PHE:HB3	1.85	0.57
24:q:263:MET:HE3	24:q:263:MET:CA	2.34	0.57
6:w:37:LEU:HB3	56:w:401:HEM:CMB	2.34	0.57
2:Ac:20:THR:HG22	4:Ad:23:MET:HE2	1.86	0.57
3:4:235:ILE:CG2	3:4:280:GLU:HB3	2.35	0.57
6:7:338:ILE:HD13	6:7:351:GLY:CA	2.33	0.57
20:m:68:PHE:CE2	25:r:117:LEU:HB3	2.38	0.57
20:m:103:MET:HE3	20:m:103:MET:CA	2.34	0.57
23:p:142:PRO:HB2	23:p:144:TRP:CD1	2.39	0.57
28:D:78:VAL:HG22	28:D:84:LEU:HD13	1.86	0.57
33:J:71:HIS:HA	33:J:75:ARG:HG3	1.86	0.57
2:Ac:34:ARG:O	2:Ac:34:ARG:HD3	2.05	0.57
51:5:377:MET:HE1	51:5:450:TYR:CE2	2.40	0.57
53:G:347:ASP:HB2	53:G:594:ALA:HB1	1.85	0.57
6:7:82:LEU:HD23	6:7:243:VAL:HG21	1.85	0.57
6:7:334:THR:O	6:7:338:ILE:HG13	2.04	0.57
10:b:84:TYR:CE1	12:d:49:ARG:HG2	2.39	0.57
12:d:113:CYS:SG	12:d:128:GLU:HG3	2.44	0.57
17:i:305:PHE:CD1	27:C:45:PRO:HG2	2.39	0.57
19:k:3:LEU:HD13	20:m:120:ASN:O	2.05	0.57
26:B:371:ILE:HD12	26:B:396:MET:HG3	1.86	0.57
48:l:90:ILE:HD11	48:l:133:THR:HG21	1.86	0.57
53:G:438:LEU:O	53:G:439:THR:OG1	2.17	0.57
3:4:245:PRO:HA	3:4:257:CYS:HB3	1.86	0.57
6:7:27:ILE:HG12	6:7:224:TYR:CE1	2.39	0.57
56:7:402:HEM:HBB2	56:7:402:HEM:CMB	2.35	0.57
10:b:105:PHE:O	10:b:107:GLY:N	2.38	0.57
26:B:201:ALA:HB3	29:E:119:TYR:CG	2.40	0.57
26:B:257:ARG:HG2	26:B:261:TRP:CD2	2.40	0.57
27:C:299:LEU:HD13	27:C:304:ILE:HD11	1.87	0.57
29:E:111:ARG:HD2	33:J:173:SER:HB2	1.87	0.57
32:I:188:LYS:O	32:I:192:ILE:HG12	2.04	0.57
35:L:78:PRO:HA	35:L:101:MET:O	2.05	0.57
37:X:125:GLU:HG2	48:l:439:PRO:HG2	1.86	0.57
6:w:40:CYS:HB3	6:w:90:PHE:CD2	2.40	0.57
6:w:119:LEU:O	6:w:123:VAL:HG23	2.04	0.57
5:6:213:PHE:O	5:6:241:ARG:HG2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:251:ASN:OD1	7:8:251:ASN:N	2.36	0.57
13:e:79:ASP:O	13:e:82:VAL:HG13	2.05	0.57
24:q:378:GLU:O	24:q:382:ILE:HG13	2.03	0.57
46:Y:61:PHE:CZ	48:l:455:LYS:HG2	2.39	0.57
1:Ab:85:LYS:NZ	1:Ab:85:LYS:HB3	2.19	0.57
5:6:121:TYR:HB3	5:6:137:LEU:HD11	1.87	0.57
6:7:53:MET:HE2	6:w:181:PHE:CE1	2.39	0.57
11:c:140:MET:HE2	48:l:283:ILE:HA	1.87	0.57
16:h:71:LYS:HB3	45:W:110:VAL:HG21	1.86	0.57
24:q:360:LEU:O	24:q:364:LEU:HG	2.04	0.57
25:r:277:TYR:CZ	31:H:66:LEU:HB3	2.39	0.57
26:B:62:TRP:CD2	26:B:181:LEU:HD13	2.40	0.57
26:B:128:ARG:HG2	26:B:132:ARG:HH12	1.69	0.57
37:O:147:TYR:O	37:O:151:LYS:HG2	2.05	0.57
44:V:18:CYS:HA	44:V:75:CYS:SG	2.44	0.57
46:Y:87:PRO:HG3	50:t:100:LYS:HA	1.86	0.57
48:l:316:THR:CG2	48:l:395:ILE:HD12	2.33	0.57
49:s:160:THR:O	49:s:164:THR:HG23	2.05	0.57
5:v:143:ALA:N	5:v:144:PRO:HD3	2.19	0.57
51:5:192:PHE:O	51:5:198:ALA:HB2	2.05	0.57
14:f:31:ILE:HD12	14:f:32:ARG:N	2.20	0.57
16:h:15:ASP:HB3	17:i:28:LEU:HD12	1.85	0.57
17:i:41:ILE:CG2	19:k:73:LEU:HD21	2.31	0.57
23:p:107:ARG:O	23:p:111:GLU:HG3	2.05	0.57
27:C:49:TRP:O	27:C:52:GLN:HG2	2.05	0.57
27:C:101:LEU:HD22	27:C:464:PHE:HZ	1.69	0.57
48:l:293:ILE:HD11	48:l:418:LEU:HD22	1.86	0.57
48:l:363:TYR:CD2	48:l:370:THR:HG21	2.40	0.57
9:a:160:MET:HE2	15:g:95:TYR:CD2	2.40	0.57
20:m:124:ASP:O	20:m:127:ILE:HG12	2.05	0.57
26:B:54:LYS:HZ2	26:B:54:LYS:H	1.52	0.57
27:C:219:PHE:O	27:C:223:VAL:HG22	2.05	0.57
31:H:63:TRP:O	31:H:67:VAL:HG23	2.04	0.57
39:Q:47:PHE:HE2	39:Q:110:ILE:HD11	1.70	0.57
7:x:136:LEU:HD11	7:x:176:PHE:CZ	2.39	0.57
3:2:104:ILE:HG21	7:x:323:ARG:HE	1.68	0.56
12:d:41:VAL:C	12:d:44:PRO:HD2	2.30	0.56
16:h:51:ARG:NH2	49:s:226:GLU:O	2.33	0.56
16:h:81:ARG:HD2	20:m:111:GLU:CD	2.30	0.56
18:j:35:SER:O	32:I:98:ARG:NH2	2.37	0.56
20:m:8:ILE:O	20:m:12:ILE:HG13	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:151:MET:HG3	27:C:220:TYR:CE2	2.40	0.56
35:L:278:VAL:HG21	35:L:348:LEU:HD12	1.86	0.56
35:L:297:GLY:O	35:L:301:GLU:HG3	2.04	0.56
48:l:124:PHE:CD2	48:l:247:LEU:HD22	2.40	0.56
48:l:292:ALA:HB2	48:l:304:PHE:CB	2.34	0.56
48:l:292:ALA:HB2	48:l:304:PHE:HB3	1.87	0.56
51:u:42:LEU:HD22	51:u:426:LEU:HB3	1.86	0.56
51:u:274:GLU:HG3	51:u:276:ARG:HE	1.70	0.56
6:w:346:PRO:O	6:w:350:ILE:HG13	2.05	0.56
2:Ac:23:LEU:HD22	4:Ad:23:MET:HE3	1.87	0.56
53:G:221:ASN:ND2	53:G:285:TRP:HB3	2.19	0.56
1:0:53:CYS:O	1:0:57:VAL:HG23	2.04	0.56
5:6:165:ALA:O	5:6:168:ASN:ND2	2.37	0.56
9:a:170:GLN:HE21	9:a:170:GLN:HA	1.70	0.56
16:h:4:PHE:HE2	17:i:21:MET:HE2	1.70	0.56
20:m:126:VAL:O	45:W:120:MET:HE2	2.04	0.56
21:n:42:SER:O	21:n:46:LYS:HB2	2.04	0.56
24:q:104:LEU:HG	24:q:108:MET:HE2	1.87	0.56
25:r:306:SER:HB2	42:T:118:PRO:HG3	1.88	0.56
26:B:345:ALA:O	26:B:346:GLN:HB2	2.04	0.56
39:Q:46:ILE:CD1	39:Q:107:LEU:HD13	2.34	0.56
43:U:263:ARG:HD3	43:U:264:GLU:H	1.70	0.56
51:5:319:GLY:CA	3:Ae:58:ALA:HB3	2.35	0.56
4:3:8:PRO:HD2	8:9:111:LYS:HB3	1.86	0.56
16:h:18:MET:O	16:h:18:MET:HG2	2.04	0.56
17:i:152:ASN:O	17:i:156:THR:HG23	2.06	0.56
17:i:180:ALA:O	17:i:184:ILE:HG13	2.05	0.56
24:q:108:MET:HB3	24:q:121:LEU:CD1	2.35	0.56
24:q:271:MET:O	24:q:275:ILE:HG13	2.06	0.56
24:q:373:ILE:HD11	24:q:444:LEU:HG	1.87	0.56
25:r:31:MET:HG2	31:H:77:LEU:HB2	1.87	0.56
26:B:371:ILE:HD11	26:B:435:VAL:HG22	1.86	0.56
27:C:186:LEU:HB2	27:C:216:MET:HE1	1.86	0.56
28:D:100:LEU:HD13	28:D:141:ILE:HD11	1.88	0.56
29:E:188:ILE:O	29:E:189:ASN:C	2.48	0.56
44:V:41:ILE:HD12	44:V:46:PRO:HG3	1.87	0.56
49:s:95:VAL:HG12	49:s:97:VAL:HG22	1.87	0.56
51:u:311:ILE:HD12	51:u:375:GLN:HB3	1.86	0.56
6:w:129:MET:CE	6:w:185:LEU:HD12	2.33	0.56
8:y:55:LEU:HD22	8:y:88:LYS:HZ3	1.69	0.56
1:Ab:37:CYS:O	1:Ab:43:CYS:HB2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:G:355:LYS:HG3	53:G:366:LEU:CD1	2.35	0.56
53:G:575:VAL:C	53:G:578:PRO:HD2	2.30	0.56
15:g:27:LYS:HG2	15:g:29:THR:H	1.69	0.56
19:k:97:GLN:O	19:k:98:CYS:HB2	2.06	0.56
24:q:207:MET:HE1	24:q:297:VAL:HG12	1.88	0.56
35:L:82:GLU:HG2	35:L:83:PRO:HD2	1.87	0.56
37:O:85:TYR:O	37:O:89:LEU:HD13	2.06	0.56
6:w:138:MET:HE1	6:w:267:HIS:O	2.05	0.56
7:x:136:LEU:HD11	7:x:176:PHE:HZ	1.69	0.56
53:G:234:LYS:N	53:G:235:PRO:HD2	2.20	0.56
6:7:123:VAL:HG22	6:7:189:ILE:HD13	1.87	0.56
18:j:7:LEU:O	18:j:11:VAL:HG23	2.06	0.56
23:p:73:CYS:HA	23:p:78:LYS:HE2	1.86	0.56
27:C:149:SER:HA	27:C:184:THR:CG2	2.36	0.56
28:D:88:ILE:CD1	28:D:96:VAL:HG11	2.35	0.56
29:E:239:LYS:HE2	29:E:239:LYS:H	1.71	0.56
51:u:179:MET:HA	51:u:179:MET:HE2	1.86	0.56
6:w:344:GLU:O	6:w:348:ILE:HG13	2.05	0.56
7:x:126:HIS:CE1	57:x:401:HEC:NA	2.72	0.56
5:6:301:ARG:HD3	51:5:95:HIS:CE1	2.40	0.56
6:7:369:THR:O	6:7:373:GLU:HG3	2.06	0.56
24:q:106:LEU:HD13	24:q:234:VAL:HG11	1.88	0.56
29:E:186:VAL:HG22	29:E:196:LEU:CD1	2.35	0.56
37:O:144:ILE:O	37:O:148:ILE:HG13	2.05	0.56
39:Q:88:LYS:HD2	39:Q:133:PHE:CD2	2.40	0.56
3:4:288:SER:O	3:4:289:ASP:HB3	2.04	0.56
5:6:111:SER:OG	5:6:122:THR:HG23	2.05	0.56
23:p:123:ILE:HG22	23:p:127:SER:OG	2.05	0.56
25:r:126:LYS:O	25:r:130:ILE:HG13	2.05	0.56
25:r:264:LEU:HD11	41:S:13:ALA:HB2	1.87	0.56
26:B:384:PRO:HD2	53:G:76:ARG:HG3	1.88	0.56
39:Q:78:LEU:HD11	39:Q:129:ILE:HG21	1.86	0.56
39:Q:88:LYS:HD2	39:Q:133:PHE:CE2	2.41	0.56
37:X:83:VAL:HG13	37:X:122:MET:CE	2.36	0.56
51:u:328:LEU:HD11	51:u:368:MET:HE2	1.86	0.56
6:w:295:VAL:HG12	6:w:299:LEU:HD12	1.87	0.56
53:G:326:VAL:HG23	53:G:626:LEU:HD13	1.88	0.56
4:3:39:ARG:O	4:3:39:ARG:HG3	2.05	0.56
6:7:8:HIS:HB3	6:7:11:MET:HB2	1.88	0.56
6:7:24:PRO:O	6:7:27:ILE:HG23	2.06	0.56
6:7:53:MET:O	6:w:176:THR:HB	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:147:ALA:HB2	24:q:173:SER:HB2	1.87	0.56
17:i:31:ILE:HG21	20:m:156:VAL:HG11	1.86	0.56
17:i:44:LEU:HD22	17:i:122:ILE:HG21	1.87	0.56
18:j:38:GLU:HB3	18:j:41:PHE:O	2.06	0.56
26:B:60:GLY:HA2	29:E:241:PRO:HA	1.87	0.56
26:B:235:VAL:HG12	26:B:240:THR:OG1	2.06	0.56
30:F:30:ARG:O	30:F:38:VAL:HG12	2.05	0.56
35:L:267:LEU:HG	35:L:370:VAL:CG2	2.34	0.56
48:l:281:GLY:O	48:l:285:THR:HG23	2.06	0.56
5:v:134:MET:HG2	5:v:233:VAL:HG21	1.88	0.56
7:8:103:LEU:HD21	7:8:291:LEU:CB	2.31	0.56
9:a:139:ILE:HG23	24:q:54:LEU:HD23	1.88	0.56
11:c:140:MET:HG3	48:l:407:TRP:HZ3	1.70	0.56
16:h:17:TRP:CH2	16:h:18:MET:HE3	2.40	0.56
17:i:110:PRO:HG2	48:l:594:THR:HG21	1.87	0.56
17:i:211:MET:HG2	17:i:333:SER:HB2	1.88	0.56
22:o:29:THR:O	22:o:33:GLN:HG3	2.06	0.56
26:B:203:ALA:HB3	26:B:206:CYS:SG	2.45	0.56
35:L:127:ARG:HD2	35:L:129:TRP:CE2	2.41	0.56
48:l:231:PRO:O	48:l:234:PRO:HD2	2.06	0.56
51:u:146:LEU:O	51:u:150:ILE:HG13	2.06	0.56
5:v:177:LEU:HD11	5:v:272:VAL:HG22	1.86	0.56
5:v:351:ILE:HD12	5:v:448:PRO:HD2	1.88	0.56
6:w:344:GLU:HG3	52:z:67:PHE:HE1	1.70	0.56
51:5:140:LEU:HD22	51:5:237:VAL:HG12	1.88	0.56
6:7:337:TRP:CH2	6:7:350:ILE:HD13	2.37	0.56
14:f:55:TRP:CD1	15:g:68:THR:HG22	2.40	0.56
19:k:23:ARG:HG3	20:m:23:LYS:HD2	1.87	0.56
26:B:317:VAL:O	26:B:327:ILE:HG13	2.06	0.56
30:F:53:VAL:HG21	35:L:76:ILE:CD1	2.36	0.56
35:L:78:PRO:HB2	35:L:103:TRP:CG	2.40	0.56
35:L:127:ARG:HD2	35:L:129:TRP:CZ2	2.41	0.56
35:L:260:PHE:HA	35:L:330:LEU:CD2	2.36	0.56
51:u:388:VAL:O	51:u:392:LYS:HG3	2.05	0.56
5:v:168:ASN:HB2	5:v:170:GLN:OE1	2.07	0.56
52:Aa:20:SER:O	52:Aa:24:GLN:HG2	2.05	0.56
8:9:106:GLU:O	8:9:110:LYS:HG3	2.06	0.55
11:c:109:LEU:O	11:c:113:ILE:HG23	2.07	0.55
17:i:250:SER:O	17:i:259:GLY:HA3	2.05	0.55
18:j:2:ASN:O	18:j:6:THR:HG23	2.06	0.55
26:B:73:PRO:HG3	26:B:147:ARG:NH1	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:222:LYS:HA	26:B:379:CYS:SG	2.46	0.55
36:N:20:PRO:HB2	36:N:77:ILE:HD13	1.86	0.55
37:O:138:LEU:O	37:O:139:MET:HB2	2.06	0.55
41:S:69:ILE:HD13	49:s:148:PHE:CB	2.35	0.55
45:W:109:SER:O	49:s:79:PRO:HD2	2.05	0.55
5:v:409:PRO:O	5:v:413:LEU:HG	2.06	0.55
9:a:80:ILE:HB	9:a:81:PRO:HD3	1.89	0.55
9:a:179:ILE:HD11	16:h:41:ILE:CB	2.36	0.55
32:I:191:ARG:O	32:I:195:ARG:HG3	2.06	0.55
41:S:69:ILE:CD1	49:s:148:PHE:HB3	2.36	0.55
7:x:263:THR:O	7:x:267:VAL:HG23	2.06	0.55
53:G:498:GLN:HG3	53:G:499:ASN:N	2.21	0.55
17:i:40:MET:HE1	17:i:44:LEU:HD21	1.88	0.55
26:B:275:LEU:HD23	26:B:289:GLU:HB2	1.89	0.55
29:E:138:THR:HA	29:E:141:MET:HE2	1.88	0.55
35:L:58:GLY:O	35:L:62:ARG:HG3	2.05	0.55
37:O:84:LEU:O	37:O:88:LYS:HG3	2.05	0.55
37:O:120:MET:HA	37:O:123:GLU:OE2	2.07	0.55
5:v:70:ARG:HD2	5:v:117:GLU:HG2	1.88	0.55
7:x:115:PHE:CE2	7:x:119:LYS:HD2	2.41	0.55
9:a:115:HIS:CG	9:a:116:PRO:HD2	2.42	0.55
17:i:311:MET:HE3	17:i:314:LYS:HD3	1.88	0.55
26:B:332:CYS:HA	26:B:335:VAL:HG12	1.88	0.55
32:I:70:ALA:HB3	32:I:107:GLY:HA2	1.87	0.55
35:L:183:GLU:HG3	35:L:195:ILE:CD1	2.35	0.55
46:Y:61:PHE:CE2	48:l:455:LYS:HG2	2.41	0.55
50:t:39:MET:HG2	50:t:58:TYR:CD1	2.41	0.55
6:w:49:LEU:O	6:w:53:MET:HG3	2.06	0.55
53:G:450:LYS:NZ	53:G:450:LYS:HB3	2.21	0.55
5:6:39:GLU:O	5:6:50:ALA:HA	2.06	0.55
6:7:59:THR:CG2	6:7:172:LYS:HA	2.36	0.55
16:h:83:ARG:HB2	45:W:97:ILE:HD13	1.88	0.55
17:i:231:SER:O	17:i:234:TRP:HD1	1.89	0.55
20:m:24:PRO:HG3	20:m:83:TRP:CE2	2.41	0.55
20:m:63:GLY:O	20:m:66:VAL:HG22	2.07	0.55
23:p:81:TYR:O	23:p:85:LEU:HG	2.04	0.55
24:q:357:THR:O	24:q:361:MET:HG3	2.07	0.55
25:r:24:GLU:HA	25:r:271:LEU:HD13	1.87	0.55
25:r:209:SER:HB3	25:r:213:VAL:HA	1.87	0.55
26:B:136:HIS:O	26:B:140:GLU:HG2	2.06	0.55
26:B:205:ILE:HG12	26:B:379:CYS:SG	2.46	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:59:PHE:HB3	60:L:401:NDP:O1N	2.06	0.55
37:O:115:GLN:O	37:O:119:ILE:HG12	2.06	0.55
48:l:88:MET:C	48:l:91:PRO:HD2	2.32	0.55
6:w:31:TRP:NE1	56:w:401:HEM:O2D	2.40	0.55
7:8:223:PRO:HG3	1:Ab:68:THR:HG22	1.88	0.55
8:9:76:LEU:HG	8:9:77:PRO:HD2	1.87	0.55
11:c:65:TYR:CZ	11:c:77:LYS:HG2	2.42	0.55
24:q:403:THR:HA	24:q:406:TYR:CD2	2.40	0.55
25:r:139:THR:HA	25:r:142:TYR:CE2	2.41	0.55
26:B:201:ALA:O	29:E:119:TYR:HB3	2.06	0.55
27:C:150:MET:O	27:C:154:GLU:HG3	2.06	0.55
48:l:529:TYR:O	48:l:533:MET:HB2	2.07	0.55
51:5:42:LEU:HD22	51:5:426:LEU:HB3	1.88	0.55
11:c:165:ASP:O	11:c:170:ARG:NH1	2.40	0.55
13:e:75:GLY:O	13:e:76:TYR:HB2	2.06	0.55
17:i:18:MET:O	17:i:22:ILE:HB	2.07	0.55
26:B:426:ALA:HB3	58:B:501:FMN:C8M	2.35	0.55
29:E:133:GLN:HA	29:E:172:ILE:O	2.06	0.55
31:H:158:CYS:O	31:H:162:CYS:HB2	2.06	0.55
39:Q:109:VAL:HG12	39:Q:113:LYS:HE3	1.89	0.55
48:l:557:TRP:O	48:l:561:ILE:HG13	2.06	0.55
6:w:246:SER:HB2	6:w:249:LEU:HB2	1.88	0.55
6:7:186:PRO:HB3	56:7:401:HEM:CBB	2.37	0.55
17:i:41:ILE:HG21	19:k:73:LEU:CD2	2.31	0.55
27:C:202:ALA:O	27:C:203:MET:HB3	2.07	0.55
35:L:122:ILE:HG22	35:L:124:LEU:HD11	1.89	0.55
37:O:120:MET:HA	37:O:123:GLU:HG2	1.89	0.55
43:U:200:TYR:OH	43:U:306:VAL:HG13	2.06	0.55
51:u:102:LYS:HG2	51:u:153:ASN:HB3	1.88	0.55
6:w:104:TYR:CD1	6:w:208:PRO:HA	2.42	0.55
6:w:270:PRO:HG2	6:w:275:LEU:HD23	1.88	0.55
11:c:81:ARG:CD	22:o:13:THR:HG21	2.37	0.55
17:i:317:PHE:HZ	43:U:143:LEU:HD21	1.72	0.55
24:q:5:ILE:HG23	24:q:104:LEU:HD11	1.89	0.55
24:q:334:TYR:O	24:q:338:HIS:N	2.38	0.55
26:B:413:TRP:O	26:B:417:LYS:HG2	2.05	0.55
28:D:164:ASN:HA	28:D:181:HIS:CE1	2.41	0.55
37:O:72:PRO:N	37:O:73:PRO:HD3	2.22	0.55
6:w:8:HIS:CD2	6:w:9:PRO:HD2	2.42	0.55
6:w:150:LEU:HB2	6:w:161:VAL:HG22	1.88	0.55
52:Aa:79:GLU:O	52:Aa:80:ASN:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:p:154:LYS:HG2	23:p:161:PHE:CZ	2.42	0.55
24:q:282:LEU:O	24:q:286:ILE:HG13	2.07	0.55
26:B:174:ARG:CA	40:R:93:LEU:HD21	2.35	0.55
26:B:226:LYS:N	26:B:227:PRO:CD	2.70	0.55
26:B:278:ILE:HG21	26:B:304:ALA:CB	2.37	0.55
38:P:32:GLY:HA3	38:P:82:PHE:O	2.07	0.55
48:l:96:VAL:O	48:l:100:ILE:HG12	2.07	0.55
48:l:122:VAL:O	48:l:126:ILE:HG13	2.07	0.55
51:u:319:GLY:HA3	3:Af:58:ALA:HB3	1.88	0.55
6:w:35:SER:O	6:w:39:ILE:HG12	2.06	0.55
25:r:179:TRP:NE1	45:W:43:LEU:HG	2.22	0.54
26:B:41:ILE:HG22	26:B:253:THR:CG2	2.24	0.54
26:B:127:ASP:O	26:B:131:ILE:HG12	2.07	0.54
27:C:466:GLU:O	27:C:469:ARG:HG3	2.07	0.54
48:l:65:ASN:HD22	48:l:65:ASN:N	2.04	0.54
51:5:368:MET:CE	51:5:368:MET:HA	2.37	0.54
3:2:145:GLY:HA3	7:x:300:LEU:HD21	1.90	0.54
3:4:258:PRO:O	3:4:259:CYS:C	2.48	0.54
15:g:74:GLY:O	15:g:78:LEU:HG	2.07	0.54
16:h:27:HIS:CD2	20:m:141:MET:HE2	2.42	0.54
17:i:114:TRP:O	17:i:118:VAL:HG23	2.08	0.54
23:p:97:LYS:HB3	23:p:97:LYS:HZ2	1.72	0.54
24:q:12:LEU:HB2	24:q:13:PRO:HD3	1.89	0.54
24:q:196:TRP:HD1	24:q:250:LEU:HB3	1.72	0.54
24:q:216:LEU:HD23	24:q:287:ALA:HB1	1.87	0.54
30:F:59:GLN:HG2	34:K:122:GLN:HA	1.89	0.54
37:O:104:PHE:HB3	37:O:110:LEU:CD2	2.35	0.54
39:Q:99:VAL:HB	61:Q:201:ZMP:O3	2.07	0.54
39:Q:105:VAL:O	39:Q:109:VAL:HG23	2.07	0.54
48:l:257:VAL:O	48:l:261:ILE:HG13	2.07	0.54
5:v:309:LEU:HD23	5:v:357:GLN:HB3	1.88	0.54
7:x:126:HIS:CE1	7:x:196:PRO:HD2	2.42	0.54
8:y:58:ASP:O	8:y:62:ARG:HG3	2.07	0.54
51:5:388:VAL:HG21	51:5:438:ALA:HA	1.88	0.54
53:G:59:GLN:CG	53:G:62:ARG:HH12	2.20	0.54
3:4:145:GLY:HA3	7:8:300:LEU:HD21	1.88	0.54
5:6:220:LEU:C	5:6:221:ILE:HD12	2.32	0.54
12:d:140:GLN:HB2	22:o:127:ILE:HG22	1.89	0.54
16:h:15:ASP:HB3	17:i:28:LEU:CD1	2.36	0.54
20:m:126:VAL:HG13	45:W:122:GLY:HA3	1.88	0.54
24:q:294:MET:HE2	24:q:294:MET:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:334:ASP:OD1	31:H:42:ASN:ND2	2.39	0.54
29:E:140:CYS:SG	55:E:301:FES:S2	3.04	0.54
42:T:125:ASN:O	42:T:129:ARG:HG3	2.07	0.54
52:Aa:19:LEU:HD22	52:Aa:24:GLN:HB3	1.90	0.54
5:6:82:LEU:HD13	5:6:158:LEU:HD11	1.89	0.54
16:h:21:GLN:HB3	16:h:37:GLU:OE1	2.06	0.54
17:i:110:PRO:HG2	48:l:594:THR:CG2	2.37	0.54
18:j:65:PHE:HA	18:j:68:GLU:OE1	2.07	0.54
19:k:76:SER:O	19:k:79:VAL:HG12	2.07	0.54
22:o:25:ILE:CG2	51:u:261:ALA:HA	2.35	0.54
27:C:175:TRP:O	27:C:178:VAL:HG12	2.08	0.54
27:C:310:LYS:HD2	27:C:324:VAL:HG23	1.90	0.54
31:H:84:ILE:HD11	32:I:84:TYR:CE1	2.42	0.54
35:L:263:PRO:HG3	35:L:339:PRO:HA	1.90	0.54
43:U:110:LEU:HD13	43:U:336:LEU:CD1	2.19	0.54
48:l:324:LEU:HB3	48:l:395:ILE:CD1	2.38	0.54
48:l:324:LEU:HB3	48:l:395:ILE:HD11	1.89	0.54
48:l:417:SER:HB3	48:l:493:VAL:HG12	1.89	0.54
56:w:402:HEM:HBB2	56:w:402:HEM:CMB	2.37	0.54
56:7:402:HEM:HHA	56:7:402:HEM:HBD1	1.88	0.54
17:i:64:ALA:O	17:i:68:MET:HG2	2.08	0.54
25:r:8:SER:O	25:r:12:PRO:HD2	2.07	0.54
28:D:108:PHE:CD1	28:D:134:SER:HB2	2.43	0.54
28:D:210:LEU:HD21	39:Q:131:ARG:NH2	2.22	0.54
35:L:111:ILE:O	35:L:114:VAL:HG12	2.07	0.54
35:L:129:TRP:CG	35:L:307:PRO:HD2	2.43	0.54
35:L:274:TYR:HB2	35:L:367:ALA:HB2	1.89	0.54
38:P:65:LEU:O	38:P:76:ASN:HA	2.08	0.54
44:V:72:LEU:HD13	44:V:76:ILE:HD12	1.89	0.54
47:Z:100:ALA:O	47:Z:104:LEU:HG	2.08	0.54
51:u:102:LYS:HG3	51:u:103:ASN:N	2.21	0.54
5:v:85:LEU:HD12	5:v:158:LEU:CD1	2.36	0.54
5:v:121:TYR:HB3	5:v:137:LEU:HD11	1.90	0.54
6:w:32:ASN:O	6:w:36:LEU:HG	2.07	0.54
51:5:116:MET:SD	51:5:142:LYS:HG2	2.48	0.54
12:d:41:VAL:O	12:d:44:PRO:HD2	2.07	0.54
22:o:118:GLU:O	22:o:118:GLU:HG2	2.07	0.54
24:q:250:LEU:O	24:q:254:THR:OG1	2.24	0.54
24:q:306:PRO:HB2	48:l:72:GLN:HE22	1.72	0.54
24:q:405:LEU:HD11	48:l:173:LEU:HD13	1.90	0.54
48:l:241:THR:OG1	48:l:242:PRO:HD3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:562:LEU:CB	48:l:563:PRO:HD3	2.38	0.54
6:w:33:PHE:CE2	6:w:96:ILE:HD12	2.43	0.54
6:w:51:LEU:HD12	6:w:83:HIS:CD2	2.41	0.54
7:x:218:GLY:O	7:x:236:PRO:HD2	2.08	0.54
16:h:81:ARG:HD2	20:m:111:GLU:CG	2.38	0.54
18:j:37:TYR:OH	25:r:208:VAL:HG11	2.08	0.54
19:k:59:MET:HG3	19:k:60:PRO:CD	2.38	0.54
24:q:127:VAL:HB	24:q:128:PRO:HD3	1.90	0.54
25:r:85:MET:O	25:r:88:PRO:HD2	2.08	0.54
37:O:135:ALA:O	37:O:138:LEU:HB2	2.08	0.54
43:U:250:GLU:HG2	43:U:251:MET:N	2.21	0.54
47:Z:67:TRP:CH2	48:l:439:PRO:HA	2.43	0.54
52:z:20:SER:HB3	52:z:23:GLU:HG3	1.89	0.54
53:G:256:ALA:HB3	53:G:517:HIS:O	2.08	0.54
53:G:322:ALA:O	53:G:326:VAL:HG22	2.08	0.54
1:O:81:CYS:O	1:O:85:LYS:HG2	2.07	0.54
5:6:227:HIS:CD2	5:6:231:LYS:HD2	2.43	0.54
26:B:287:THR:HB	29:E:225:CYS:SG	2.48	0.54
28:D:153:ILE:O	28:D:178:PHE:HA	2.08	0.54
45:W:141:ILE:H	45:W:141:ILE:HD12	1.73	0.54
48:l:306:THR:HG22	48:l:336:LYS:CG	2.37	0.54
6:w:138:MET:HB2	6:w:255:ASN:ND2	2.23	0.54
3:4:152:ASN:O	3:4:156:GLN:HG3	2.08	0.54
5:6:168:ASN:HB2	5:6:170:GLN:HE22	1.73	0.54
16:h:4:PHE:CE2	17:i:21:MET:HE2	2.43	0.54
20:m:11:THR:O	20:m:15:ILE:HG13	2.08	0.54
24:q:36:LEU:HD23	24:q:39:LEU:HD12	1.89	0.54
26:B:210:THR:HG22	26:B:224:ARG:HD2	1.89	0.54
26:B:213:ILE:HG23	26:B:235:VAL:CA	2.38	0.54
29:E:44:THR:HB	29:E:45:PRO:HD2	1.89	0.54
42:T:151:VAL:O	49:s:207:LYS:NZ	2.32	0.54
44:V:121:THR:O	44:V:125:VAL:HG23	2.08	0.54
51:5:328:LEU:HD13	51:5:371:PHE:HB3	1.89	0.54
6:7:362:ILE:HA	6:7:366:MET:CE	2.38	0.54
10:b:21:ARG:HA	10:b:24:LYS:HG2	1.90	0.54
15:g:41:TYR:CE2	15:g:45:LEU:HD11	2.43	0.54
17:i:261:MET:HG3	17:i:262:PRO:HD3	1.90	0.54
41:S:37:ARG:HD2	41:S:48:MET:HG2	1.90	0.54
42:T:139:PRO:HD3	45:W:69:ILE:HD13	1.89	0.54
48:l:37:LYS:NZ	48:l:98:TRP:HE1	2.06	0.54
48:l:155:ILE:HD11	48:l:248:HIS:CE1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:201:ILE:HG22	48:l:266:LEU:HD11	1.90	0.54
2:l:43:ILE:O	2:l:47:ILE:HG13	2.08	0.53
3:2:217:ARG:NH1	3:2:275:ALA:O	2.39	0.53
3:4:225:ARG:HH22	3:4:278:ASN:HB3	1.73	0.53
11:c:86:ARG:HH12	11:c:99:LEU:HD12	1.73	0.53
11:c:184:TYR:CD1	50:t:36:GLU:HA	2.42	0.53
17:i:88:LYS:HD2	17:i:148:SER:HB3	1.90	0.53
25:r:134:ARG:HH22	25:r:206:GLU:CD	2.16	0.53
26:B:222:LYS:HG2	26:B:379:CYS:SG	2.48	0.53
26:B:317:VAL:HG22	26:B:356:VAL:HG22	1.91	0.53
26:B:332:CYS:HA	26:B:335:VAL:CG1	2.38	0.53
26:B:364:VAL:HB	26:B:449:ARG:HH12	1.73	0.53
27:C:284:VAL:HG13	27:C:444:MET:HG2	1.90	0.53
48:l:65:ASN:ND2	48:l:78:LEU:HB3	2.23	0.53
48:l:264:TYR:N	48:l:265:PRO:HD2	2.23	0.53
5:v:47:LEU:HD11	5:v:238:LEU:HD13	1.89	0.53
5:v:125:CYS:HB3	5:v:133:LEU:HD22	1.90	0.53
6:w:48:GLY:HA3	56:w:402:HEM:C3C	2.42	0.53
53:G:35:PHE:O	53:G:101:ASN:HA	2.08	0.53
5:6:259:ARG:HB3	5:6:444:LEU:HD13	1.89	0.53
5:6:262:ASN:OD1	5:6:442:GLY:HA2	2.09	0.53
14:f:55:TRP:NE1	15:g:68:THR:HG22	2.23	0.53
27:C:354:LEU:O	45:W:11:PRO:HG3	2.09	0.53
34:K:8:ARG:O	34:K:12:GLN:HG3	2.08	0.53
35:L:234:PRO:O	35:L:262:GLY:HA3	2.08	0.53
6:w:314:SER:O	6:w:318:ARG:HD3	2.08	0.53
6:w:337:TRP:O	6:w:341:GLN:HG2	2.09	0.53
53:G:47:THR:O	53:G:96:VAL:HG22	2.07	0.53
53:G:76:ARG:NH2	53:G:90:ALA:HB2	2.23	0.53
7:8:122:CYS:SG	7:8:198:LEU:HD12	2.49	0.53
8:9:14:LEU:CD2	8:9:17:ILE:HD11	2.38	0.53
13:e:91:PHE:HA	13:e:95:PHE:CD2	2.43	0.53
19:k:76:SER:OG	20:m:172:THR:HG23	2.08	0.53
19:k:80:MET:HE2	19:k:80:MET:HA	1.89	0.53
24:q:257:MET:O	24:q:260:PRO:HD2	2.08	0.53
26:B:210:THR:CG2	26:B:224:ARG:HB2	2.38	0.53
26:B:319:PRO:HG3	26:B:347:THR:CB	2.35	0.53
27:C:204:THR:HG22	27:C:208:TRP:CE2	2.43	0.53
32:I:67:PHE:CZ	32:I:69:LEU:HD21	2.43	0.53
35:L:215:MET:HE2	35:L:221:VAL:HG13	1.89	0.53
5:v:90:THR:HG23	5:v:95:SER:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:w:338:ILE:HD11	6:w:350:ILE:CG2	2.33	0.53
1:Ab:37:CYS:SG	1:Ab:78:ARG:HG3	2.48	0.53
3:2:194:PRO:HG2	3:2:236:GLY:HA3	1.90	0.53
5:6:233:VAL:HG22	5:6:236:ARG:HH12	1.73	0.53
6:7:21:LEU:HD12	6:7:22:PRO:HD2	1.90	0.53
7:8:118:TYR:HA	7:8:122:CYS:HB3	1.89	0.53
7:8:315:LEU:O	7:8:318:ARG:HB3	2.09	0.53
15:g:12:PRO:HD3	16:h:8:LYS:HZ1	1.73	0.53
18:j:67:LEU:HD22	19:k:65:VAL:HA	1.90	0.53
20:m:27:ILE:O	20:m:31:LEU:HG	2.08	0.53
24:q:233:ALA:HA	24:q:320:GLY:HA2	1.90	0.53
24:q:457:PRO:HG2	24:q:458:LEU:HD12	1.90	0.53
26:B:170:GLN:HG3	40:R:86:PHE:CD1	2.43	0.53
26:B:339:PHE:CE1	26:B:349:LEU:HD23	2.44	0.53
26:B:455:LEU:O	26:B:458:GLN:HG3	2.08	0.53
35:L:222:PRO:HB3	35:L:286:TYR:CZ	2.44	0.53
53:G:217:GLU:OE2	53:G:409:PHE:HD1	1.92	0.53
2:1:17:ARG:HD3	2:1:20:THR:HG23	1.91	0.53
5:6:111:SER:HB3	3:Ae:59:LEU:CG	2.38	0.53
6:7:214:ASP:HB3	52:Aa:9:THR:HB	1.91	0.53
6:7:217:LYS:HG3	52:Aa:8:LEU:HD13	1.90	0.53
6:7:218:ILE:HD11	6:7:224:TYR:CE2	2.43	0.53
6:7:270:PRO:HD2	6:7:275:LEU:CD2	2.37	0.53
31:H:135:ARG:NH2	31:H:141:ARG:HG3	2.23	0.53
51:u:206:GLU:CD	51:u:206:GLU:H	2.17	0.53
51:u:390:ARG:O	51:u:394:ILE:HG13	2.09	0.53
3:2:235:ILE:CG2	3:2:280:GLU:HB3	2.39	0.53
6:7:47:THR:HG23	6:7:79:ILE:CG2	2.35	0.53
7:8:310:HIS:O	52:Aa:21:PRO:HB3	2.08	0.53
9:a:115:HIS:O	9:a:119:ARG:HG3	2.08	0.53
12:d:40:LEU:O	12:d:44:PRO:HG2	2.08	0.53
14:f:55:TRP:O	14:f:59:ILE:HG13	2.08	0.53
23:p:141:VAL:HG13	23:p:142:PRO:HD2	1.91	0.53
24:q:128:PRO:O	24:q:132:ILE:HG13	2.09	0.53
25:r:200:LEU:HD13	25:r:282:TYR:HB3	1.90	0.53
26:B:102:MET:HE1	26:B:240:THR:C	2.34	0.53
6:w:59:THR:HG23	6:w:172:LYS:HA	1.90	0.53
6:w:368:ILE:O	6:w:372:ILE:HG13	2.08	0.53
2:1:30:LEU:HD11	4:3:42:LEU:HD21	1.91	0.53
5:6:190:LEU:CD1	3:Ae:64:GLU:HG3	2.38	0.53
16:h:27:HIS:NE2	20:m:141:MET:HE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:163:ILE:O	20:m:167:VAL:HG23	2.09	0.53
24:q:333:ASN:O	24:q:337:VAL:HG22	2.09	0.53
27:C:389:LYS:HG3	53:G:144:MET:HG3	1.90	0.53
28:D:204:LEU:HD12	28:D:205:SER:N	2.24	0.53
51:u:83:ASN:OD1	51:u:85:LYS:HG3	2.09	0.53
51:u:360:CYS:SG	51:u:365:ILE:HG12	2.48	0.53
5:v:61:ILE:HD12	5:v:130:ILE:HD12	1.90	0.53
53:G:534:VAL:HG22	53:G:534:VAL:O	2.09	0.53
16:h:26:PRO:CD	19:k:55:LEU:HD13	2.39	0.53
17:i:93:VAL:HG13	48:l:599:MET:CE	2.32	0.53
18:j:63:LEU:HD22	20:m:63:GLY:HA2	1.91	0.53
24:q:11:LEU:HB3	24:q:100:ILE:HD13	1.90	0.53
24:q:216:LEU:CD2	24:q:287:ALA:HB1	2.39	0.53
26:B:71:LYS:HB2	26:B:71:LYS:HZ3	1.74	0.53
26:B:88:ARG:HD2	26:B:274:LYS:HE2	1.91	0.53
27:C:143:ASP:OD1	27:C:143:ASP:N	2.40	0.53
35:L:201:ILE:CG2	35:L:237:ILE:HA	2.39	0.53
35:L:275:ILE:HG23	35:L:348:LEU:HD11	1.90	0.53
43:U:148:ALA:CB	43:U:159:VAL:HG11	2.37	0.53
48:l:243:VAL:O	48:l:247:LEU:HG	2.08	0.53
48:l:319:ILE:HG22	48:l:319:ILE:O	2.08	0.53
51:5:95:HIS:HB3	51:5:164:GLU:HG3	1.91	0.53
53:G:569:GLN:NE2	53:G:619:ASP:HB3	2.24	0.53
5:6:293:LEU:HD21	5:6:361:ILE:HD12	1.91	0.53
12:d:162:ARG:O	12:d:166:GLU:HG3	2.09	0.53
16:h:16:ARG:HA	16:h:19:THR:HG23	1.90	0.53
24:q:361:MET:HB2	24:q:441:ILE:CD1	2.39	0.53
26:B:292:MET:HE1	26:B:349:LEU:CD2	2.39	0.53
28:D:216:VAL:HG13	28:D:218:ARG:HB3	1.91	0.53
29:E:148:ILE:O	29:E:152:ILE:HG13	2.09	0.53
31:H:83:THR:HG22	32:I:82:PRO:O	2.09	0.53
32:I:85:ASP:OD2	32:I:88:ARG:HG3	2.09	0.53
34:K:44:TYR:HE2	34:K:83:PRO:HB3	1.73	0.53
48:l:230:HIS:N	48:l:231:PRO:CD	2.72	0.53
48:l:366:MET:HA	48:l:445:GLU:OE1	2.09	0.53
48:l:417:SER:HB3	48:l:493:VAL:CG1	2.39	0.53
52:Aa:15:ILE:HA	51:5:276:ARG:O	2.08	0.53
51:5:429:TRP:O	51:5:433:ILE:HG13	2.09	0.53
51:5:440:VAL:O	51:5:444:VAL:HG23	2.09	0.53
5:6:104:GLU:OE2	51:5:324:MET:HG3	2.09	0.53
5:6:125:CYS:SG	5:6:130:ILE:HA	2.49	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:69:ILE:HA	6:7:73:VAL:CG2	2.39	0.53
6:7:119:LEU:O	6:7:123:VAL:HG23	2.09	0.53
21:n:29:ARG:O	21:n:33:GLU:HG3	2.09	0.53
25:r:205:SER:OG	25:r:279:ARG:NH1	2.34	0.53
27:C:103:LEU:HD11	27:C:115:CYS:SG	2.48	0.53
34:K:42:ASP:OD1	34:K:46:ASN:N	2.42	0.53
35:L:349:ARG:HA	35:L:352:ARG:HD3	1.91	0.53
37:O:104:PHE:HB3	37:O:110:LEU:CG	2.38	0.53
38:P:68:ARG:HH11	53:G:359:ASN:HD21	1.57	0.53
48:l:297:ASP:O	48:l:301:ILE:HG13	2.09	0.53
51:u:145:GLU:HG2	51:u:249:HIS:NE2	2.23	0.53
7:x:144:GLU:O	7:x:147:LYS:HG2	2.08	0.53
8:y:55:LEU:HD22	8:y:88:LYS:NZ	2.24	0.53
53:G:347:ASP:CB	53:G:594:ALA:HB1	2.38	0.53
53:G:473:MET:HE2	53:G:475:VAL:HG22	1.91	0.53
5:6:407:VAL:CG1	5:6:411:THR:HB	2.39	0.52
5:6:421:ASP:N	5:6:421:ASP:OD1	2.43	0.52
16:h:74:LYS:HB2	16:h:74:LYS:NZ	2.24	0.52
17:i:186:HIS:O	17:i:190:MET:HG3	2.09	0.52
26:B:170:GLN:HE22	40:R:93:LEU:HD12	1.74	0.52
27:C:344:ARG:HB3	45:W:21:TYR:O	2.09	0.52
35:L:52:THR:CG2	35:L:114:VAL:HG22	2.39	0.52
35:L:301:GLU:OE2	35:L:311:ARG:HD3	2.09	0.52
46:Y:65:MET:O	46:Y:69:ILE:HG13	2.10	0.52
51:u:388:VAL:HG21	51:u:438:ALA:HA	1.90	0.52
5:v:326:PHE:HD2	3:Af:66:PRO:O	1.92	0.52
6:w:51:LEU:HG	6:w:79:ILE:HG22	1.91	0.52
6:w:239:LEU:O	6:w:243:VAL:HG23	2.09	0.52
51:5:300:ASP:C	51:5:303:PRO:HD2	2.34	0.52
3:2:216:LEU:HD13	3:2:269:ARG:HD2	1.90	0.52
3:4:244:VAL:HG23	6:w:264:THR:HG23	1.91	0.52
6:7:226:ILE:HG23	7:8:308:LYS:HG3	1.91	0.52
11:c:101:TRP:CD1	22:o:47:TYR:HB2	2.44	0.52
13:e:57:GLU:OE1	43:U:328:ARG:HD3	2.09	0.52
15:g:32:ARG:HB3	17:i:339:MET:HE1	1.92	0.52
18:j:44:MET:HE1	27:C:102:ARG:HH21	1.74	0.52
20:m:14:VAL:O	20:m:18:VAL:HG23	2.10	0.52
24:q:8:THR:O	24:q:11:LEU:HB2	2.10	0.52
24:q:369:LEU:HD13	48:l:149:ILE:HG13	1.91	0.52
31:H:101:HIS:CD2	59:H:301:SF4:S3	3.02	0.52
31:H:211:TYR:CZ	54:M:39:PRO:HG3	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:65:MET:HE1	32:I:120:VAL:CG1	2.38	0.52
43:U:88:PHE:CD1	43:U:159:VAL:HG13	2.44	0.52
46:Y:39:HIS:C	46:Y:40:ILE:HD12	2.34	0.52
46:Y:44:TYR:HD2	47:Z:33:PRO:HD2	1.74	0.52
48:l:368:PHE:HE2	48:l:454:ILE:HB	1.74	0.52
6:w:303:LEU:HD22	6:w:306:MET:CE	2.39	0.52
56:w:402:HEM:HBC2	56:w:402:HEM:CMC	2.35	0.52
53:G:638:THR:O	53:G:642:VAL:HG23	2.08	0.52
3:2:173:ILE:HD11	3:2:195:LEU:CD2	2.39	0.52
3:4:127:SER:O	3:4:131:ARG:HG3	2.08	0.52
3:4:190:TRP:CZ2	3:4:295:GLY:HA2	2.44	0.52
5:6:209:VAL:O	5:6:213:PHE:HB2	2.09	0.52
20:m:45:LEU:HD22	20:m:50:SER:CA	2.22	0.52
23:p:106:LEU:HD22	23:p:110:GLU:OE1	2.10	0.52
24:q:77:LEU:O	24:q:81:GLN:HG3	2.09	0.52
24:q:244:MET:HE3	24:q:309:PHE:CD2	2.44	0.52
25:r:259:PHE:O	25:r:263:THR:HG23	2.09	0.52
27:C:224:SER:CB	27:C:230:ALA:HB1	2.39	0.52
27:C:262:ASP:CG	27:C:344:ARG:HH22	2.17	0.52
32:I:98:ARG:HA	32:I:125:PRO:CD	2.39	0.52
39:Q:47:PHE:CE2	39:Q:110:ILE:HD11	2.44	0.52
39:Q:56:ARG:O	39:Q:60:GLU:HG3	2.09	0.52
42:T:138:TYR:CD1	42:T:139:PRO:HD2	2.44	0.52
44:V:96:ALA:O	44:V:100:THR:HG23	2.09	0.52
48:l:482:MET:SD	48:l:487:LYS:HG2	2.49	0.52
6:w:138:MET:HB2	6:w:255:ASN:HD22	1.74	0.52
7:x:291:LEU:HD11	7:x:295:MET:HE3	1.90	0.52
52:z:19:LEU:HD22	52:z:23:GLU:HB2	1.91	0.52
5:6:414:GLN:HA	5:6:417:ASP:OD2	2.09	0.52
6:7:314:SER:O	6:7:318:ARG:HD3	2.10	0.52
14:f:48:LEU:O	14:f:52:VAL:HG23	2.09	0.52
14:f:62:HIS:O	14:f:66:VAL:HG23	2.09	0.52
24:q:30:HIS:O	24:q:34:ILE:HG13	2.09	0.52
30:F:53:VAL:HG21	35:L:76:ILE:HD13	1.90	0.52
31:H:128:ILE:HD11	59:H:301:SF4:S3	2.49	0.52
35:L:164:HIS:HA	60:L:401:NDP:H5N	1.92	0.52
5:v:231:LYS:HB2	5:v:231:LYS:NZ	2.23	0.52
53:G:450:LYS:HB3	53:G:450:LYS:HZ3	1.74	0.52
17:i:183:SER:O	17:i:187:MET:HG2	2.09	0.52
22:o:33:GLN:OE1	23:p:51:TYR:HB3	2.08	0.52
26:B:58:SER:O	29:E:241:PRO:HD3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:167:ILE:HD12	27:C:369:VAL:HG21	1.91	0.52
28:D:103:HIS:HB2	28:D:107:GLN:HG2	1.91	0.52
37:O:133:ILE:HD13	37:O:133:ILE:N	2.25	0.52
51:u:317:THR:CB	3:Af:53:VAL:HG13	2.40	0.52
5:v:89:LEU:HD22	5:v:150:GLU:HB3	1.91	0.52
5:v:295:ALA:C	3:Af:46:LEU:HD13	2.34	0.52
5:v:320:PRO:HB3	3:Af:75:LEU:CB	2.40	0.52
5:6:257:GLU:OE1	5:6:450:VAL:HG22	2.10	0.52
7:8:216:LEU:HB3	7:8:249:ILE:HD11	1.92	0.52
24:q:96:ILE:O	24:q:100:ILE:HG13	2.08	0.52
26:B:297:LYS:HB2	26:B:311:TRP:CH2	2.45	0.52
27:C:126:THR:O	27:C:130:ILE:HG13	2.10	0.52
27:C:143:ASP:OD1	27:C:154:GLU:HG2	2.10	0.52
27:C:368:LYS:HG2	27:C:386:HIS:HE1	1.75	0.52
33:J:77:VAL:HG22	33:J:99:MET:HG2	1.90	0.52
35:L:206:ASP:CG	35:L:208:PHE:H	2.18	0.52
39:Q:54:ALA:O	39:Q:58:VAL:HG23	2.09	0.52
47:Z:49:GLN:HE22	47:Z:59:ASP:HB3	1.75	0.52
51:u:221:SER:O	51:u:225:LYS:HD3	2.08	0.52
5:v:61:ILE:HG12	5:v:225:VAL:HG21	1.91	0.52
6:w:307:LEU:HD11	6:w:363:LEU:HD23	1.91	0.52
5:6:89:LEU:HD22	5:6:150:GLU:HB3	1.92	0.52
6:7:25:SER:HB2	6:7:218:ILE:HG23	1.90	0.52
7:8:136:LEU:HD22	7:8:140:CYS:SG	2.50	0.52
17:i:243:LEU:O	17:i:247:THR:HG23	2.10	0.52
26:B:102:MET:CE	26:B:231:ALA:HA	2.39	0.52
26:B:122:PRO:HB2	26:B:322:SER:OG	2.09	0.52
28:D:119:VAL:HG11	28:D:122:ARG:HD2	1.92	0.52
31:H:88:PHE:CE2	34:K:30:ALA:HA	2.43	0.52
39:Q:48:SER:HB2	39:Q:53:GLU:HB3	1.91	0.52
39:Q:124:LYS:NZ	39:Q:128:HIS:HB3	2.25	0.52
42:T:97:ALA:HB1	42:T:105:VAL:CG2	2.40	0.52
5:v:165:ALA:O	5:v:168:ASN:ND2	2.43	0.52
6:w:139:SER:H	6:w:255:ASN:ND2	2.07	0.52
6:w:196:HIS:HE1	56:w:401:HEM:ND	2.07	0.52
7:8:160:ASN:O	7:x:184:GLU:HG2	2.09	0.52
16:h:65:GLU:HB2	16:h:71:LYS:HZ1	1.73	0.52
19:k:6:MET:HB2	20:m:119:PHE:CD1	2.44	0.52
24:q:194:PHE:CZ	44:V:124:LEU:HD21	2.45	0.52
34:K:78:ASP:OD1	34:K:81:MET:HG3	2.10	0.52
37:X:114:ASP:O	37:X:118:ILE:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:114:ARG:HA	50:t:114:ARG:NE	2.25	0.52
51:u:134:LYS:HE3	5:v:384:MET:HE3	1.91	0.52
5:v:142:ALA:C	5:v:144:PRO:HD3	2.34	0.52
6:w:138:MET:HE2	6:w:254:ASP:CB	2.38	0.52
57:x:401:HEC:HMC1	57:x:401:HEC:CBC	2.39	0.52
51:5:396:ARG:O	51:5:400:VAL:HG13	2.10	0.52
53:G:341:ILE:HD13	53:G:367:CYS:HB2	1.92	0.52
17:i:268:GLN:HA	24:q:165:VAL:CG1	2.33	0.52
24:q:171:THR:HG22	24:q:184:HIS:HE1	1.74	0.52
26:B:328:PRO:HD3	26:B:441:HIS:CG	2.44	0.52
35:L:319:MET:HE1	35:L:322:MET:HE3	1.91	0.52
46:Y:87:PRO:HB3	50:t:100:LYS:HG2	1.92	0.52
48:l:94:LEU:HD23	48:l:125:LEU:HD21	1.92	0.52
48:l:315:VAL:O	48:l:319:ILE:HG12	2.09	0.52
5:v:180:ALA:HB1	5:v:256:GLY:O	2.10	0.52
6:w:253:PRO:HD2	7:x:206:HIS:CE1	2.45	0.52
6:w:281:LEU:HD12	6:w:290:GLY:C	2.35	0.52
6:w:303:LEU:HD22	6:w:306:MET:HE1	1.92	0.52
18:j:106:TRP:CE2	25:r:291:LYS:HD2	2.45	0.52
24:q:289:SER:HB2	24:q:406:TYR:OH	2.10	0.52
27:C:299:LEU:O	27:C:304:ILE:HG23	2.09	0.52
28:D:201:ASP:OD1	28:D:201:ASP:N	2.41	0.52
32:I:51:ASP:HA	32:I:54:VAL:HG22	1.91	0.52
33:J:86:ASN:HB3	53:G:224:ASP:OD2	2.10	0.52
43:U:291:ARG:HH22	43:U:294:HIS:HD2	1.58	0.52
44:V:103:ALA:O	44:V:106:ARG:HD3	2.10	0.52
5:v:106:VAL:HG21	5:v:133:LEU:CD1	2.40	0.52
8:y:76:LEU:HG	8:y:77:PRO:HD2	1.92	0.52
51:5:141:PRO:HA	51:5:245:LEU:HD13	1.91	0.52
17:i:321:LYS:O	17:i:321:LYS:HD3	2.10	0.51
24:q:375:LEU:HG	24:q:375:LEU:O	2.09	0.51
25:r:20:LEU:HD13	41:S:12:MET:HE1	1.93	0.51
25:r:31:MET:HE1	25:r:272:TRP:HA	1.92	0.51
27:C:91:GLY:HA3	27:C:101:LEU:O	2.10	0.51
27:C:172:ARG:O	27:C:176:ILE:HG13	2.10	0.51
54:M:46:SER:O	54:M:52:ASN:ND2	2.42	0.51
3:Ae:49:PHE:O	3:Ae:50:CYS:C	2.53	0.51
9:a:181:HIS:CD2	16:h:38:LYS:HD2	2.44	0.51
27:C:145:LEU:HD13	27:C:430:ILE:HG21	1.91	0.51
29:E:100:LYS:O	29:E:104:ILE:HG13	2.11	0.51
35:L:215:MET:CE	35:L:221:VAL:HG13	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:54:PHE:CD1	48:l:58:GLY:HA2	2.46	0.51
48:l:372:ALA:HA	48:l:458:LEU:HD21	1.92	0.51
5:v:70:ARG:O	5:v:185:ALA:CB	2.57	0.51
5:v:295:ALA:HA	3:Af:46:LEU:HD22	1.92	0.51
2:Ac:30:LEU:HG	4:Ad:34:TRP:HB2	1.92	0.51
3:Af:65:SER:HB3	3:Af:66:PRO:HD2	1.90	0.51
5:6:322:ASP:OD2	3:Ae:72:ARG:HB2	2.09	0.51
9:a:185:THR:H	16:h:30:PRO:HD3	1.75	0.51
12:d:98:VAL:O	12:d:102:ILE:HG13	2.10	0.51
15:g:77:LEU:HD12	15:g:77:LEU:O	2.10	0.51
16:h:101:LYS:HE3	16:h:101:LYS:CA	2.41	0.51
17:i:68:MET:SD	19:k:37:MET:HE2	2.51	0.51
28:D:88:ILE:HD11	28:D:96:VAL:HG11	1.91	0.51
28:D:168:ARG:HB2	28:D:187:ILE:HD11	1.92	0.51
31:H:196:LYS:HD2	31:H:197:TRP:NE1	2.25	0.51
43:U:213:VAL:HG12	43:U:217:GLN:HE21	1.75	0.51
48:l:488:MET:O	48:l:492:ILE:HG13	2.09	0.51
50:t:39:MET:HE1	50:t:41:ALA:HB3	1.91	0.51
51:u:142:LYS:O	51:u:146:LEU:HG	2.10	0.51
5:v:134:MET:SD	5:v:233:VAL:HG11	2.50	0.51
51:5:38:TYR:CZ	51:5:42:LEU:HD11	2.45	0.51
7:8:310:HIS:CE1	52:Aa:21:PRO:HB2	2.45	0.51
12:d:99:ASP:O	12:d:103:VAL:HG23	2.10	0.51
12:d:146:LEU:HD21	12:d:155:CYS:HB2	1.93	0.51
24:q:318:ALA:CB	24:q:373:ILE:HG13	2.41	0.51
25:r:215:TYR:HD2	25:r:219:PRO:HB2	1.76	0.51
27:C:448:HIS:HB3	27:C:452:ASP:CB	2.40	0.51
28:D:68:ILE:HD13	36:N:44:TYR:HA	1.93	0.51
48:l:188:TRP:CZ2	48:l:209:PRO:HG2	2.44	0.51
7:x:168:ARG:CG	7:x:169:PRO:HD2	2.40	0.51
3:4:196:PHE:O	3:4:233:ILE:HA	2.11	0.51
56:7:402:HEM:HBA1	56:7:402:HEM:CHA	2.40	0.51
10:b:14:GLN:OE1	23:p:206:PRO:HG3	2.11	0.51
11:c:169:GLU:OE2	50:t:43:GLN:HG3	2.11	0.51
18:j:44:MET:HG3	39:Q:122:VAL:CG2	2.40	0.51
18:j:109:LYS:HE2	18:j:109:LYS:HA	1.93	0.51
19:k:44:SER:O	19:k:48:ILE:HG12	2.10	0.51
25:r:238:THR:OG1	25:r:266:LEU:HD13	2.11	0.51
27:C:261:ILE:HD11	27:C:340:VAL:HG13	1.91	0.51
31:H:196:LYS:HD3	34:K:113:HIS:CE1	2.45	0.51
37:O:83:VAL:HG13	37:O:122:MET:CE	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:S:16:LEU:C	41:S:19:PRO:HD2	2.35	0.51
48:l:347:ILE:HD13	48:l:354:GLN:HG2	1.92	0.51
51:u:445:CYS:O	51:u:449:PHE:HB2	2.11	0.51
5:v:174:LEU:HD11	3:Af:67:VAL:HB	1.93	0.51
53:G:360:ARG:HD2	53:G:632:MET:HB3	1.93	0.51
3:2:222:ASP:O	3:2:226:VAL:HG22	2.11	0.51
6:7:137:GLN:HE22	6:7:260:ASN:HB3	1.74	0.51
6:7:218:ILE:HD11	6:7:224:TYR:CD2	2.45	0.51
7:8:265:SER:OG	1:Ab:90:LEU:HD11	2.10	0.51
7:8:315:LEU:HB3	8:9:71:MET:SD	2.51	0.51
11:c:101:TRP:CZ3	22:o:62:ASP:HA	2.45	0.51
18:j:93:PHE:CZ	18:j:97:LEU:HD11	2.45	0.51
35:L:60:LEU:CD2	35:L:124:LEU:HD23	2.41	0.51
35:L:203:GLY:N	35:L:206:ASP:HB2	2.26	0.51
37:O:131:PRO:HB2	37:O:133:ILE:CD1	2.41	0.51
39:Q:101:ASP:O	39:Q:105:VAL:HG23	2.10	0.51
44:V:140:LYS:HD3	44:V:141:VAL:N	2.26	0.51
5:v:257:GLU:HA	5:v:438:MET:O	2.09	0.51
53:G:569:GLN:HE21	53:G:619:ASP:HB3	1.75	0.51
3:Ae:48:PRO:O	3:Ae:64:GLU:N	2.42	0.51
6:7:278:TYR:O	6:7:282:ARG:HG3	2.09	0.51
8:9:13:TRP:CG	8:9:14:LEU:N	2.79	0.51
11:c:70:MET:HE3	22:o:86:THR:HG22	1.91	0.51
11:c:115:ASN:HA	48:l:166:THR:HG22	1.93	0.51
15:g:46:ILE:O	15:g:50:ILE:HG13	2.10	0.51
20:m:61:LEU:O	25:r:114:TYR:OH	2.20	0.51
24:q:290:SER:HA	24:q:319:HIS:NE2	2.26	0.51
27:C:149:SER:HA	27:C:184:THR:HG22	1.91	0.51
27:C:175:TRP:HA	27:C:178:VAL:HG12	1.91	0.51
27:C:196:HIS:O	27:C:200:ILE:HG12	2.10	0.51
41:S:14:ALA:O	41:S:18:ILE:HG13	2.11	0.51
48:l:233:LEU:HB3	48:l:234:PRO:HD3	1.93	0.51
48:l:289:ALA:HB1	48:l:418:LEU:HB2	1.93	0.51
49:s:147:PHE:CZ	49:s:151:ILE:HD11	2.46	0.51
51:u:304:LEU:HD13	51:u:354:LEU:HD22	1.91	0.51
5:v:392:PHE:O	5:v:396:VAL:HG23	2.11	0.51
53:G:241:ARG:HG2	53:G:243:TRP:CH2	2.46	0.51
3:2:225:ARG:NH2	3:2:278:ASN:HB3	2.25	0.51
5:6:180:ALA:HB2	5:6:258:ILE:HG13	1.91	0.51
6:7:348:ILE:O	6:7:352:GLN:HG3	2.11	0.51
9:a:156:VAL:HG21	15:g:92:MET:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:242:SER:O	17:i:246:VAL:HG23	2.10	0.51
24:q:1:MET:CE	24:q:111:THR:HG21	2.40	0.51
26:B:154:ALA:HB2	26:B:193:PHE:CZ	2.45	0.51
26:B:225:LEU:HB2	33:J:160:TYR:CE2	2.45	0.51
26:B:388:GLY:O	26:B:392:MET:HG3	2.10	0.51
26:B:405:ARG:HH22	54:M:49:LEU:HD11	1.76	0.51
27:C:143:ASP:HB2	27:C:144:ARG:HH11	1.76	0.51
35:L:110:SER:O	35:L:113:LYS:HG2	2.10	0.51
37:O:133:ILE:O	37:O:137:LYS:HG2	2.10	0.51
6:w:65:SER:O	6:w:69:ILE:HG13	2.09	0.51
52:z:4:GLU:O	52:z:8:LEU:HG	2.10	0.51
51:5:373:GLN:O	51:5:377:MET:HG2	2.10	0.51
3:Ae:40:VAL:HG22	3:Ae:42:CYS:H	1.75	0.51
6:7:49:LEU:O	6:7:53:MET:HG3	2.10	0.51
12:d:169:ALA:O	12:d:171:LYS:HG3	2.10	0.51
17:i:313:MET:HE3	43:U:96:ALA:HB2	1.93	0.51
19:k:37:MET:HG3	19:k:67:ALA:HB1	1.91	0.51
26:B:284:HIS:ND1	29:E:228:ALA:HB3	2.26	0.51
27:C:151:MET:HG3	27:C:220:TYR:CZ	2.45	0.51
27:C:285:THR:HA	36:N:12:VAL:HG23	1.93	0.51
28:D:61:PHE:HZ	28:D:106:ALA:HB2	1.74	0.51
48:l:173:LEU:O	48:l:177:ILE:HG13	2.11	0.51
48:l:280:LEU:O	48:l:284:THR:HG23	2.10	0.51
51:u:384:THR:O	51:u:388:VAL:HG23	2.11	0.51
5:6:90:THR:HG23	5:6:95:SER:HA	1.93	0.51
11:c:101:TRP:CZ3	22:o:60:ILE:HG22	2.46	0.51
16:h:26:PRO:O	16:h:29:ILE:HG13	2.10	0.51
17:i:58:LYS:HG2	48:l:584:ILE:HD11	1.93	0.51
17:i:268:GLN:HG2	17:i:272:LYS:HE3	1.93	0.51
26:B:366:ALA:HA	29:E:141:MET:HE1	1.93	0.51
29:E:224:SER:C	29:E:226:GLU:H	2.20	0.51
34:K:23:TYR:O	34:K:26:VAL:HG12	2.10	0.51
37:O:105:MET:CG	37:O:139:MET:HG2	2.41	0.51
37:O:133:ILE:HG12	37:O:134:ASP:N	2.26	0.51
39:Q:107:LEU:HD12	39:Q:110:ILE:HD12	1.92	0.51
43:U:258:LEU:HD11	43:U:278:LEU:HD11	1.93	0.51
43:U:327:ASP:O	43:U:331:GLN:HG3	2.10	0.51
46:Y:88:ASP:N	46:Y:89:PRO:HD2	2.25	0.51
48:l:305:SER:O	48:l:309:GLN:HG2	2.11	0.51
51:u:300:ASP:O	51:u:303:PRO:HD2	2.11	0.51
7:x:182:ASN:HB2	7:x:183:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:G:171:THR:CG2	53:G:173:MET:HG2	2.41	0.51
53:G:355:LYS:HG3	53:G:366:LEU:HD13	1.92	0.51
4:3:23:MET:O	4:3:27:VAL:HG23	2.10	0.50
4:3:39:ARG:O	4:3:43:ASP:HB2	2.11	0.50
5:6:292:VAL:HG11	5:6:366:LEU:HD11	1.93	0.50
5:6:322:ASP:O	3:Ae:68:LEU:HD11	2.11	0.50
10:b:93:LYS:HB3	10:b:96:THR:HG21	1.92	0.50
17:i:112:HIS:CE1	17:i:164:ILE:HD13	2.46	0.50
18:j:1:MET:SD	45:W:142:TRP:HB3	2.51	0.50
18:j:44:MET:HE1	27:C:102:ARG:NH2	2.25	0.50
24:q:451:PRO:O	24:q:455:LEU:HG	2.11	0.50
31:H:131:GLU:HG3	31:H:144:ARG:HD2	1.92	0.50
39:Q:49:ARG:HD3	39:Q:49:ARG:N	2.26	0.50
6:w:26:ASN:ND2	6:w:207:ASN:HB2	2.25	0.50
6:7:357:LEU:O	6:7:361:ILE:HG13	2.10	0.50
16:h:20:ILE:HB	16:h:37:GLU:OE2	2.11	0.50
20:m:15:ILE:HG23	20:m:97:LEU:HD21	1.92	0.50
25:r:26:LYS:HG2	25:r:36:GLY:HA3	1.93	0.50
27:C:170:PRO:HG2	27:C:173:ALA:CB	2.42	0.50
27:C:259:PHE:O	27:C:263:GLU:HG3	2.11	0.50
31:H:86:TYR:CE2	32:I:171:GLU:HG2	2.46	0.50
31:H:142:THR:O	31:H:187:LYS:NZ	2.35	0.50
32:I:174:LEU:O	32:I:178:LEU:HG	2.12	0.50
35:L:206:ASP:OD1	35:L:207:ARG:N	2.44	0.50
35:L:215:MET:HE2	35:L:222:PRO:HD2	1.92	0.50
35:L:342:LEU:HA	35:L:361:MET:HE1	1.93	0.50
36:N:35:LEU:HD13	36:N:49:GLU:HG3	1.93	0.50
37:O:134:ASP:O	37:O:138:LEU:HD13	2.12	0.50
43:U:85:LEU:HD22	43:U:158:GLY:CA	2.40	0.50
43:U:312:ILE:HG22	43:U:314:VAL:HG23	1.93	0.50
44:V:72:LEU:CD1	44:V:76:ILE:HD12	2.41	0.50
51:u:191:ALA:HB1	51:u:270:PHE:CE2	2.46	0.50
7:x:212:VAL:O	7:x:216:LEU:HG	2.11	0.50
51:5:179:MET:CE	51:5:282:LEU:HD13	2.38	0.50
51:5:405:GLY:O	51:5:408:PRO:HD2	2.11	0.50
53:G:387:LEU:CD1	53:G:514:ASN:HB3	2.38	0.50
1:0:33:VAL:CG1	1:0:85:LYS:HB2	2.42	0.50
3:4:194:PRO:HG2	3:4:244:VAL:HG22	1.92	0.50
9:a:54:LEU:HD23	10:b:27:GLU:HA	1.92	0.50
15:g:17:PRO:HG2	15:g:83:TYR:OH	2.11	0.50
16:h:87:ILE:HD11	16:h:92:TYR:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:75:ILE:HD12	19:k:40:LEU:HD22	1.92	0.50
22:o:5:LYS:HB2	22:o:5:LYS:HZ2	1.77	0.50
22:o:25:ILE:HG12	22:o:30:ARG:NE	2.27	0.50
24:q:142:ARG:NH2	27:C:43:TRP:O	2.41	0.50
24:q:412:ILE:HD11	48:l:152:PHE:HZ	1.76	0.50
25:r:298:LEU:O	25:r:302:MET:HG3	2.11	0.50
35:L:163:SER:HA	35:L:179:LYS:HE3	1.93	0.50
51:u:404:ASP:O	51:u:408:PRO:HG2	2.11	0.50
5:v:59:SER:HB2	5:v:130:ILE:HG12	1.93	0.50
5:v:261:GLN:HG3	5:v:261:GLN:O	2.10	0.50
53:G:41:VAL:HG22	53:G:43:VAL:HG13	1.93	0.50
5:6:91:THR:HB	5:6:143:ALA:O	2.12	0.50
6:7:300:ILE:HD11	6:7:363:LEU:HD21	1.92	0.50
16:h:94:PRO:HG2	16:h:99:LEU:HD11	1.93	0.50
17:i:100:MET:HE3	17:i:111:PHE:CZ	2.47	0.50
17:i:171:ASN:ND2	27:C:59:TYR:HB2	2.26	0.50
20:m:28:TYR:HA	20:m:31:LEU:CG	2.38	0.50
22:o:6:TYR:O	22:o:8:PRO:HD3	2.10	0.50
25:r:34:ARG:HG2	32:I:82:PRO:CA	2.40	0.50
26:B:68:ILE:HG23	26:B:75:TRP:CZ3	2.40	0.50
32:I:189:ARG:HG3	35:L:82:GLU:OE2	2.11	0.50
33:J:163:ASN:O	33:J:171:ARG:HA	2.12	0.50
35:L:68:LEU:HA	35:L:71:MET:HE2	1.93	0.50
35:L:160:ILE:CD1	35:L:194:THR:HB	2.42	0.50
43:U:228:GLU:O	43:U:231:ILE:HG13	2.11	0.50
43:U:353:TRP:O	43:U:357:LYS:HB2	2.12	0.50
6:w:121:PHE:CZ	6:w:298:ILE:HB	2.46	0.50
53:G:64:CYS:CB	53:G:75:CYS:HB3	2.26	0.50
7:8:126:HIS:CD2	7:8:195:PRO:HB2	2.46	0.50
9:a:179:ILE:HG23	16:h:22:SER:HB3	1.94	0.50
10:b:87:LYS:CE	12:d:49:ARG:HG3	2.41	0.50
16:h:25:GLN:HB3	16:h:26:PRO:HD2	1.93	0.50
17:i:26:TRP:HB3	17:i:74:ILE:HD13	1.94	0.50
18:j:3:ILE:O	18:j:7:LEU:HG	2.11	0.50
25:r:316:PRO:CG	45:W:57:ARG:HB3	2.37	0.50
26:B:355:ILE:HD13	29:E:139:PRO:HG3	1.93	0.50
27:C:62:LYS:HG3	27:C:63:GLU:HG3	1.92	0.50
27:C:399:PRO:HB3	36:N:115:PRO:HG3	1.93	0.50
29:E:200:ASP:O	29:E:204:ILE:HG13	2.12	0.50
33:J:79:ILE:HG12	33:J:99:MET:HG3	1.94	0.50
33:J:111:LEU:HD11	34:K:126:PRO:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:319:GLY:HA3	3:Af:58:ALA:CB	2.41	0.50
51:u:338:CYS:HB3	51:u:368:MET:SD	2.52	0.50
5:v:60:ARG:NH1	5:v:124:GLU:HG2	2.27	0.50
5:v:322:ASP:C	3:Af:68:LEU:HD11	2.36	0.50
3:4:244:VAL:HG11	6:w:262:LEU:O	2.12	0.50
10:b:11:ARG:HE	23:p:206:PRO:HB3	1.77	0.50
11:c:166:LEU:HB3	11:c:169:GLU:HB2	1.93	0.50
14:f:70:LYS:HB2	14:f:70:LYS:NZ	2.26	0.50
17:i:216:PHE:O	17:i:220:ILE:HG13	2.11	0.50
18:j:73:LEU:HD12	20:m:55:MET:SD	2.52	0.50
22:o:5:LYS:HE3	22:o:7:LYS:HD2	1.93	0.50
23:p:174:SER:O	23:p:178:GLU:HG3	2.11	0.50
31:H:198:GLU:HG2	34:K:108:TYR:HE1	1.75	0.50
36:N:106:GLU:HG3	36:N:107:PRO:CD	2.34	0.50
37:O:92:LYS:NZ	37:O:92:LYS:HB3	2.26	0.50
7:x:228:LEU:HD11	7:x:234:PHE:CB	2.42	0.50
6:7:260:ASN:HD22	6:7:261:PRO:HD2	1.76	0.50
11:c:140:MET:SD	48:l:283:ILE:HG12	2.52	0.50
12:d:32:TYR:O	12:d:36:ILE:HG13	2.11	0.50
17:i:267:ILE:O	17:i:271:THR:HG23	2.12	0.50
24:q:137:GLY:O	27:C:42:GLN:HG3	2.12	0.50
26:B:62:TRP:CZ3	26:B:181:LEU:HB3	2.46	0.50
26:B:87:GLY:HA3	58:B:501:FMN:O2P	2.12	0.50
26:B:231:ALA:O	26:B:239:PRO:HA	2.12	0.50
35:L:215:MET:CE	35:L:222:PRO:HD2	2.42	0.50
41:S:40:HIS:H	41:S:44:GLN:NE2	2.09	0.50
48:l:227:PHE:N	48:l:284:THR:HG22	2.26	0.50
51:u:114:GLU:HG2	5:v:298:HIS:HB2	1.93	0.50
5:v:371:VAL:HG12	5:v:375:LYS:HD2	1.93	0.50
53:G:169:VAL:HG21	53:G:222:ILE:HD11	1.94	0.50
1:0:42:LYS:HD2	1:0:45:LYS:HD3	1.93	0.50
3:4:171:SER:HB2	6:w:168:PHE:HZ	1.75	0.50
13:e:98:VAL:HG11	24:q:71:TRP:CZ3	2.47	0.50
17:i:230:LEU:HD21	17:i:244:MET:HE1	1.94	0.50
17:i:276:ILE:C	17:i:279:PRO:HD2	2.37	0.50
31:H:115:ALA:HB3	31:H:140:ARG:HG2	1.94	0.50
35:L:160:ILE:HD13	35:L:194:THR:HB	1.93	0.50
35:L:294:ARG:NH1	35:L:311:ARG:HB3	2.26	0.50
36:N:98:LYS:N	36:N:99:PRO:HD3	2.27	0.50
37:O:104:PHE:HB3	37:O:110:LEU:CD1	2.42	0.50
43:U:123:PRO:HB2	43:U:180:PHE:CD1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:X:144:ILE:O	37:X:148:ILE:HG13	2.11	0.50
48:l:86:SER:O	48:l:90:ILE:HG13	2.11	0.50
6:w:117:VAL:HG21	6:w:302:ILE:HD13	1.94	0.50
6:w:119:LEU:HD21	6:w:192:LEU:CB	2.40	0.50
7:x:142:THR:HG23	7:x:145:GLU:H	1.75	0.50
7:x:154:GLU:OE2	7:x:169:PRO:HA	2.11	0.50
2:Ac:43:ILE:O	2:Ac:47:ILE:HG13	2.12	0.50
53:G:245:THR:HB	53:G:264:SER:OG	2.11	0.50
6:7:138:MET:HE3	6:7:252:ASP:OD2	2.12	0.50
17:i:86:ILE:O	17:i:87:THR:HG23	2.12	0.50
24:q:263:MET:HA	24:q:263:MET:CE	2.41	0.50
26:B:152:ARG:O	26:B:193:PHE:HA	2.12	0.50
26:B:423:THR:HG21	26:B:428:GLY:HA3	1.92	0.50
27:C:228:MET:CG	32:I:167:PRO:HG3	2.41	0.50
31:H:200:GLU:OE1	34:K:87:HIS:HB3	2.11	0.50
51:u:38:TYR:CZ	51:u:42:LEU:HD11	2.46	0.50
51:u:276:ARG:HB2	52:z:16:THR:HG23	1.93	0.50
5:v:182:TYR:O	5:v:187:ALA:HB2	2.12	0.50
6:w:24:PRO:HB2	6:w:27:ILE:HG23	1.93	0.50
6:w:185:LEU:HD23	6:w:188:ILE:HD12	1.93	0.50
1:0:32:THR:O	1:0:36:GLN:HG3	2.12	0.49
9:a:80:ILE:O	9:a:84:ILE:HG13	2.12	0.49
10:b:108:ASP:HA	10:b:114:GLY:O	2.12	0.49
16:h:63:PHE:HE2	17:i:83:GLN:HE21	1.60	0.49
16:h:94:PRO:HG2	16:h:99:LEU:HD21	1.94	0.49
19:k:33:LEU:HA	19:k:36:MET:HE2	1.92	0.49
22:o:96:GLY:N	22:o:97:PRO:HD2	2.27	0.49
24:q:7:PRO:O	24:q:11:LEU:HD23	2.12	0.49
24:q:401:MET:SD	48:l:177:ILE:HG12	2.52	0.49
26:B:326:LEU:HD12	26:B:326:LEU:C	2.37	0.49
27:C:122:LEU:HG	27:C:122:LEU:O	2.12	0.49
27:C:391:TYR:HD1	31:H:122:VAL:HG21	1.77	0.49
28:D:221:ALA:O	28:D:222:GLU:HG2	2.12	0.49
30:F:37:LYS:HD3	30:F:37:LYS:N	2.25	0.49
51:u:397:ASN:HA	51:u:400:VAL:CG2	2.42	0.49
3:Ae:45:PRO:C	3:Ae:47:GLY:H	2.18	0.49
1:0:60:ARG:HB3	1:0:63:THR:HB	1.93	0.49
3:4:145:GLY:O	7:8:296:MET:HE1	2.11	0.49
5:6:233:VAL:CG2	5:6:236:ARG:HH12	2.25	0.49
6:7:211:ILE:HD12	8:9:37:THR:HA	1.93	0.49
11:c:127:ASN:O	11:c:131:LYS:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:54:ARG:NH2	17:i:306:PRO:HB3	2.12	0.49
16:h:15:ASP:CB	17:i:28:LEU:HD12	2.42	0.49
20:m:45:LEU:N	20:m:45:LEU:HD23	2.26	0.49
24:q:214:LEU:O	24:q:217:PRO:HD2	2.12	0.49
24:q:237:LYS:HD2	24:q:316:MET:HB3	1.93	0.49
25:r:212:ASN:O	32:l:99:GLN:NE2	2.45	0.49
27:C:376:GLU:HA	27:C:379:THR:HG22	1.93	0.49
28:D:92:GLY:C	28:D:95:PRO:HD2	2.37	0.49
31:H:38:TYR:CZ	54:M:106:LEU:HD13	2.45	0.49
31:H:188:GLU:HG3	34:K:127:TYR:OH	2.11	0.49
49:s:188:VAL:CG1	49:s:194:TRP:HB2	2.42	0.49
6:w:9:PRO:O	6:w:13:ILE:HG12	2.12	0.49
6:w:98:VAL:HG22	56:w:401:HEM:CBC	2.41	0.49
52:z:73:LYS:HG2	52:z:74:ASN:N	2.27	0.49
3:4:204:GLU:O	3:4:208:GLU:HG2	2.12	0.49
6:7:200:LEU:CD2	56:7:402:HEM:HAA1	2.42	0.49
10:b:118:PRO:O	10:b:120:MET:N	2.43	0.49
13:e:112:TYR:HD2	24:q:43:ASN:HD21	1.60	0.49
19:k:25:HIS:CE1	19:k:89:TYR:HE1	2.30	0.49
24:q:201:MET:O	24:q:205:VAL:HG23	2.12	0.49
27:C:228:MET:O	27:C:229:HIS:HB2	2.12	0.49
38:P:24:CYS:HB2	38:P:27:SER:HB2	1.94	0.49
48:l:213:LEU:HB2	48:l:273:VAL:HG21	1.94	0.49
5:v:271:LEU:HD22	5:v:453:LEU:HD13	1.95	0.49
7:x:268:ALA:HA	7:x:271:VAL:HG12	1.95	0.49
57:x:401:HEC:HMB3	57:x:401:HEC:CBB	2.43	0.49
51:5:306:VAL:O	51:5:310:ILE:HG13	2.12	0.49
51:5:384:THR:O	51:5:388:VAL:HG23	2.13	0.49
53:G:643:ARG:NH1	53:G:656:TYR:OH	2.45	0.49
1:0:29:PRO:O	1:0:33:VAL:HG23	2.12	0.49
3:4:240:HIS:HB3	55:4:301:FES:S1	2.52	0.49
5:6:326:PHE:HD2	3:Ae:66:PRO:O	1.96	0.49
12:d:114:GLN:HG2	48:l:199:GLN:HB3	1.95	0.49
35:L:301:GLU:CG	35:L:310:THR:HG23	2.42	0.49
44:V:97:GLY:O	44:V:100:THR:OG1	2.25	0.49
48:l:227:PHE:H	48:l:284:THR:HG22	1.76	0.49
48:l:332:HIS:HA	48:l:335:PHE:CE2	2.47	0.49
7:x:323:ARG:HB3	7:x:323:ARG:NH1	2.27	0.49
1:0:30:LEU:O	1:0:34:ARG:HG3	2.12	0.49
3:2:254:GLY:HA3	3:2:264:TYR:O	2.12	0.49
5:6:125:CYS:HB3	5:6:133:LEU:HD22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:313:VAL:HG11	5:6:350:VAL:HG13	1.94	0.49
5:6:410:SER:O	5:6:414:GLN:HG3	2.11	0.49
6:7:254:ASP:O	6:7:257:THR:HG22	2.13	0.49
8:9:57:ASN:CA	8:9:60:VAL:HG22	2.40	0.49
14:f:70:LYS:HB2	14:f:70:LYS:HZ2	1.78	0.49
17:i:68:MET:HG3	19:k:36:MET:CE	2.39	0.49
17:i:261:MET:CG	17:i:262:PRO:HD3	2.42	0.49
20:m:9:LEU:O	20:m:39:VAL:CG1	2.59	0.49
26:B:284:HIS:HD2	26:B:305:GLY:HA3	1.77	0.49
27:C:170:PRO:HG2	27:C:173:ALA:HB2	1.94	0.49
29:E:155:LYS:NZ	29:E:206:ASP:OD1	2.34	0.49
31:H:135:ARG:HG3	31:H:137:ASP:H	1.78	0.49
43:U:170:VAL:CG1	43:U:239:ILE:HG23	2.41	0.49
53:G:691:ILE:HG23	53:G:714:VAL:HG21	1.94	0.49
3:4:201:THR:O	3:4:205:ILE:HG13	2.13	0.49
5:6:216:ALA:HB3	5:6:244:LEU:N	2.24	0.49
11:c:186:ILE:HB	50:t:97:LYS:HG3	1.95	0.49
13:e:65:ASN:HB3	24:q:427:LYS:HE3	1.93	0.49
18:j:68:GLU:HG3	20:m:161:LEU:HD13	1.94	0.49
22:o:3:PHE:HB3	23:p:115:TYR:CG	2.47	0.49
25:r:214:GLU:HA	32:I:98:ARG:HD2	1.93	0.49
25:r:306:SER:O	25:r:310:MET:HG2	2.12	0.49
28:D:103:HIS:HA	28:D:106:ALA:O	2.12	0.49
35:L:241:SER:O	35:L:245:ILE:HG12	2.12	0.49
35:L:301:GLU:HG2	35:L:310:THR:HG23	1.94	0.49
37:O:80:LYS:O	37:O:84:LEU:HD23	2.12	0.49
37:O:92:LYS:HD3	37:O:114:ASP:CG	2.38	0.49
38:P:16:LEU:HD21	38:P:67:ALA:HB1	1.95	0.49
48:l:90:ILE:HD11	48:l:133:THR:CG2	2.43	0.49
48:l:197:ASP:O	48:l:201:ILE:HG13	2.12	0.49
6:w:331:ASP:OD2	6:w:358:TYR:HB2	2.11	0.49
53:G:367:CYS:HB3	53:G:533:GLY:O	2.13	0.49
53:G:400:ILE:HG13	53:G:427:LEU:HD11	1.94	0.49
2:1:19:SER:HB2	4:3:23:MET:CB	2.39	0.49
3:4:284:TYR:HB3	3:4:294:VAL:HG13	1.93	0.49
17:i:30:TRP:HZ2	19:k:37:MET:HE1	1.75	0.49
17:i:254:LEU:HD21	17:i:290:LEU:HD11	1.95	0.49
20:m:28:TYR:HB3	20:m:83:TRP:CH2	2.47	0.49
26:B:257:ARG:HG2	26:B:261:TRP:CG	2.48	0.49
27:C:252:GLU:O	27:C:255:LYS:HG2	2.12	0.49
27:C:345:GLN:O	27:C:349:ILE:HG13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:D:87:PHE:HE1	28:D:144:LYS:HE2	1.78	0.49
34:K:55:PHE:CZ	34:K:58:ARG:HG3	2.48	0.49
35:L:231:VAL:HG22	35:L:267:LEU:CD2	2.35	0.49
43:U:149:LEU:O	43:U:153:LEU:HG	2.13	0.49
48:l:226:GLN:HA	48:l:284:THR:HG21	1.94	0.49
48:l:400:ASN:HA	48:l:409:LEU:HD11	1.94	0.49
51:5:328:LEU:HD11	51:5:368:MET:HE2	1.94	0.49
3:2:235:ILE:HG21	3:2:280:GLU:HB3	1.95	0.49
5:6:168:ASN:HB2	5:6:170:GLN:NE2	2.27	0.49
6:7:294:LEU:HD23	6:7:294:LEU:C	2.37	0.49
6:7:338:ILE:CD1	6:7:350:ILE:HG22	2.42	0.49
9:a:59:PRO:HG3	24:q:350:THR:O	2.12	0.49
17:i:254:LEU:CD2	24:q:154:LEU:HD11	2.43	0.49
18:j:92:LEU:O	18:j:96:ILE:HG13	2.12	0.49
19:k:10:MET:O	19:k:14:ILE:HG13	2.13	0.49
22:o:81:ARG:O	22:o:83:THR:HG23	2.12	0.49
24:q:109:THR:CG2	24:q:121:LEU:HB3	2.43	0.49
25:r:132:ALA:O	25:r:136:VAL:HG23	2.12	0.49
28:D:67:GLU:O	28:D:70:PRO:HD3	2.13	0.49
28:D:71:LYS:HB2	36:N:99:PRO:O	2.13	0.49
28:D:161:LYS:HG3	28:D:161:LYS:O	2.13	0.49
37:O:131:PRO:HB2	37:O:133:ILE:HD13	1.95	0.49
42:T:154:HIS:ND1	42:T:155:PRO:HD2	2.28	0.49
49:s:115:LYS:HB3	49:s:116:PRO:CD	2.43	0.49
51:u:373:GLN:OE1	51:u:474:GLY:HA3	2.12	0.49
6:w:217:LYS:HG3	52:z:8:LEU:HD13	1.93	0.49
6:w:268:ILE:N	6:w:268:ILE:HD12	2.28	0.49
51:5:415:ARG:O	51:5:419:THR:HG23	2.12	0.49
3:4:168:LEU:O	3:4:171:SER:HB3	2.13	0.49
5:6:392:PHE:O	5:6:396:VAL:HG23	2.12	0.49
6:7:25:SER:HB3	6:7:216:ASP:OD2	2.12	0.49
6:7:265:PRO:HG2	6:7:268:ILE:HG12	1.94	0.49
10:b:80:TRP:HD1	12:d:41:VAL:HG13	1.77	0.49
11:c:42:PRO:HD3	11:c:74:ASP:OD1	2.12	0.49
17:i:145:ILE:O	17:i:149:ILE:HG13	2.13	0.49
17:i:162:ILE:HD12	17:i:282:MET:HG2	1.95	0.49
21:n:24:GLY:HA2	24:q:6:ILE:HD12	1.95	0.49
23:p:205:LEU:HD13	23:p:209:TRP:CZ2	2.48	0.49
24:q:129:THR:O	24:q:133:ILE:HG13	2.13	0.49
24:q:389:SER:HB3	24:q:392:THR:HG23	1.95	0.49
27:C:191:MET:SD	32:I:77:MET:HE1	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:272:ARG:HH22	31:H:63:TRP:HA	1.78	0.49
31:H:38:TYR:HB3	54:M:104:TRP:HE3	1.76	0.49
31:H:114:ILE:HD12	59:H:302:SF4:S4	2.52	0.49
39:Q:85:GLY:O	39:Q:89:VAL:HG23	2.13	0.49
41:S:7:PRO:O	41:S:11:VAL:HG23	2.13	0.49
43:U:211:VAL:HG22	43:U:262:ALA:HB2	1.94	0.49
43:U:216:ILE:O	43:U:220:ILE:HG13	2.12	0.49
48:l:217:LEU:C	48:l:217:LEU:HD23	2.38	0.49
48:l:410:LEU:O	48:l:414:ILE:HG13	2.13	0.49
5:v:65:ILE:HG12	5:v:218:MET:HG2	1.95	0.49
5:v:149:TRP:CD1	5:v:150:GLU:HG3	2.48	0.49
7:x:238:PHE:CD2	7:x:243:ILE:HG13	2.47	0.49
51:5:120:LEU:HD13	51:5:133:ILE:CG1	2.42	0.49
51:5:142:LYS:HB2	51:5:142:LYS:HZ2	1.78	0.49
54:M:28:TYR:O	54:M:30:GLU:N	2.45	0.49
3:4:258:PRO:O	3:4:260:HIS:N	2.45	0.49
6:7:334:THR:HG22	6:7:338:ILE:HD11	1.94	0.49
7:8:113:ARG:O	7:8:117:VAL:HG23	2.13	0.49
8:9:63:ILE:O	8:9:67:LEU:HG	2.12	0.49
9:a:107:PRO:HB2	9:a:112:TYR:CZ	2.48	0.49
11:c:169:GLU:HG2	50:t:56:ARG:HH11	1.77	0.49
17:i:311:MET:HG2	43:U:311:THR:CG2	2.43	0.49
20:m:2:THR:HA	20:m:5:ILE:HD11	1.95	0.49
24:q:231:LEU:HA	24:q:235:LEU:HB2	1.94	0.49
25:r:66:SER:HA	25:r:122:ALA:O	2.12	0.49
26:B:159:ARG:HD2	26:B:162:PHE:CD2	2.47	0.49
27:C:197:ALA:HA	27:C:200:ILE:HG12	1.94	0.49
27:C:221:GLU:O	27:C:225:GLY:N	2.41	0.49
28:D:218:ARG:HD2	39:Q:127:THR:CA	2.36	0.49
35:L:52:THR:HG23	35:L:114:VAL:HG22	1.94	0.49
35:L:273:GLN:HG3	35:L:283:PHE:CD2	2.48	0.49
43:U:97:ASP:N	43:U:97:ASP:OD1	2.45	0.49
48:l:83:ASP:CG	48:l:262:ARG:HH12	2.20	0.49
51:u:37:THR:OG1	51:u:40:GLN:HG3	2.13	0.49
7:x:97:TRP:CE2	7:x:209:GLU:HG3	2.48	0.49
51:5:95:HIS:HB3	51:5:164:GLU:CG	2.43	0.49
51:5:368:MET:HA	51:5:368:MET:HE3	1.95	0.49
3:2:128:SER:O	3:2:132:LYS:HD3	2.12	0.48
3:2:179:ASP:O	3:2:181:PRO:HD3	2.13	0.48
5:6:355:TYR:O	5:6:359:LYS:HG3	2.11	0.48
11:c:58:ARG:HE	22:o:35:GLU:CD	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:81:GLN:HG3	15:g:85:TYR:HE2	1.77	0.48
17:i:259:GLY:O	17:i:262:PRO:HD2	2.13	0.48
17:i:313:MET:CE	43:U:96:ALA:HB2	2.42	0.48
25:r:149:ILE:O	25:r:153:VAL:HG22	2.13	0.48
29:E:158:ILE:HD13	29:E:164:THR:HG23	1.95	0.48
29:E:180:CYS:SG	55:E:301:FES:S1	3.10	0.48
43:U:80:ALA:CB	43:U:87:HIS:HB2	2.43	0.48
37:X:120:MET:O	37:X:123:GLU:HG2	2.12	0.48
49:s:87:LEU:O	49:s:91:LYS:HG3	2.13	0.48
6:w:36:LEU:CD2	6:w:232:ALA:HA	2.42	0.48
7:x:238:PHE:CG	7:x:243:ILE:HG13	2.48	0.48
6:7:294:LEU:HD23	6:7:294:LEU:O	2.13	0.48
17:i:190:MET:HE1	17:i:208:TYR:CD2	2.48	0.48
17:i:278:MET:HB3	17:i:279:PRO:HD3	1.95	0.48
17:i:311:MET:HG2	43:U:311:THR:HG21	1.94	0.48
24:q:89:THR:HG22	24:q:93:LYS:HE3	1.94	0.48
25:r:61:LEU:C	25:r:61:LEU:HD22	2.38	0.48
25:r:263:THR:O	25:r:267:THR:HG23	2.13	0.48
26:B:446:LEU:O	26:B:450:MET:HG3	2.13	0.48
29:E:143:ARG:HG3	29:E:183:ALA:HB3	1.95	0.48
42:T:150:ASP:O	42:T:159:GLN:HB3	2.13	0.48
5:6:180:ALA:HB1	5:6:256:GLY:O	2.12	0.48
7:8:108:HIS:CD2	7:8:111:ILE:HD12	2.49	0.48
15:g:80:ARG:HG2	17:i:345:SER:HA	1.94	0.48
17:i:78:LEU:HD22	17:i:84:TRP:CZ2	2.47	0.48
17:i:273:ASN:O	17:i:274:GLU:HB2	2.14	0.48
26:B:35:LEU:CD2	26:B:40:ARG:HG2	2.42	0.48
26:B:102:MET:HE1	26:B:240:THR:N	2.28	0.48
32:I:133:MET:SD	32:I:173:LEU:HD22	2.53	0.48
34:K:4:VAL:O	34:K:8:ARG:HG3	2.13	0.48
37:O:76:LEU:HB2	37:O:155:TYR:CE2	2.48	0.48
51:u:397:ASN:HA	51:u:400:VAL:HG22	1.95	0.48
5:v:410:SER:O	5:v:414:GLN:HG3	2.12	0.48
52:Aa:47:LEU:O	52:Aa:47:LEU:HD13	2.13	0.48
52:Aa:68:GLU:O	52:Aa:72:ARG:HG2	2.13	0.48
54:M:58:ASP:O	54:M:62:GLU:HG3	2.13	0.48
3:Af:45:PRO:HB2	3:Af:48:PRO:HB3	1.95	0.48
2:1:41:ASP:OD1	7:x:288:ARG:NE	2.46	0.48
6:7:117:VAL:HG21	6:7:302:ILE:HD13	1.94	0.48
13:e:89:VAL:HG11	24:q:29:VAL:CG2	2.43	0.48
17:i:89:MET:HG3	17:i:95:MET:SD	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:10:ARG:HG3	22:o:11:LEU:HG	1.94	0.48
24:q:73:LEU:HB3	24:q:74:PRO:HD3	1.96	0.48
25:r:307:LEU:HA	25:r:310:MET:CE	2.43	0.48
27:C:200:ILE:HD11	27:C:274:TRP:HE1	1.77	0.48
35:L:257:THR:O	35:L:328:PRO:HD2	2.13	0.48
37:X:104:PHE:HB3	37:X:110:LEU:HD12	1.95	0.48
37:X:140:CYS:HB3	37:X:143:GLU:HG2	1.95	0.48
48:l:12:LEU:HD22	48:l:129:MET:HB3	1.95	0.48
48:l:105:MET:HB3	48:l:449:LEU:HD13	1.95	0.48
51:u:302:VAL:HB	51:u:303:PRO:HD3	1.95	0.48
5:v:170:GLN:HG2	3:Af:67:VAL:HG13	1.95	0.48
6:w:119:LEU:CD2	6:w:192:LEU:HB2	2.42	0.48
53:G:618:GLU:O	53:G:622:ILE:HG13	2.11	0.48
12:d:107:GLN:C	12:d:111:LYS:HZ2	2.21	0.48
17:i:198:THR:HA	17:i:201:THR:HG23	1.94	0.48
21:n:10:ASP:HB2	24:q:19:LYS:HD2	1.96	0.48
23:p:164:ARG:HG2	23:p:168:LYS:HE3	1.95	0.48
27:C:57:VAL:HG13	27:C:58:MET:O	2.14	0.48
27:C:418:VAL:CG2	27:C:426:TYR:HB3	2.43	0.48
29:E:73:GLY:HA2	40:R:106:GLN:O	2.13	0.48
51:u:220:VAL:O	51:u:224:TYR:HB2	2.14	0.48
5:v:326:PHE:O	5:v:336:PHE:HA	2.13	0.48
6:w:24:PRO:HB2	6:w:27:ILE:CG2	2.43	0.48
1:0:78:ARG:O	1:0:82:VAL:HG23	2.12	0.48
5:6:60:ARG:HD3	5:6:393:LEU:HD22	1.96	0.48
5:6:84:ARG:HD2	3:Ae:60:PRO:HB2	1.94	0.48
6:7:150:LEU:HB2	6:7:161:VAL:HG22	1.96	0.48
12:d:115:GLN:HG2	48:l:62:ILE:HG22	1.94	0.48
16:h:98:HIS:ND1	45:W:128:ARG:HD3	2.29	0.48
18:j:8:LEU:O	18:j:12:THR:HG23	2.12	0.48
19:k:38:LEU:O	19:k:42:ILE:HG12	2.13	0.48
24:q:208:PRO:HG3	24:q:216:LEU:CD1	2.42	0.48
27:C:102:ARG:O	27:C:118:HIS:HB2	2.13	0.48
28:D:225:GLU:HG3	33:J:118:ALA:HB2	1.95	0.48
31:H:98:ARG:HD2	31:H:156:GLY:CA	2.44	0.48
35:L:114:VAL:CG1	35:L:115:VAL:HG13	2.43	0.48
35:L:216:ARG:NH1	35:L:351:HIS:HB3	2.29	0.48
35:L:363:ASP:OD1	35:L:364:VAL:N	2.47	0.48
37:O:103:HIS:CB	37:O:106:LYS:HE3	2.43	0.48
43:U:215:GLU:O	43:U:219:ARG:HG3	2.13	0.48
45:W:121:MET:HE2	45:W:137:THR:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:19:ILE:HD11	48:l:122:VAL:HB	1.96	0.48
48:l:62:ILE:HG21	48:l:199:GLN:HE22	1.79	0.48
50:t:96:VAL:HG12	50:t:100:LYS:HE3	1.95	0.48
1:0:65:GLU:HB3	52:z:78:TYR:CD1	2.49	0.48
2:1:44:TYR:O	2:1:48:ASN:ND2	2.39	0.48
11:c:111:MET:HE2	24:q:278:ARG:NH1	2.29	0.48
18:j:5:LEU:HD22	25:r:6:ILE:CD1	2.44	0.48
20:m:103:MET:HA	20:m:103:MET:CE	2.40	0.48
26:B:262:PHE:CE2	26:B:272:GLY:HA3	2.49	0.48
27:C:160:ALA:HB2	27:C:404:THR:OG1	2.13	0.48
33:J:137:PHE:HA	33:J:140:LYS:HE3	1.96	0.48
48:l:152:PHE:CD1	48:l:168:ALA:HB1	2.48	0.48
48:l:560:THR:O	48:l:565:THR:HG23	2.13	0.48
49:s:115:LYS:HB3	49:s:116:PRO:HD3	1.96	0.48
7:x:133:TYR:HA	7:x:136:LEU:CD1	2.43	0.48
51:5:49:GLN:O	51:5:60:ALA:HA	2.14	0.48
51:5:74:TRP:CZ2	51:5:411:GLU:HA	2.49	0.48
5:6:258:ILE:O	5:6:439:ALA:HA	2.14	0.48
5:6:293:LEU:CD2	5:6:361:ILE:HD12	2.43	0.48
24:q:18:SER:OG	24:q:23:ILE:HG22	2.14	0.48
26:B:169:LEU:O	26:B:173:ILE:HG13	2.14	0.48
27:C:240:GLN:HB3	31:H:96:ARG:HH22	1.78	0.48
27:C:340:VAL:O	27:C:344:ARG:HG3	2.14	0.48
37:O:133:ILE:H	37:O:133:ILE:CD1	2.26	0.48
43:U:213:VAL:O	43:U:217:GLN:HG3	2.13	0.48
45:W:106:VAL:O	49:s:81:ILE:HD12	2.14	0.48
48:l:375:ILE:HD12	48:l:458:LEU:CD2	2.43	0.48
51:5:338:CYS:HB2	51:5:368:MET:SD	2.53	0.48
53:G:326:VAL:HG23	53:G:626:LEU:CD1	2.43	0.48
3:Af:45:PRO:HB3	3:Af:66:PRO:CD	2.43	0.48
1:0:33:VAL:HG12	1:0:82:VAL:HG22	1.96	0.48
5:6:108:GLY:HA3	5:6:133:LEU:HD21	1.96	0.48
7:8:126:HIS:CE1	7:8:196:PRO:HD2	2.49	0.48
25:r:35:LYS:H	31:H:83:THR:HG21	1.77	0.48
29:E:177:LEU:HB2	29:E:185:MET:HE1	1.95	0.48
35:L:201:ILE:HA	35:L:235:VAL:O	2.13	0.48
35:L:266:TYR:CE2	35:L:369:THR:HG22	2.48	0.48
51:u:158:ASP:O	51:u:161:ILE:HB	2.13	0.48
51:5:276:ARG:NH2	51:5:466:PRO:O	2.44	0.48
51:5:318:TYR:CE1	3:Ae:55:GLY:HA2	2.49	0.48
51:5:473:SER:HA	51:5:476:PHE:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:G:471:LYS:HG3	53:G:510:TRP:CD2	2.49	0.48
3:Af:47:GLY:H	3:Af:66:PRO:HB3	1.77	0.48
2:1:36:PHE:HZ	7:x:295:MET:CB	2.26	0.48
3:4:140:ALA:O	3:4:144:VAL:HG23	2.12	0.48
5:6:195:TYR:CE2	5:6:196:ARG:HG2	2.48	0.48
11:c:70:MET:HE1	48:l:552:LEU:HD13	1.96	0.48
14:f:69:TYR:HD1	15:g:22:SER:O	1.97	0.48
16:h:86:LEU:HD21	45:W:97:ILE:O	2.13	0.48
17:i:262:PRO:O	17:i:266:ILE:HG13	2.13	0.48
23:p:55:GLN:O	23:p:59:LEU:HG	2.14	0.48
24:q:4:ILE:HD13	24:q:37:ILE:HG22	1.95	0.48
24:q:23:ILE:HD11	24:q:92:LYS:HE2	1.96	0.48
24:q:366:ASN:HD22	24:q:407:SER:HB3	1.78	0.48
25:r:164:THR:O	25:r:168:THR:HG23	2.13	0.48
25:r:272:TRP:CZ2	31:H:74:LEU:HB2	2.49	0.48
26:B:219:LYS:HG2	33:J:173:SER:O	2.14	0.48
26:B:230:PRO:HA	26:B:233:VAL:O	2.14	0.48
26:B:246:GLU:O	26:B:250:VAL:HG13	2.13	0.48
27:C:112:VAL:HG12	27:C:448:HIS:O	2.14	0.48
31:H:186:ASN:HB2	34:K:124:TYR:OH	2.14	0.48
35:L:76:ILE:HG21	35:L:101:MET:HE2	1.96	0.48
35:L:126:GLY:H	60:L:401:NDP:H52A	1.79	0.48
40:R:95:LYS:HE2	40:R:96:PHE:CZ	2.49	0.48
2:Ac:19:SER:HB3	4:Ad:23:MET:HB3	1.96	0.48
51:5:79:SER:HA	51:5:82:GLU:OE1	2.14	0.48
53:G:347:ASP:O	53:G:351:LEU:HG	2.14	0.48
3:2:265:ASP:OD1	3:2:269:ARG:N	2.46	0.47
5:6:170:GLN:CD	5:6:170:GLN:H	2.21	0.47
5:6:227:HIS:N	5:6:228:PRO:HD2	2.29	0.47
6:7:156:ILE:HG13	6:7:157:GLY:H	1.78	0.47
10:b:93:LYS:HB3	10:b:96:THR:HG23	1.95	0.47
14:f:29:PHE:CZ	43:U:102:ASP:HB3	2.49	0.47
17:i:65:THR:HG22	19:k:19:LEU:HD23	1.95	0.47
19:k:37:MET:HG3	19:k:67:ALA:CB	2.44	0.47
19:k:97:GLN:HA	48:l:582:GLY:HA3	1.96	0.47
24:q:163:ALA:O	24:q:167:ILE:HG13	2.14	0.47
26:B:91:ALA:HB1	26:B:93:PHE:CE2	2.49	0.47
27:C:112:VAL:HG13	27:C:112:VAL:O	2.13	0.47
37:O:87:LEU:HG	37:O:122:MET:HE1	1.95	0.47
37:O:104:PHE:CB	37:O:110:LEU:HD11	2.44	0.47
5:v:338:ILE:HG21	5:v:354:ALA:HB1	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:146:LEU:O	51:5:150:ILE:HG13	2.14	0.47
51:5:302:VAL:HB	51:5:303:PRO:HD3	1.95	0.47
53:G:389:THR:OG1	53:G:511:LYS:O	2.32	0.47
3:2:111:ASP:OD1	3:2:111:ASP:N	2.45	0.47
5:6:409:PRO:O	5:6:413:LEU:HD13	2.14	0.47
9:a:161:ARG:HH11	44:V:141:VAL:HB	1.79	0.47
14:f:30:TYR:CD2	14:f:34:PRO:HG3	2.49	0.47
15:g:32:ARG:HD2	17:i:339:MET:HE1	1.96	0.47
18:j:113:TRP:O	18:j:114:ALA:HB3	2.14	0.47
20:m:70:TYR:CE2	20:m:74:MET:HE3	2.50	0.47
24:q:294:MET:O	24:q:298:ILE:HG13	2.14	0.47
24:q:306:PRO:O	24:q:310:MET:HG3	2.14	0.47
25:r:8:SER:O	25:r:12:PRO:HG2	2.13	0.47
25:r:202:GLU:HG2	25:r:209:SER:O	2.14	0.47
25:r:277:TYR:CZ	31:H:70:LEU:HD13	2.49	0.47
27:C:147:TYR:CE2	27:C:463:VAL:HG23	2.48	0.47
27:C:468:ASP:HA	28:D:188:LEU:CD2	2.44	0.47
29:E:215:LYS:HG3	29:E:215:LYS:O	2.14	0.47
35:L:84:TYR:HA	35:L:87:MET:HE2	1.95	0.47
35:L:273:GLN:HG3	35:L:283:PHE:HD2	1.79	0.47
46:Y:71:TRP:CZ3	47:Z:97:ALA:HB1	2.48	0.47
7:x:322:TYR:HB2	8:y:61:PHE:CE1	2.49	0.47
52:Aa:51:PRO:HB2	52:Aa:52:PRO:HD3	1.95	0.47
3:2:173:ILE:HD12	3:2:175:ILE:CD1	2.34	0.47
5:6:121:TYR:CB	5:6:137:LEU:HD11	2.44	0.47
5:6:181:ALA:O	5:6:254:ARG:N	2.44	0.47
5:6:425:ILE:HG22	5:6:429:LYS:NZ	2.30	0.47
8:9:85:GLU:CD	8:9:85:GLU:H	2.22	0.47
13:e:87:MET:HG3	13:e:88:ARG:N	2.29	0.47
17:i:247:THR:O	17:i:251:MET:HG3	2.13	0.47
24:q:399:ASN:O	24:q:403:THR:HG23	2.14	0.47
25:r:6:ILE:O	25:r:10:ILE:HG13	2.15	0.47
25:r:54:LYS:HD3	32:I:61:SER:HB2	1.97	0.47
26:B:168:ASN:OD1	40:R:81:TYR:HE2	1.97	0.47
28:D:216:VAL:HG21	28:D:218:ARG:NH2	2.29	0.47
31:H:86:TYR:CG	31:H:87:PRO:HA	2.49	0.47
31:H:88:PHE:CZ	34:K:30:ALA:HA	2.49	0.47
31:H:116:CYS:N	59:H:302:SF4:S4	2.68	0.47
33:J:77:VAL:CG2	33:J:99:MET:HG2	2.44	0.47
37:O:126:PHE:CE1	37:O:148:ILE:HD13	2.49	0.47
39:Q:91:GLU:HG2	39:Q:95:LYS:HZ1	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:V:37:SER:O	44:V:41:ILE:HG12	2.14	0.47
48:l:10:THR:O	48:l:14:ILE:HG13	2.14	0.47
49:s:157:GLU:HB2	49:s:158:PRO:HD3	1.96	0.47
5:v:295:ALA:HB1	3:Af:46:LEU:CB	2.45	0.47
51:5:454:PRO:HG3	51:5:475:MET:HG3	1.95	0.47
53:G:414:PHE:CE2	53:G:418:ILE:HD11	2.49	0.47
54:M:12:ARG:HG3	54:M:13:ASN:N	2.28	0.47
16:h:91:LYS:NZ	16:h:91:LYS:HB2	2.29	0.47
22:o:49:LEU:HD23	23:p:208:LEU:HD21	1.97	0.47
27:C:133:LYS:O	27:C:425:PRO:HD2	2.13	0.47
28:D:210:LEU:HD21	39:Q:131:ARG:HH22	1.80	0.47
48:l:504:LEU:O	48:l:507:THR:OG1	2.30	0.47
51:u:247:GLN:O	51:u:251:SER:HB2	2.15	0.47
7:x:214:SER:O	7:x:218:GLY:N	2.47	0.47
53:G:522:GLN:O	53:G:526:LEU:HG	2.15	0.47
6:7:223:TYR:HB3	7:8:312:TRP:NE1	2.29	0.47
6:7:277:ALA:HB1	6:7:294:LEU:HG	1.96	0.47
7:8:313:SER:OG	52:Aa:24:GLN:NE2	2.48	0.47
12:d:54:GLN:O	12:d:58:LYS:HG3	2.15	0.47
13:e:98:VAL:HG11	24:q:71:TRP:HZ3	1.80	0.47
15:g:41:TYR:O	15:g:45:LEU:HG	2.14	0.47
16:h:105:ARG:O	45:W:82:ARG:HD3	2.15	0.47
17:i:70:LEU:O	17:i:74:ILE:HG13	2.14	0.47
20:m:7:PHE:O	20:m:11:THR:HG23	2.15	0.47
22:o:3:PHE:CZ	23:p:112:GLU:HG3	2.50	0.47
26:B:212:LEU:HD23	26:B:212:LEU:O	2.14	0.47
28:D:63:GLN:HG3	54:M:69:VAL:HG12	1.96	0.47
29:E:132:ILE:CD1	29:E:169:PHE:HB3	2.45	0.47
39:Q:65:TRP:O	39:Q:69:VAL:HG23	2.14	0.47
46:Y:83:HIS:O	46:Y:85:PRO:HD3	2.15	0.47
48:l:41:SER:O	48:l:45:THR:HG23	2.14	0.47
48:l:343:SER:O	48:l:347:ILE:HG13	2.14	0.47
49:s:178:ARG:HD3	49:s:178:ARG:HA	1.66	0.47
51:5:405:GLY:O	51:5:409:VAL:HG23	2.15	0.47
5:6:271:LEU:O	5:6:337:GLY:HA3	2.13	0.47
5:6:322:ASP:HB2	3:Ae:72:ARG:HB2	1.97	0.47
5:6:322:ASP:C	3:Ae:68:LEU:HD11	2.40	0.47
9:a:82:VAL:HG11	13:e:104:THR:HG21	1.95	0.47
18:j:69:ILE:HD11	25:r:148:ILE:HG13	1.96	0.47
24:q:243:MET:HA	24:q:246:ILE:HG22	1.96	0.47
24:q:307:TRP:HA	24:q:310:MET:HE2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:q:400:MET:CE	48:l:183:VAL:HG21	2.43	0.47
25:r:179:TRP:CG	25:r:180:PRO:HD3	2.50	0.47
27:C:299:LEU:HD22	27:C:304:ILE:HD13	1.96	0.47
36:N:26:ILE:O	36:N:30:LYS:HG3	2.14	0.47
49:s:121:MET:HA	49:s:121:MET:CE	2.40	0.47
6:w:69:ILE:HA	6:w:73:VAL:CG2	2.45	0.47
2:Ac:56:ILE:HB	2:Ac:59:LYS:HE2	1.96	0.47
53:G:141:ASP:O	53:G:145:MET:HG2	2.15	0.47
53:G:358:LEU:O	53:G:361:VAL:HG23	2.13	0.47
3:4:216:LEU:CD1	3:4:269:ARG:HD2	2.40	0.47
5:6:378:LEU:HD22	3:Ae:38:ARG:NH1	2.30	0.47
11:c:86:ARG:HD3	11:c:98:ARG:O	2.14	0.47
12:d:27:PRO:HB2	12:d:32:TYR:CE2	2.50	0.47
17:i:13:VAL:HG13	17:i:36:ASN:ND2	2.29	0.47
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.96	0.47
17:i:203:LEU:HD21	17:i:261:MET:HE2	1.97	0.47
17:i:344:SER:O	17:i:347:ASN:HB3	2.15	0.47
17:i:346:LEU:HD12	17:i:347:ASN:N	2.29	0.47
18:j:67:LEU:HD21	19:k:68:ALA:CB	2.44	0.47
22:o:20:PRO:HA	23:p:107:ARG:HH12	1.79	0.47
24:q:412:ILE:O	24:q:416:ARG:HB2	2.15	0.47
27:C:163:LYS:HD2	28:D:81:PHE:HB2	1.97	0.47
29:E:59:ASN:O	29:E:63:ILE:HG13	2.14	0.47
29:E:191:ASN:HB3	29:E:216:PRO:HB3	1.96	0.47
29:E:196:LEU:HD13	29:E:201:ILE:HG12	1.97	0.47
31:H:111:GLU:O	31:H:141:ARG:NH1	2.48	0.47
32:I:67:PHE:HZ	32:I:113:MET:HE2	1.77	0.47
35:L:57:THR:HG21	35:L:86:THR:HG22	1.97	0.47
43:U:51:THR:HG21	43:U:153:LEU:HD22	1.95	0.47
43:U:162:GLU:O	43:U:163:ARG:HB2	2.15	0.47
46:Y:79:ALA:O	46:Y:80:VAL:HG13	2.15	0.47
48:l:304:PHE:CZ	48:l:526:LEU:HD22	2.49	0.47
49:s:136:GLU:O	49:s:140:VAL:HG23	2.14	0.47
51:u:49:GLN:O	51:u:60:ALA:HA	2.15	0.47
5:v:85:LEU:CD1	5:v:158:LEU:HD12	2.41	0.47
6:w:112:THR:HG22	6:w:196:HIS:NE2	2.29	0.47
6:w:237:LEU:O	6:w:241:ILE:HG13	2.14	0.47
6:w:294:LEU:HD23	6:w:294:LEU:C	2.40	0.47
7:x:103:LEU:HD13	7:x:291:LEU:HD13	1.97	0.47
7:x:142:THR:HG22	7:x:145:GLU:CG	2.44	0.47
7:x:203:ARG:CG	7:x:279:SER:HB3	2.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ac:53:TRP:O	2:Ac:57:LYS:N	2.48	0.47
53:G:402:LEU:HD23	53:G:475:VAL:HB	1.96	0.47
3:2:142:THR:OG1	7:x:303:LEU:HB3	2.14	0.47
5:6:177:LEU:HD11	5:6:272:VAL:CG2	2.44	0.47
6:7:27:ILE:HG23	6:7:224:TYR:OH	2.14	0.47
7:8:125:CYS:C	7:8:179:PRO:HG2	2.40	0.47
19:k:8:ILE:HD13	19:k:42:ILE:CG2	2.44	0.47
22:o:5:LYS:HE3	22:o:7:LYS:CD	2.45	0.47
24:q:66:LEU:HD21	24:q:110:PHE:HB2	1.97	0.47
24:q:266:MET:HE2	24:q:395:LEU:HD12	1.95	0.47
26:B:318:ILE:CD1	26:B:326:LEU:HB3	2.44	0.47
26:B:383:THR:HB	26:B:384:PRO:HD3	1.96	0.47
35:L:168:ASP:CG	35:L:170:LYS:HE3	2.40	0.47
37:O:84:LEU:HB3	37:O:88:LYS:HZ3	1.77	0.47
43:U:51:THR:O	43:U:54:LYS:HG3	2.14	0.47
43:U:245:LYS:O	43:U:249:PRO:HG2	2.15	0.47
48:l:232:TRP:HZ3	48:l:248:HIS:HD2	1.63	0.47
5:6:40:PHE:CZ	5:6:48:VAL:HG11	2.50	0.47
5:6:42:ARG:HD3	5:6:48:VAL:CG2	2.45	0.47
5:6:375:LYS:O	5:6:379:LYS:HG3	2.15	0.47
7:8:168:ARG:HH12	7:8:171:LYS:HG2	1.80	0.47
20:m:104:VAL:O	20:m:108:LEU:HG	2.14	0.47
23:p:205:LEU:HD13	23:p:209:TRP:CE2	2.50	0.47
25:r:20:LEU:HD23	25:r:228:TYR:HB3	1.97	0.47
26:B:316:ALA:HB2	26:B:442:PHE:CE1	2.50	0.47
35:L:76:ILE:CG2	35:L:101:MET:HE2	2.45	0.47
43:U:213:VAL:N	43:U:214:PRO:HD2	2.29	0.47
45:W:110:VAL:HG13	45:W:110:VAL:O	2.14	0.47
48:l:268:GLU:HG3	48:l:320:ASN:OD1	2.15	0.47
48:l:271:LYS:O	48:l:275:THR:HG23	2.14	0.47
51:u:449:PHE:O	51:u:475:MET:HE3	2.15	0.47
5:v:40:PHE:CE1	5:v:406:TYR:HB2	2.49	0.47
7:x:172:LEU:HD12	7:x:173:SER:N	2.29	0.47
51:5:283:PRO:O	51:5:284:LEU:HD13	2.14	0.47
53:G:127:ASP:O	53:G:131:CYS:N	2.48	0.47
3:2:157:PHE:O	3:2:160:SER:OG	2.29	0.47
3:2:262:SER:OG	55:2:301:FES:S2	2.64	0.47
3:4:235:ILE:HG22	3:4:280:GLU:HB3	1.97	0.47
5:6:67:ALA:HB1	5:6:208:TYR:HE1	1.80	0.47
5:6:214:THR:O	5:6:218:MET:HG3	2.15	0.47
5:6:227:HIS:O	5:6:231:LYS:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:227:HIS:HD2	5:6:231:LYS:HD2	1.78	0.47
16:h:17:TRP:CZ2	20:m:150:GLY:HA2	2.50	0.47
24:q:353:PRO:O	24:q:356:ALA:HB3	2.15	0.47
29:E:152:ILE:HD11	29:E:201:ILE:HG13	1.96	0.47
35:L:101:MET:HE1	35:L:114:VAL:HA	1.96	0.47
48:l:213:LEU:HB3	48:l:273:VAL:HG11	1.97	0.47
51:u:121:ASN:OD1	5:v:300:LYS:HD3	2.15	0.47
51:u:274:GLU:CD	51:u:276:ARG:HE	2.23	0.47
51:u:287:VAL:HB	51:u:358:PHE:CZ	2.50	0.47
6:w:25:SER:HB3	6:w:218:ILE:CG2	2.44	0.47
6:w:41:LEU:HA	6:w:90:PHE:HE2	1.79	0.47
52:z:37:ASN:OD1	52:z:40:ARG:NH1	2.47	0.47
53:G:389:THR:N	53:G:514:ASN:OD1	2.38	0.47
2:1:30:LEU:HD21	4:3:48:ILE:HG21	1.97	0.46
6:7:41:LEU:HD12	56:7:401:HEM:HBB1	1.96	0.46
6:7:89:MET:HE2	6:7:235:MET:HG3	1.96	0.46
7:8:116:GLN:O	7:8:120:GLN:NE2	2.47	0.46
17:i:261:MET:N	17:i:262:PRO:HD2	2.30	0.46
23:p:197:PRO:O	23:p:207:PRO:HD2	2.15	0.46
25:r:168:THR:HG22	45:W:57:ARG:NH2	2.29	0.46
26:B:225:LEU:C	26:B:227:PRO:HD2	2.40	0.46
27:C:255:LYS:HA	45:W:19:ILE:HG23	1.97	0.46
41:S:67:GLU:HG2	41:S:68:ASN:N	2.30	0.46
43:U:353:TRP:HZ3	43:U:356:LEU:HD12	1.79	0.46
37:X:86:VAL:CG2	37:X:125:GLU:HG3	2.45	0.46
5:v:177:LEU:HD21	5:v:272:VAL:HG11	1.96	0.46
7:x:190:ASN:HB3	57:x:401:HEC:CMD	2.45	0.46
4:Ad:23:MET:O	4:Ad:27:VAL:HG23	2.15	0.46
53:G:618:GLU:HB3	53:G:621:LYS:HG3	1.96	0.46
3:4:189:LYS:HZ3	6:w:261:PRO:HB2	1.80	0.46
3:4:257:CYS:HB2	3:4:259:CYS:SG	2.55	0.46
9:a:170:GLN:HA	9:a:170:GLN:NE2	2.30	0.46
22:o:39:ILE:HG23	22:o:42:ARG:HH21	1.80	0.46
27:C:146:ASP:CG	27:C:463:VAL:HG11	2.40	0.46
27:C:190:ILE:HG21	27:C:213:ARG:HG3	1.96	0.46
31:H:118:LEU:HD22	31:H:163:PRO:HD3	1.97	0.46
34:K:27:LEU:O	34:K:31:ASN:HA	2.14	0.46
48:l:51:LEU:HG	48:l:55:MET:HE3	1.97	0.46
48:l:128:MET:HG2	48:l:251:THR:HG22	1.98	0.46
5:v:320:PRO:HB3	3:Af:75:LEU:HB2	1.96	0.46
52:z:25:ARG:NH1	52:z:28:PRO:HA	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:199:HIS:HB2	3:2:231:TRP:CZ3	2.50	0.46
6:7:113:TRP:O	6:7:117:VAL:HG23	2.16	0.46
10:b:5:THR:OG1	10:b:8:GLU:HG3	2.16	0.46
12:d:43:ARG:HB3	12:d:44:PRO:HD3	1.97	0.46
12:d:170:ALA:O	12:d:171:LYS:HB2	2.15	0.46
25:r:198:PHE:CD1	25:r:285:LEU:HD13	2.50	0.46
26:B:267:ARG:HD2	26:B:293:SER:HB3	1.96	0.46
29:E:134:VAL:HG22	29:E:186:VAL:HG12	1.97	0.46
35:L:235:VAL:HG22	35:L:261:VAL:HA	1.97	0.46
48:l:154:LEU:HD12	48:l:247:LEU:HD11	1.97	0.46
49:s:102:LEU:HD23	49:s:148:PHE:HZ	1.80	0.46
5:v:51:SER:HA	5:v:222:GLY:O	2.15	0.46
5:v:95:SER:O	5:v:99:ILE:HG13	2.15	0.46
6:w:26:ASN:HD21	6:w:207:ASN:HB2	1.79	0.46
6:w:225:THR:O	6:w:229:ILE:HG13	2.16	0.46
3:2:240:HIS:CE1	3:2:274:PRO:HB2	2.51	0.46
3:4:177:LEU:O	3:4:178:SER:OG	2.26	0.46
11:c:126:TRP:HA	11:c:129:MET:HE2	1.95	0.46
17:i:49:ASN:O	17:i:53:THR:HG23	2.15	0.46
20:m:159:TRP:CZ2	20:m:163:ILE:HD11	2.51	0.46
24:q:313:THR:HA	24:q:316:MET:HE2	1.97	0.46
25:r:185:TRP:NE1	25:r:238:THR:HG22	2.24	0.46
26:B:98:LYS:HA	26:B:101:PHE:CD2	2.50	0.46
26:B:138:LEU:HD22	26:B:245:VAL:HG13	1.98	0.46
26:B:170:GLN:OE1	26:B:197:VAL:HB	2.16	0.46
27:C:377:MET:HG3	27:C:378:LYS:N	2.29	0.46
31:H:144:ARG:HB2	34:K:130:THR:HG23	1.97	0.46
7:x:243:ILE:HG23	7:x:245:MET:N	2.30	0.46
3:Ae:45:PRO:C	3:Ae:47:GLY:N	2.72	0.46
3:Af:45:PRO:HB2	3:Af:48:PRO:HD3	1.98	0.46
3:Af:53:VAL:CG1	3:Af:60:PRO:HD2	2.46	0.46
3:4:186:MET:HB3	3:4:188:PHE:CZ	2.50	0.46
6:7:88:SER:HB3	6:7:272:TRP:HE1	1.79	0.46
6:7:133:LEU:HA	6:7:175:LEU:HD11	1.98	0.46
6:7:267:HIS:NE2	6:7:269:LYS:HE3	2.30	0.46
11:c:81:ARG:HD2	22:o:13:THR:HG21	1.98	0.46
17:i:51:ARG:HG3	27:C:75:VAL:CG2	2.46	0.46
17:i:222:SER:HA	17:i:237:MET:HE1	1.97	0.46
19:k:63:LEU:HD23	19:k:63:LEU:C	2.40	0.46
24:q:245:ARG:O	24:q:248:THR:HG23	2.15	0.46
34:K:105:ALA:C	34:K:106:ARG:HD2	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:P:83:SER:OG	38:P:86:GLN:HG3	2.15	0.46
41:S:22:ALA:O	41:S:26:ILE:HG13	2.16	0.46
44:V:62:THR:CG2	44:V:104:ARG:HD3	2.32	0.46
48:l:95:PHE:CZ	48:l:456:ARG:HB3	2.50	0.46
48:l:144:TRP:CZ2	48:l:223:LYS:CG	2.99	0.46
5:v:371:VAL:O	5:v:375:LYS:HG3	2.15	0.46
53:G:588:ALA:O	53:G:592:LYS:HD2	2.15	0.46
4:3:3:SER:HA	4:3:6:LEU:HD22	1.97	0.46
6:7:331:ASP:OD2	6:7:357:LEU:HB3	2.15	0.46
13:e:74:HIS:O	24:q:431:THR:HG22	2.15	0.46
15:g:110:THR:HG22	15:g:113:GLU:HG3	1.97	0.46
16:h:77:SER:HB3	20:m:122:LEU:CD1	2.42	0.46
25:r:206:GLU:CD	27:C:451:ALA:HB2	2.40	0.46
25:r:308:PRO:HA	25:r:313:SER:OG	2.16	0.46
26:B:389:VAL:HA	26:B:392:MET:HE2	1.97	0.46
27:C:208:TRP:CZ3	27:C:267:MET:HG3	2.50	0.46
28:D:119:VAL:CG1	28:D:122:ARG:HD2	2.46	0.46
31:H:119:CYS:CB	59:H:302:SF4:S3	3.01	0.46
35:L:122:ILE:CG2	35:L:124:LEU:HD11	2.45	0.46
35:L:274:TYR:O	35:L:278:VAL:HG22	2.15	0.46
41:S:40:HIS:H	41:S:44:GLN:HE22	1.63	0.46
51:u:317:THR:HB	3:Af:53:VAL:HG11	1.95	0.46
5:v:320:PRO:HA	3:Af:75:LEU:HG	1.96	0.46
51:5:226:ALA:N	51:5:227:PRO:HD2	2.30	0.46
53:G:82:ILE:HD11	53:G:89:VAL:HG21	1.96	0.46
3:2:173:ILE:HG12	3:2:190:TRP:CD1	2.51	0.46
6:7:129:MET:HE1	6:7:185:LEU:HD12	1.96	0.46
7:8:295:MET:HE1	2:Ac:40:ALA:HB2	1.97	0.46
15:g:13:LEU:HD11	16:h:4:PHE:HB3	1.98	0.46
15:g:24:PRO:CD	49:s:237:PRO:HG3	2.46	0.46
15:g:84:MET:HG2	17:i:344:SER:O	2.15	0.46
17:i:182:SER:HB2	17:i:293:TYR:OH	2.15	0.46
17:i:256:PRO:HD3	24:q:124:ALA:CB	2.46	0.46
24:q:197:LEU:O	24:q:201:MET:HG2	2.16	0.46
26:B:342:LEU:HD13	26:B:349:LEU:HA	1.98	0.46
27:C:284:VAL:CG1	27:C:444:MET:HG2	2.46	0.46
37:O:141:PRO:O	37:O:145:VAL:HG23	2.16	0.46
43:U:50:ARG:O	43:U:53:ARG:HG2	2.16	0.46
45:W:93:GLU:OE2	45:W:127:LEU:HD12	2.16	0.46
45:W:121:MET:HE1	45:W:136:ALA:CB	2.45	0.46
46:Y:47:PHE:HA	47:Z:73:PHE:CZ	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:591:PHE:O	48:l:595:ILE:HG13	2.14	0.46
51:u:477:TRP:HB3	51:u:479:ARG:HG2	1.96	0.46
6:w:41:LEU:O	6:w:45:ILE:HG13	2.16	0.46
7:x:142:THR:HG22	7:x:145:GLU:HG3	1.96	0.46
7:x:234:PHE:CE1	7:x:241:GLN:HB3	2.50	0.46
51:5:216:LEU:O	51:5:220:VAL:HG23	2.15	0.46
5:6:89:LEU:HD11	5:6:154:LEU:HD12	1.97	0.46
5:6:115:THR:O	5:6:116:ARG:C	2.57	0.46
5:6:182:TYR:O	5:6:187:ALA:HB2	2.15	0.46
5:6:354:ALA:O	5:6:358:VAL:HG23	2.16	0.46
5:6:383:LEU:HD12	51:5:136:LEU:HD22	1.97	0.46
24:q:243:MET:O	24:q:247:THR:HG23	2.15	0.46
25:r:200:LEU:HD13	25:r:282:TYR:CB	2.46	0.46
35:L:97:GLN:OE1	35:L:97:GLN:HA	2.16	0.46
43:U:102:ASP:HB2	43:U:104:LYS:HE2	1.98	0.46
46:Y:54:GLN:HE21	48:l:446:ASN:CB	2.24	0.46
48:l:125:LEU:O	48:l:129:MET:HG2	2.16	0.46
48:l:409:LEU:O	48:l:413:LEU:HG	2.16	0.46
48:l:561:ILE:O	48:l:565:THR:OG1	2.33	0.46
50:t:52:MET:O	50:t:56:ARG:HG3	2.16	0.46
5:v:324:SER:CB	3:Af:68:LEU:HG	2.46	0.46
8:y:110:LYS:NZ	4:Ad:6:LEU:O	2.47	0.46
52:z:51:PRO:HD2	52:z:52:PRO:HD3	1.98	0.46
3:2:244:VAL:O	3:2:244:VAL:HG13	2.16	0.46
5:6:70:ARG:HH22	5:6:332:ASP:HB2	1.81	0.46
5:6:106:VAL:HG21	5:6:133:LEU:HD13	1.98	0.46
13:e:52:THR:O	43:U:317:PRO:HB3	2.15	0.46
24:q:336:ARG:NH2	24:q:429:SER:HA	2.30	0.46
25:r:105:MET:HE1	25:r:162:LEU:HD21	1.98	0.46
25:r:310:MET:O	42:T:123:TYR:HB2	2.15	0.46
26:B:375:LYS:HE3	26:B:390:ASP:OD1	2.15	0.46
27:C:90:PHE:HZ	27:C:454:VAL:HG22	1.79	0.46
27:C:103:LEU:HD12	27:C:117:PRO:HA	1.97	0.46
27:C:159:LEU:HD13	27:C:159:LEU:HA	1.82	0.46
28:D:121:THR:OG1	33:J:128:PHE:HA	2.16	0.46
28:D:152:PRO:HG2	39:Q:44:LYS:HE2	1.97	0.46
29:E:180:CYS:SG	55:E:301:FES:S2	3.12	0.46
42:T:155:PRO:O	42:T:156:GLN:HB2	2.15	0.46
46:Y:40:ILE:HD12	46:Y:40:ILE:N	2.31	0.46
51:u:274:GLU:CG	51:u:276:ARG:HE	2.27	0.46
6:w:8:HIS:O	6:w:12:LYS:N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:w:142:GLY:O	6:w:146:ILE:HG12	2.16	0.46
3:2:173:ILE:HG23	3:2:190:TRP:CD1	2.47	0.46
5:6:290:GLN:HB2	5:6:336:PHE:HE1	1.80	0.46
15:g:2:THR:HG22	15:g:3:MET:N	2.31	0.46
22:o:103:TYR:O	22:o:107:THR:HG23	2.16	0.46
26:B:77:LEU:O	26:B:81:LYS:HG3	2.16	0.46
27:C:259:PHE:HB3	27:C:260:ARG:NH1	2.31	0.46
33:J:169:ARG:NH1	40:R:105:ARG:HH12	2.14	0.46
35:L:119:ASN:ND2	35:L:120:VAL:HG23	2.18	0.46
35:L:278:VAL:CG2	35:L:348:LEU:HD12	2.46	0.46
41:S:15:CYS:O	41:S:19:PRO:HD3	2.15	0.46
43:U:297:ARG:HA	43:U:300:VAL:CG2	2.45	0.46
47:Z:73:PHE:CG	48:l:435:PRO:HG3	2.50	0.46
48:l:565:THR:O	48:l:569:ILE:HG13	2.15	0.46
5:v:121:TYR:HB3	5:v:137:LEU:CD1	2.46	0.46
7:x:130:TYR:HB2	7:x:199:SER:OG	2.16	0.46
54:M:12:ARG:HD3	54:M:20:LEU:HD12	1.97	0.46
3:Ae:75:LEU:O	3:Ae:76:CYS:C	2.59	0.46
3:Af:45:PRO:HB3	3:Af:66:PRO:HD3	1.98	0.46
5:6:127:ARG:HH21	5:6:224:GLY:CA	2.28	0.45
6:7:106:SER:HA	6:7:313:ARG:HH21	1.81	0.45
7:8:218:GLY:O	7:8:236:PRO:HD2	2.16	0.45
7:8:245:MET:HB2	57:8:401:HEC:C1D	2.45	0.45
7:8:314:VAL:CG2	52:Aa:21:PRO:HG3	2.46	0.45
11:c:78:LEU:HD11	11:c:104:PRO:HB2	1.98	0.45
16:h:89:GLU:HB3	16:h:91:LYS:CE	2.45	0.45
25:r:222:MET:HA	25:r:225:MET:HE3	1.98	0.45
27:C:190:ILE:HD11	27:C:257:PHE:CZ	2.51	0.45
28:D:87:PHE:CE1	28:D:144:LYS:HE2	2.50	0.45
35:L:59:PHE:CE2	35:L:237:ILE:HD13	2.50	0.45
43:U:291:ARG:HH22	43:U:294:HIS:CD2	2.32	0.45
44:V:69:ILE:HG13	44:V:100:THR:CG2	2.40	0.45
45:W:129:THR:HG23	45:W:132:GLU:H	1.82	0.45
48:l:102:GLU:HA	48:l:105:MET:HE3	1.98	0.45
5:v:338:ILE:HD11	5:v:358:VAL:HG21	1.98	0.45
6:w:82:LEU:HD23	6:w:243:VAL:HG21	1.98	0.45
6:w:133:LEU:HA	6:w:175:LEU:HD11	1.98	0.45
3:4:270:ILE:HG22	3:4:278:ASN:OD1	2.17	0.45
5:6:47:LEU:CD2	5:6:234:ALA:HB1	2.47	0.45
5:6:111:SER:CB	3:Ae:59:LEU:HG	2.42	0.45
6:7:195:VAL:HG12	6:7:199:PHE:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:261:MET:HB3	17:i:337:LEU:HD12	1.98	0.45
21:n:17:VAL:N	21:n:18:PRO:HD2	2.31	0.45
22:o:5:LYS:C	22:o:5:LYS:HD3	2.39	0.45
29:E:169:PHE:CE2	29:E:209:LYS:HG3	2.44	0.45
35:L:256:LYS:HZ1	35:L:258:PHE:HZ	1.63	0.45
35:L:359:SER:HB2	35:L:363:ASP:OD2	2.17	0.45
38:P:20:ARG:HB2	38:P:66:TRP:HB2	1.98	0.45
43:U:75:LEU:O	43:U:79:ILE:HG13	2.17	0.45
43:U:142:LEU:HA	43:U:165:ILE:HG21	1.98	0.45
48:l:76:LEU:HD11	48:l:196:TRP:CZ3	2.52	0.45
48:l:188:TRP:HZ2	48:l:209:PRO:HG2	1.80	0.45
48:l:395:ILE:O	48:l:399:VAL:HG23	2.15	0.45
50:t:97:LYS:O	50:t:101:GLU:HG3	2.17	0.45
7:x:268:ALA:O	7:x:271:VAL:HG12	2.16	0.45
52:z:33:LYS:C	52:z:36:PRO:HD2	2.41	0.45
52:Aa:79:GLU:HG2	52:Aa:80:ASN:N	2.28	0.45
2:Ac:11:TYR:OH	51:5:451:ASP:HB3	2.16	0.45
53:G:577:ALA:HB3	53:G:578:PRO:HD3	1.98	0.45
15:g:27:LYS:NZ	15:g:27:LYS:HB3	2.31	0.45
17:i:215:MET:HG3	17:i:251:MET:SD	2.56	0.45
18:j:5:LEU:O	18:j:9:THR:HG23	2.16	0.45
22:o:83:THR:H	22:o:86:THR:HG1	1.64	0.45
22:o:111:LYS:O	22:o:114:LYS:HE2	2.16	0.45
23:p:217:ARG:O	23:p:220:PRO:HG3	2.16	0.45
26:B:451:GLN:O	26:B:455:LEU:HG	2.15	0.45
27:C:144:ARG:HD2	59:I:201:SF4:S4	2.55	0.45
27:C:159:LEU:HD22	27:C:177:ARG:HH21	1.82	0.45
27:C:197:ALA:HA	27:C:200:ILE:CG1	2.46	0.45
27:C:305:GLN:HB3	54:M:104:TRP:CE3	2.51	0.45
27:C:322:PHE:CG	27:C:349:ILE:HD11	2.50	0.45
28:D:111:LEU:HD23	28:D:131:ASN:O	2.15	0.45
35:L:125:VAL:HG13	60:L:401:NDP:C4A	2.46	0.45
36:N:55:LYS:O	36:N:59:VAL:HG23	2.16	0.45
6:w:309:THR:OG1	6:w:370:SER:HB2	2.16	0.45
6:w:338:ILE:HD13	6:w:351:GLY:N	2.31	0.45
54:M:96:THR:HB	54:M:97:PRO:HD2	1.98	0.45
3:2:230:GLU:HB2	3:2:231:TRP:CD1	2.52	0.45
5:6:214:THR:OG1	5:6:217:ARG:HD3	2.17	0.45
10:b:76:LEU:HA	10:b:76:LEU:HD23	1.71	0.45
24:q:60:SER:HB2	24:q:457:PRO:HA	1.97	0.45
25:r:117:LEU:HD13	25:r:117:LEU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:66:LYS:O	26:B:70:LEU:HG	2.16	0.45
26:B:205:ILE:HG21	26:B:379:CYS:SG	2.57	0.45
27:C:197:ALA:HB1	27:C:202:ALA:HB3	1.99	0.45
45:W:74:LEU:O	45:W:78:GLU:HG3	2.14	0.45
46:Y:47:PHE:CE1	48:l:364:LYS:HD3	2.46	0.45
46:Y:55:LEU:H	46:Y:55:LEU:HD12	1.82	0.45
48:l:470:ASN:HD22	48:l:470:ASN:N	2.15	0.45
51:u:265:PHE:HE2	51:u:350:GLU:HG2	1.80	0.45
5:v:49:ILE:HD13	5:v:231:LYS:HA	1.98	0.45
5:6:106:VAL:HG21	5:6:133:LEU:CD1	2.47	0.45
9:a:96:ALA:HB2	12:d:61:TYR:CE2	2.51	0.45
18:j:78:ALA:O	18:j:81:THR:HG23	2.16	0.45
24:q:451:PRO:HA	24:q:454:ILE:HD11	1.97	0.45
25:r:102:VAL:HG11	25:r:154:LEU:HD11	1.97	0.45
27:C:62:LYS:HG3	27:C:63:GLU:H	1.82	0.45
30:F:84:ILE:C	30:F:84:ILE:HD12	2.42	0.45
41:S:37:ARG:HG3	49:s:170:GLY:O	2.16	0.45
44:V:66:ILE:HD11	44:V:101:LEU:HB2	1.98	0.45
48:l:34:ASN:O	48:l:38:THR:HG23	2.16	0.45
50:t:108:LEU:HD23	50:t:111:ARG:NH1	2.30	0.45
51:u:103:ASN:HB2	51:u:149:ASP:OD2	2.17	0.45
51:u:405:GLY:O	51:u:408:PRO:HD2	2.17	0.45
6:w:311:LYS:HG2	6:w:374:ASN:ND2	2.32	0.45
3:2:191:ARG:HD2	6:7:168:PHE:CD2	2.51	0.45
56:7:402:HEM:HMC2	56:7:402:HEM:CBC	2.34	0.45
18:j:109:LYS:HE2	18:j:109:LYS:CA	2.46	0.45
24:q:118:PHE:O	24:q:122:PHE:HB3	2.16	0.45
25:r:145:THR:O	25:r:149:ILE:HG13	2.17	0.45
25:r:258:ASN:O	25:r:262:LYS:HG3	2.16	0.45
25:r:307:LEU:CD1	25:r:310:MET:HE3	2.47	0.45
26:B:41:ILE:HG13	26:B:42:PHE:CD2	2.51	0.45
26:B:284:HIS:CD2	26:B:305:GLY:HA3	2.52	0.45
27:C:90:PHE:CZ	27:C:454:VAL:HG22	2.51	0.45
27:C:241:ASP:OD1	27:C:242:LEU:N	2.50	0.45
35:L:124:LEU:N	35:L:124:LEU:HD12	2.32	0.45
48:l:5:ALA:HB2	48:l:61:MET:CE	2.41	0.45
48:l:30:ASN:O	48:l:33:PRO:HD2	2.15	0.45
48:l:32:TYR:N	48:l:33:PRO:HD2	2.32	0.45
48:l:184:LEU:HD23	48:l:184:LEU:C	2.41	0.45
51:u:233:ALA:HB1	51:u:237:VAL:HG11	1.98	0.45
53:G:339:ALA:HB3	53:G:542:PRO:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:177:LEU:HD22	3:4:231:TRP:CE3	2.51	0.45
5:6:121:TYR:HB3	5:6:137:LEU:CD1	2.46	0.45
6:7:37:LEU:HD22	6:7:90:PHE:CE1	2.52	0.45
7:8:224:THR:HB	1:Ab:67:CYS:SG	2.57	0.45
7:8:322:TYR:HB2	8:9:61:PHE:CD1	2.52	0.45
13:e:109:LEU:HD12	13:e:109:LEU:HA	1.83	0.45
19:k:43:MET:O	19:k:47:ILE:HG13	2.17	0.45
19:k:59:MET:HG3	19:k:60:PRO:N	2.31	0.45
20:m:52:LEU:O	20:m:56:VAL:CG2	2.61	0.45
26:B:128:ARG:HD2	26:B:162:PHE:CZ	2.52	0.45
26:B:182:ILE:HD12	26:B:195:VAL:HG22	1.99	0.45
27:C:292:TYR:C	28:D:162:ALA:HB2	2.41	0.45
27:C:376:GLU:O	27:C:380:SER:OG	2.30	0.45
31:H:180:HIS:CE1	35:L:95:LEU:HD21	2.51	0.45
37:O:110:LEU:HB2	37:O:114:ASP:CB	2.46	0.45
48:l:293:ILE:HD11	48:l:418:LEU:HB3	1.98	0.45
5:v:121:TYR:CB	5:v:137:LEU:HD11	2.47	0.45
5:v:184:ASN:O	5:v:185:ALA:C	2.59	0.45
5:v:289:LEU:HB2	5:v:424:VAL:HG13	1.99	0.45
56:w:401:HEM:HBB2	56:w:401:HEM:HMB1	1.99	0.45
53:G:76:ARG:O	53:G:116:VAL:HG21	2.17	0.45
53:G:514:ASN:C	53:G:515:ILE:HD12	2.42	0.45
3:2:166:ASP:OD1	3:2:166:ASP:N	2.49	0.45
9:a:110:TRP:CD1	9:a:110:TRP:H	2.34	0.45
14:f:47:THR:HG23	15:g:65:LEU:HD22	1.98	0.45
18:j:69:ILE:O	18:j:73:LEU:HG	2.17	0.45
22:o:112:LYS:HB2	22:o:112:LYS:HE3	1.61	0.45
23:p:179:VAL:O	23:p:183:GLN:HG3	2.16	0.45
24:q:303:ILE:HG22	24:q:305:THR:HG23	1.98	0.45
27:C:190:ILE:HG23	27:C:209:MET:HB3	1.99	0.45
27:C:244:LEU:HD21	45:W:7:LYS:HG2	1.98	0.45
27:C:272:ARG:NH2	31:H:63:TRP:HA	2.32	0.45
35:L:174:ARG:HG2	35:L:177:ARG:HH22	1.82	0.45
45:W:121:MET:HE1	45:W:136:ALA:HB3	1.98	0.45
51:u:92:PHE:O	51:u:96:LEU:HG	2.17	0.45
6:w:237:LEU:HB2	7:x:297:MET:HG2	1.97	0.45
7:x:119:LYS:HG3	7:x:120:GLN:HG3	1.99	0.45
51:5:278:ARG:HB2	51:5:462:ILE:HD11	1.99	0.45
3:Ae:52:GLY:HA2	3:Ae:61:ALA:HA	1.99	0.45
3:4:292:VAL:HG13	3:4:292:VAL:O	2.17	0.45
6:7:26:ASN:ND2	6:7:207:ASN:HB2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:185:GLU:CD	50:t:37:ARG:HA	2.41	0.45
13:e:67:TYR:HA	13:e:70:ASN:O	2.17	0.45
25:r:134:ARG:NH2	25:r:206:GLU:OE2	2.50	0.45
26:B:44:ASN:HB2	26:B:59:ARG:NE	2.32	0.45
27:C:266:GLU:OE1	45:W:25:LEU:HG	2.16	0.45
28:D:181:HIS:CD2	28:D:183:ASP:H	2.34	0.45
31:H:58:ALA:O	31:H:62:LEU:HB2	2.17	0.45
38:P:30:SER:OG	38:P:63:PRO:HG3	2.17	0.45
45:W:100:ASP:OD1	45:W:100:ASP:N	2.47	0.45
48:l:37:LYS:HZ1	48:l:98:TRP:HE1	1.63	0.45
48:l:362:LEU:HD22	48:l:366:MET:HE2	1.98	0.45
48:l:532:ILE:HG13	48:l:533:MET:N	2.32	0.45
7:x:276:ARG:O	7:x:276:ARG:HD3	2.16	0.45
53:G:124:HIS:CD2	59:G:801:SF4:S1	3.10	0.45
6:7:8:HIS:O	6:7:12:LYS:N	2.45	0.45
6:7:41:LEU:O	6:7:45:ILE:HG13	2.18	0.45
7:8:107:ASP:O	7:8:111:ILE:HG13	2.18	0.45
9:a:157:ARG:HG2	9:a:168:TRP:CZ3	2.52	0.45
10:b:11:ARG:HD2	23:p:198:PRO:HA	1.99	0.45
11:c:166:LEU:HB2	11:c:170:ARG:NH1	2.32	0.45
17:i:51:ARG:HG3	27:C:75:VAL:HG21	1.98	0.45
19:k:15:ALA:HB3	19:k:36:MET:HG2	1.99	0.45
35:L:119:ASN:HB2	35:L:157:GLU:CD	2.41	0.45
35:L:175:TYR:CD1	35:L:175:TYR:C	2.95	0.45
43:U:80:ALA:HB1	43:U:85:LEU:O	2.17	0.45
50:t:3:ALA:O	50:t:6:ALA:HB3	2.17	0.45
51:u:96:LEU:CD1	51:u:156:LEU:HD23	2.46	0.45
5:v:67:ALA:O	5:v:119:MET:HG3	2.16	0.45
5:v:323:VAL:N	3:Af:68:LEU:HD11	2.32	0.45
7:x:96:PRO:HA	7:x:100:ARG:NE	2.31	0.45
52:Aa:19:LEU:HD23	52:Aa:20:SER:H	1.80	0.45
51:5:96:LEU:HD21	51:5:164:GLU:HB2	1.99	0.45
53:G:445:LEU:HD22	53:G:460:HIS:HE1	1.81	0.45
3:2:246:ILE:N	3:2:256:TYR:O	2.48	0.44
3:4:235:ILE:HG21	3:4:280:GLU:HB3	1.99	0.44
6:7:119:LEU:HD22	6:7:189:ILE:HG23	1.99	0.44
6:7:302:ILE:O	6:7:305:PRO:HD2	2.17	0.44
10:b:12:LEU:HB3	10:b:16:ARG:NH1	2.32	0.44
11:c:160:GLN:NE2	50:t:101:GLU:OE2	2.50	0.44
13:e:79:ASP:HB2	13:e:82:VAL:HG11	1.96	0.44
16:h:17:TRP:CD1	16:h:17:TRP:H	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:254:LEU:CD2	17:i:290:LEU:HD11	2.47	0.44
19:k:78:LEU:HD23	19:k:78:LEU:C	2.41	0.44
20:m:9:LEU:HB3	20:m:39:VAL:HG13	1.99	0.44
21:n:30:ARG:O	21:n:33:GLU:HB2	2.18	0.44
24:q:207:MET:HG3	24:q:239:GLY:HA3	1.99	0.44
26:B:130:ILE:HD11	26:B:275:LEU:CD1	2.47	0.44
26:B:228:PRO:HG3	33:J:160:TYR:HD2	1.82	0.44
29:E:137:THR:HB	55:E:301:FES:S2	2.57	0.44
31:H:112:ARG:O	31:H:164:VAL:HG21	2.17	0.44
31:H:114:ILE:O	31:H:140:ARG:HD3	2.17	0.44
32:I:51:ASP:O	32:I:54:VAL:HG22	2.16	0.44
32:I:84:TYR:O	32:I:85:ASP:C	2.60	0.44
35:L:36:ILE:HG23	53:G:615:LEU:HG	1.99	0.44
35:L:263:PRO:CG	35:L:339:PRO:HA	2.47	0.44
37:X:155:TYR:O	37:X:156:GLU:HG3	2.17	0.44
48:l:284:THR:OG1	48:l:311:GLY:HA3	2.16	0.44
48:l:458:LEU:O	48:l:462:ILE:HG13	2.18	0.44
51:u:300:ASP:C	51:u:303:PRO:HD2	2.42	0.44
5:v:326:PHE:CZ	3:Af:65:SER:HB2	2.52	0.44
7:x:168:ARG:NH1	7:x:171:LYS:HE3	2.31	0.44
4:Ad:45:VAL:O	4:Ad:49:ASN:HB2	2.16	0.44
3:Af:46:LEU:HG	3:Af:47:GLY:H	1.81	0.44
5:6:383:LEU:HD12	51:5:136:LEU:CD2	2.47	0.44
6:7:35:SER:O	6:7:39:ILE:HG12	2.17	0.44
6:7:207:ASN:ND2	6:7:213:SER:HB3	2.32	0.44
7:8:126:HIS:NE2	7:8:196:PRO:HD2	2.32	0.44
7:8:142:THR:HG23	7:8:145:GLU:H	1.82	0.44
7:8:322:TYR:HB2	8:9:61:PHE:CG	2.52	0.44
12:d:85:MET:HE1	24:q:182:TRP:CD1	2.51	0.44
26:B:114:VAL:HA	26:B:155:TYR:O	2.17	0.44
26:B:381:GLN:NE2	26:B:424:ILE:HD11	2.32	0.44
28:D:126:PHE:HB2	28:D:147:THR:HG23	1.99	0.44
29:E:185:MET:HE3	29:E:185:MET:HB3	1.59	0.44
31:H:118:LEU:HD21	31:H:161:ALA:O	2.17	0.44
31:H:189:LYS:NZ	31:H:193:ASN:HD21	2.15	0.44
38:P:35:ASP:O	38:P:38:GLU:HG2	2.17	0.44
48:l:3:PRO:O	48:l:7:LEU:HD23	2.17	0.44
5:v:206:HIS:O	5:v:210:GLN:HG3	2.18	0.44
5:v:326:PHE:CE2	3:Af:65:SER:HB2	2.52	0.44
6:w:120:LEU:O	6:w:124:MET:HG3	2.16	0.44
7:x:283:HIS:O	7:x:287:LYS:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:140:LEU:O	51:5:144:VAL:HG23	2.17	0.44
53:G:341:ILE:HB	53:G:547:LEU:HD23	2.00	0.44
53:G:349:GLU:H	53:G:349:GLU:HG2	1.49	0.44
1:0:65:GLU:HB3	52:z:78:TYR:CG	2.52	0.44
3:4:237:VAL:HG12	3:4:242:GLY:HA2	1.99	0.44
5:6:194:ASP:HA	5:6:197:ILE:HG12	1.99	0.44
20:m:4:TYR:O	20:m:8:ILE:HG13	2.17	0.44
21:n:28:ASP:OD2	24:q:3:LYS:HG3	2.17	0.44
21:n:47:ARG:HH22	21:n:53:GLU:CD	2.25	0.44
23:p:133:TYR:O	48:l:161:ARG:HG2	2.17	0.44
25:r:38:ASN:ND2	32:I:88:ARG:HD2	2.33	0.44
26:B:322:SER:O	26:B:434:PRO:HG3	2.17	0.44
27:C:344:ARG:NH2	45:W:23:ARG:HA	2.32	0.44
28:D:238:PRO:HB2	33:J:90:GLY:HA3	2.00	0.44
30:F:78:GLU:HA	30:F:119:ARG:O	2.17	0.44
35:L:56:ALA:HA	35:L:61:GLY:HA3	1.98	0.44
51:u:140:LEU:HD22	51:u:237:VAL:HG12	1.99	0.44
51:u:314:TYR:HB3	51:u:341:PHE:HD2	1.81	0.44
5:v:214:THR:HB	5:v:243:GLY:O	2.17	0.44
8:y:14:LEU:O	8:y:18:ARG:HG3	2.17	0.44
51:5:465:LEU:HD12	51:5:466:PRO:HD2	1.99	0.44
53:G:636:TYR:HB2	53:G:642:VAL:HG22	1.98	0.44
1:0:33:VAL:HG13	1:0:85:LYS:HB2	1.99	0.44
2:1:58:HIS:HA	2:1:61:GLU:HG2	1.99	0.44
5:6:85:LEU:HD13	5:6:158:LEU:HD12	1.99	0.44
5:6:358:VAL:HG11	5:6:431:PHE:CD2	2.53	0.44
6:7:364:VAL:C	6:7:367:PRO:HD2	2.42	0.44
13:e:112:TYR:HB3	24:q:45:LEU:HD23	1.99	0.44
16:h:65:GLU:HB2	16:h:71:LYS:NZ	2.32	0.44
17:i:175:LEU:HD13	17:i:219:LEU:HD22	1.99	0.44
22:o:18:LEU:HD11	23:p:114:TRP:CB	2.47	0.44
23:p:150:HIS:CG	23:p:151:PRO:HD2	2.52	0.44
24:q:3:LYS:O	24:q:7:PRO:HG2	2.17	0.44
24:q:213:HIS:O	24:q:217:PRO:HD3	2.17	0.44
27:C:361:GLU:H	27:C:361:GLU:HG3	1.51	0.44
29:E:138:THR:O	29:E:142:LEU:HG	2.16	0.44
29:E:195:ASP:OD2	29:E:218:PRO:HB3	2.18	0.44
33:J:115:SER:OG	53:G:267:THR:HB	2.17	0.44
41:S:57:VAL:HG23	41:S:59:ARG:HB2	1.99	0.44
2:Ac:13:LEU:HD22	2:Ac:13:LEU:HA	1.83	0.44
53:G:223:ILE:HG23	53:G:232:THR:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:G:325:ARG:HE	53:G:325:ARG:HB2	1.51	0.44
53:G:372:PHE:H	53:G:532:PRO:HB2	1.81	0.44
3:2:244:VAL:O	3:2:244:VAL:CG1	2.65	0.44
5:6:221:ILE:HD12	5:6:221:ILE:N	2.33	0.44
6:7:112:THR:HG22	6:7:196:HIS:ND1	2.32	0.44
6:7:253:PRO:HD2	7:8:206:HIS:CE1	2.52	0.44
17:i:13:VAL:HG23	17:i:39:ALA:CB	2.47	0.44
19:k:8:ILE:CG2	19:k:43:MET:HG2	2.47	0.44
26:B:130:ILE:HD11	26:B:275:LEU:HD12	2.00	0.44
27:C:194:THR:HG23	27:C:206:PHE:HD2	1.83	0.44
27:C:278:THR:HA	27:C:281:ILE:HG12	1.99	0.44
27:C:361:GLU:HG2	54:M:44:GLY:CA	2.44	0.44
29:E:115:VAL:O	29:E:119:TYR:HD2	2.01	0.44
34:K:65:THR:O	34:K:73:THR:OG1	2.34	0.44
35:L:54:PHE:CZ	35:L:114:VAL:HG11	2.53	0.44
43:U:83:LEU:HG	43:U:272:VAL:HG13	1.99	0.44
43:U:174:ALA:O	43:U:178:GLN:HG2	2.17	0.44
43:U:241:ASN:O	43:U:245:LYS:HB2	2.17	0.44
43:U:281:ASP:O	43:U:286:PRO:HG2	2.18	0.44
45:W:141:ILE:HD12	45:W:141:ILE:N	2.33	0.44
48:l:529:TYR:N	48:l:530:PRO:HD2	2.32	0.44
50:t:22:MET:HG2	50:t:105:GLU:HG3	2.00	0.44
6:w:332:LEU:HD21	6:w:358:TYR:CE1	2.53	0.44
51:5:61:SER:HA	51:5:233:ALA:O	2.17	0.44
51:5:220:VAL:O	51:5:224:TYR:HB2	2.17	0.44
51:5:310:ILE:HG21	51:5:379:LEU:HD21	1.99	0.44
51:5:348:TYR:HB2	51:5:351:THR:O	2.16	0.44
53:G:562:LYS:HA	53:G:562:LYS:HD3	1.83	0.44
6:7:310:SER:HB2	6:7:370:SER:HB3	1.99	0.44
9:a:163:ARG:HH22	15:g:102:ASP:CG	2.25	0.44
17:i:17:THR:HG21	17:i:133:TRP:NE1	2.32	0.44
19:k:44:SER:HB3	19:k:59:MET:HE3	1.98	0.44
20:m:159:TRP:O	20:m:163:ILE:HG12	2.17	0.44
26:B:113:LEU:HD12	26:B:241:THR:O	2.18	0.44
27:C:417:LEU:HD11	27:C:425:PRO:HB3	2.00	0.44
28:D:114:LEU:HD13	28:D:130:TYR:CD2	2.53	0.44
35:L:128:GLU:OE2	35:L:207:ARG:HD2	2.17	0.44
44:V:62:THR:HG22	44:V:104:ARG:CD	2.31	0.44
47:Z:52:LEU:HA	47:Z:55:ARG:HG2	2.00	0.44
48:l:120:TYR:CB	48:l:154:LEU:HD21	2.47	0.44
48:l:132:VAL:HG13	48:l:258:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:416:THR:O	48:l:419:THR:OG1	2.26	0.44
51:u:96:LEU:HD21	51:u:216:LEU:HD13	2.00	0.44
51:u:409:VAL:O	51:u:413:ILE:HG13	2.18	0.44
5:v:50:ALA:HB3	5:v:221:ILE:HD12	1.98	0.44
51:5:157:GLU:O	51:5:161:ILE:HG13	2.17	0.44
51:5:319:GLY:HA3	3:Ae:58:ALA:CB	2.40	0.44
53:G:170:LYS:N	53:G:232:THR:O	2.44	0.44
5:6:320:PRO:HG2	5:6:343:GLN:HE21	1.83	0.44
16:h:85:LYS:HD2	16:h:85:LYS:C	2.43	0.44
17:i:98:MET:HE3	17:i:98:MET:HB2	1.94	0.44
18:j:61:THR:HG21	18:j:105:GLU:OE1	2.18	0.44
19:k:43:MET:HE2	19:k:43:MET:HA	1.99	0.44
19:k:48:ILE:HG21	19:k:56:ALA:C	2.42	0.44
25:r:138:GLN:O	25:r:142:TYR:HD2	2.01	0.44
27:C:468:ASP:HA	28:D:188:LEU:HD22	1.99	0.44
28:D:89:HIS:CG	28:D:90:PRO:HD2	2.53	0.44
32:I:193:TRP:O	32:I:196:ARG:HG2	2.18	0.44
33:J:71:HIS:NE2	33:J:120:PRO:HD2	2.33	0.44
35:L:60:LEU:HA	35:L:237:ILE:HD11	1.99	0.44
35:L:358:THR:HG22	39:Q:77:GLN:HE21	1.83	0.44
42:T:112:GLY:O	42:T:116:ILE:HG13	2.17	0.44
48:l:63:ILE:O	48:l:79:SER:HA	2.18	0.44
51:u:74:TRP:CZ2	51:u:411:GLU:HA	2.53	0.44
5:v:217:ARG:NH2	5:v:246:LEU:O	2.50	0.44
5:v:354:ALA:O	5:v:358:VAL:HG23	2.18	0.44
51:5:392:LYS:O	51:5:396:ARG:HG3	2.18	0.44
51:5:409:VAL:O	51:5:413:ILE:HG13	2.18	0.44
53:G:278:HIS:CE1	53:G:280:ASP:HB2	2.52	0.44
53:G:343:GLY:O	53:G:346:VAL:HG22	2.18	0.44
2:1:4:PRO:HB2	2:1:9:ARG:HE	1.82	0.44
3:2:113:ARG:HH12	51:u:271:THR:HG21	1.82	0.44
3:2:173:ILE:HD11	3:2:195:LEU:HD22	2.00	0.44
6:7:377:LEU:HD23	6:7:377:LEU:HA	1.88	0.44
8:9:57:ASN:O	8:9:60:VAL:HG22	2.17	0.44
10:b:16:ARG:HD2	37:X:150:ASP:OD2	2.18	0.44
18:j:5:LEU:HD23	18:j:9:THR:HG23	2.00	0.44
19:k:23:ARG:HD3	20:m:23:LYS:HB2	1.99	0.44
24:q:141:GLU:HB2	24:q:222:GLU:CD	2.43	0.44
27:C:174:GLN:HA	27:C:177:ARG:HD3	2.00	0.44
29:E:132:ILE:HD11	29:E:169:PHE:CD1	2.53	0.44
34:K:106:ARG:HG2	34:K:108:TYR:OH	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:242:LYS:HE2	35:L:335:ILE:HD13	1.99	0.44
38:P:19:ILE:HA	38:P:66:TRP:O	2.17	0.44
43:U:63:THR:HA	43:U:161:LEU:O	2.17	0.44
43:U:82:LYS:HB2	43:U:272:VAL:HG21	2.00	0.44
37:X:120:MET:HA	37:X:123:GLU:HG2	1.98	0.44
46:Y:43:ARG:HB3	46:Y:46:GLN:CG	2.35	0.44
51:u:206:GLU:O	51:u:210:LYS:HG3	2.18	0.44
51:u:310:ILE:HG21	51:u:379:LEU:HD21	1.99	0.44
51:u:405:GLY:C	51:u:408:PRO:HD2	2.43	0.44
5:v:68:GLY:O	5:v:208:TYR:OH	2.34	0.44
5:v:70:ARG:HB3	5:v:116:ARG:O	2.18	0.44
8:y:46:GLU:O	8:y:50:ARG:HG3	2.18	0.44
53:G:217:GLU:HG2	53:G:412:PRO:HG3	2.00	0.44
3:2:193:LYS:HB2	3:2:193:LYS:HE2	1.80	0.44
3:4:189:LYS:HZ1	6:w:261:PRO:HG2	1.83	0.44
15:g:81:GLN:HG3	15:g:85:TYR:CE2	2.53	0.44
16:h:26:PRO:HD3	19:k:55:LEU:CD1	2.46	0.44
17:i:194:LEU:N	17:i:195:PRO:HD2	2.32	0.44
18:j:5:LEU:HD22	25:r:6:ILE:HD12	1.99	0.44
23:p:59:LEU:HD21	37:X:112:SER:HB2	2.00	0.44
24:q:247:THR:HB	24:q:304:GLN:NE2	2.28	0.44
24:q:325:MET:HE1	24:q:441:ILE:CD1	2.47	0.44
26:B:236:PHE:O	33:J:166:TRP:HE3	1.98	0.44
28:D:93:VAL:HG11	28:D:153:ILE:HD11	1.99	0.44
31:H:157:PHE:C	31:H:159:GLN:H	2.25	0.44
33:J:86:ASN:HD21	53:G:284:GLU:HB3	1.82	0.44
35:L:268:LEU:O	35:L:272:VAL:HG23	2.18	0.44
37:O:72:PRO:N	37:O:73:PRO:CD	2.81	0.44
39:Q:66:TYR:CE2	39:Q:86:ARG:HD3	2.52	0.44
39:Q:67:ARG:HE	39:Q:67:ARG:HB3	1.29	0.44
45:W:81:ARG:HH22	49:s:141:ASN:HD22	1.66	0.44
48:l:370:THR:O	48:l:374:ILE:HG13	2.18	0.44
6:w:218:ILE:HD11	6:w:224:TYR:CE2	2.53	0.44
6:w:237:LEU:HD13	7:x:297:MET:HG2	2.00	0.44
52:z:20:SER:O	52:z:24:GLN:HG2	2.18	0.44
53:G:679:LEU:H	53:G:679:LEU:HG	1.56	0.44
6:7:27:ILE:HD12	6:7:31:TRP:HB3	2.00	0.43
6:7:137:GLN:HE21	6:7:141:TRP:HE1	1.66	0.43
7:8:202:VAL:HG11	7:8:276:ARG:HG2	1.99	0.43
7:8:236:PRO:HA	7:8:241:GLN:HG3	1.98	0.43
7:8:314:VAL:HG23	52:Aa:21:PRO:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:137:ALA:HB3	17:i:138:PRO:HD3	2.00	0.43
19:k:24:SER:O	19:k:89:TYR:HA	2.18	0.43
25:r:129:LEU:O	25:r:133:LEU:HD23	2.18	0.43
26:B:126:LYS:HG3	26:B:127:ASP:N	2.33	0.43
26:B:152:ARG:CZ	40:R:101:PRO:HD3	2.48	0.43
26:B:201:ALA:HB3	29:E:119:TYR:CD1	2.53	0.43
27:C:277:ARG:NH2	27:C:451:ALA:HB1	2.33	0.43
28:D:229:GLU:HB2	33:J:117:THR:HG22	1.99	0.43
29:E:149:LEU:O	29:E:153:GLN:HG3	2.18	0.43
31:H:149:MET:HE2	31:H:185:TYR:CE2	2.53	0.43
31:H:198:GLU:HB3	34:K:109:ILE:HG12	2.00	0.43
38:P:73:GLN:OE1	38:P:73:GLN:N	2.50	0.43
39:Q:107:LEU:HD12	39:Q:107:LEU:HA	1.75	0.43
5:v:212:HIS:HD2	5:v:217:ARG:HH12	1.66	0.43
6:w:216:ASP:OD2	8:y:64:LYS:HG3	2.18	0.43
7:x:123:SER:O	7:x:179:PRO:HB3	2.18	0.43
7:x:245:MET:HE2	57:x:401:HEC:C1A	2.48	0.43
52:Aa:61:THR:O	52:Aa:65:GLN:HG3	2.18	0.43
53:G:473:MET:HE2	53:G:475:VAL:CG2	2.48	0.43
2:1:21:PHE:CE2	2:1:25:ILE:HD11	2.53	0.43
3:2:257:CYS:HB3	3:2:262:SER:HB2	2.00	0.43
6:7:297:SER:O	6:7:300:ILE:HG22	2.17	0.43
9:a:97:GLU:O	12:d:62:TYR:HA	2.18	0.43
22:o:59:VAL:HG13	24:q:423:ILE:HG12	2.00	0.43
24:q:116:ILE:HD12	24:q:116:ILE:HA	1.82	0.43
25:r:201:THR:O	25:r:210:GLY:HA3	2.19	0.43
25:r:277:TYR:HB3	27:C:273:ILE:HD12	1.99	0.43
26:B:357:MET:HG2	26:B:361:THR:HG21	1.98	0.43
30:F:71:ILE:HD11	30:F:115:GLY:CA	2.43	0.43
35:L:299:LEU:HD13	35:L:299:LEU:C	2.42	0.43
37:X:128:PHE:CZ	37:X:148:ILE:HG12	2.53	0.43
48:l:217:LEU:HD23	48:l:217:LEU:O	2.18	0.43
48:l:426:ILE:HG13	48:l:427:ILE:N	2.33	0.43
49:s:117:ASN:OD1	49:s:140:VAL:HG13	2.18	0.43
50:t:69:CYS:SG	50:t:70:LYS:N	2.91	0.43
50:t:74:PHE:HA	50:t:75:PRO:C	2.44	0.43
51:u:342:GLN:HE21	51:u:342:GLN:HB2	1.60	0.43
5:v:295:ALA:O	3:Af:46:LEU:CD1	2.62	0.43
6:w:21:LEU:HD12	6:w:22:PRO:HD2	2.00	0.43
6:w:37:LEU:HD13	56:w:401:HEM:C3B	2.52	0.43
2:Ac:53:TRP:O	2:Ac:57:LYS:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:5:274:GLU:HA	51:5:456:VAL:O	2.18	0.43
3:Ae:65:SER:HB2	3:Ae:66:PRO:CD	2.46	0.43
6:7:300:ILE:HD11	6:7:363:LEU:CD2	2.48	0.43
7:8:122:CYS:CA	57:8:401:HEC:HAB	2.47	0.43
10:b:84:TYR:HE1	12:d:49:ARG:HG2	1.81	0.43
15:g:16:LEU:HD13	15:g:16:LEU:HA	1.78	0.43
16:h:2:PRO:HB2	17:i:21:MET:HE3	1.98	0.43
19:k:61:ILE:HD12	20:m:143:ILE:HG23	1.99	0.43
19:k:62:ILE:HD12	19:k:62:ILE:N	2.33	0.43
23:p:180:LYS:HE3	23:p:180:LYS:HB3	1.87	0.43
25:r:1:MET:HA	25:r:4:ILE:HD13	1.99	0.43
25:r:276:SER:HA	27:C:267:MET:HE1	1.99	0.43
25:r:277:TYR:CE1	31:H:66:LEU:HB3	2.53	0.43
27:C:148:VAL:HG12	27:C:188:ASN:HA	1.99	0.43
27:C:418:VAL:HG22	27:C:426:TYR:HB3	2.00	0.43
28:D:114:LEU:HG	28:D:170:ILE:HD11	1.99	0.43
31:H:114:ILE:CD1	31:H:116:CYS:HB3	2.49	0.43
31:H:211:TYR:CE1	54:M:39:PRO:HG3	2.54	0.43
32:I:127:PRO:HB3	32:I:189:ARG:HH22	1.83	0.43
34:K:105:ALA:O	34:K:106:ARG:HD2	2.18	0.43
35:L:152:LYS:HD2	35:L:152:LYS:HA	1.87	0.43
35:L:198:PRO:HG2	60:L:401:NDP:C5N	2.49	0.43
37:X:76:LEU:HD22	37:X:154:VAL:HG12	2.00	0.43
5:v:106:VAL:HG21	5:v:133:LEU:HD13	2.01	0.43
2:Ac:10:LEU:HD22	2:Ac:14:LEU:HD11	2.00	0.43
53:G:585:PRO:HB2	53:G:616:ALA:HA	2.00	0.43
4:3:46:PRO:C	4:3:48:ILE:H	2.25	0.43
17:i:244:MET:HE2	17:i:244:MET:HB3	1.84	0.43
22:o:6:TYR:CE2	22:o:15:PRO:HD3	2.54	0.43
22:o:10:ARG:CZ	22:o:10:ARG:HB2	2.48	0.43
24:q:200:ILE:HG23	24:q:204:MET:HG3	2.00	0.43
24:q:200:ILE:HG23	24:q:204:MET:CG	2.48	0.43
24:q:266:MET:HA	24:q:269:MET:HE3	1.99	0.43
28:D:124:ASN:ND2	28:D:148:ASP:OD1	2.52	0.43
29:E:140:CYS:HA	29:E:183:ALA:HB1	2.01	0.43
35:L:226:LEU:HD11	35:L:285:PRO:HB2	2.00	0.43
35:L:236:TYR:CE2	35:L:343:LYS:HE2	2.54	0.43
35:L:363:ASP:OD1	35:L:364:VAL:HG13	2.17	0.43
37:O:118:ILE:HG13	37:O:119:ILE:N	2.34	0.43
48:l:227:PHE:H	48:l:284:THR:CG2	2.32	0.43
48:l:441:VAL:HG13	48:l:443:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:108:HIS:O	49:s:112:GLN:HG2	2.18	0.43
51:u:257:TYR:HB3	51:u:261:ALA:O	2.19	0.43
5:v:112:VAL:HA	5:v:120:ALA:O	2.18	0.43
5:v:191:TYR:CE1	3:Af:62:THR:HG21	2.54	0.43
6:w:15:ASN:OD1	6:w:19:ILE:HB	2.18	0.43
7:x:121:VAL:O	57:x:401:HEC:HMC3	2.18	0.43
53:G:139:LEU:HD12	53:G:139:LEU:HA	1.86	0.43
53:G:414:PHE:O	53:G:418:ILE:HG13	2.18	0.43
3:2:161:MET:HB3	6:7:177:ARG:HH12	1.82	0.43
5:6:97:PHE:O	5:6:101:ARG:HB2	2.19	0.43
11:c:123:PRO:HD2	48:l:525:MET:HE1	2.00	0.43
24:q:216:LEU:HB3	24:q:217:PRO:HD3	2.00	0.43
27:C:128:LYS:HB2	28:D:198:PHE:CD1	2.53	0.43
27:C:374:ARG:NH2	31:H:165:ASP:OD1	2.51	0.43
29:E:188:ILE:O	29:E:190:ASP:N	2.51	0.43
30:F:67:ALA:HB2	31:H:111:GLU:HG2	2.00	0.43
32:I:67:PHE:CE1	32:I:113:MET:HE2	2.54	0.43
43:U:246:THR:C	43:U:249:PRO:HD2	2.43	0.43
45:W:108:GLU:HA	49:s:81:ILE:HD13	1.99	0.43
48:l:230:HIS:N	48:l:231:PRO:HD3	2.33	0.43
53:G:323:LEU:HA	53:G:326:VAL:HG22	2.00	0.43
1:0:79:ASP:HB3	7:x:93:PRO:HG2	1.99	0.43
14:f:58:LEU:HD13	15:g:72:PHE:CD1	2.53	0.43
15:g:12:PRO:HD3	16:h:8:LYS:HZ2	1.83	0.43
17:i:236:LYS:HB2	17:i:311:MET:HE1	2.00	0.43
17:i:299:SER:HA	17:i:305:PHE:CE1	2.53	0.43
25:r:74:ALA:HB3	25:r:75:PRO:HD3	2.00	0.43
26:B:367:ILE:O	26:B:371:ILE:HG13	2.17	0.43
27:C:120:GLY:CA	28:D:188:LEU:HA	2.49	0.43
29:E:173:GLU:H	29:E:173:GLU:HG2	1.64	0.43
32:I:65:MET:HE1	32:I:97:PRO:HG3	1.99	0.43
35:L:78:PRO:HB3	35:L:114:VAL:HG21	2.00	0.43
35:L:101:MET:HE3	35:L:114:VAL:HA	2.00	0.43
38:P:18:GLU:OE1	38:P:20:ARG:HD3	2.18	0.43
39:Q:59:ARG:O	39:Q:63:ARG:HG3	2.18	0.43
44:V:117:TYR:O	44:V:121:THR:HG23	2.19	0.43
45:W:83:VAL:HG13	45:W:124:LEU:HD21	2.00	0.43
45:W:105:LYS:HZ2	49:s:81:ILE:HD11	1.82	0.43
48:l:54:PHE:CZ	48:l:84:TYR:HB2	2.53	0.43
48:l:229:LEU:O	48:l:232:TRP:HD1	2.02	0.43
48:l:439:PRO:O	48:l:441:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:v:375:LYS:O	5:v:379:LYS:HD3	2.18	0.43
6:w:113:TRP:O	6:w:117:VAL:HG23	2.19	0.43
8:y:111:LYS:HB3	4:Ad:8:PRO:HD2	2.00	0.43
2:Ac:34:ARG:HH21	4:Ad:50:GLY:C	2.26	0.43
51:5:70:THR:O	51:5:233:ALA:HA	2.19	0.43
51:5:417:LEU:HD23	51:5:417:LEU:HA	1.90	0.43
53:G:594:ALA:O	53:G:605:GLN:HA	2.18	0.43
3:2:175:ILE:HB	3:2:292:VAL:HG13	2.00	0.43
3:2:194:PRO:O	3:2:236:GLY:N	2.46	0.43
5:6:106:VAL:HG23	5:6:108:GLY:H	1.84	0.43
7:8:168:ARG:NH1	7:8:174:ASP:OD2	2.50	0.43
7:8:198:LEU:HD22	7:8:201:ILE:HG21	2.01	0.43
10:b:117:ILE:HG13	10:b:118:PRO:HD2	1.99	0.43
11:c:140:MET:HE2	48:l:283:ILE:HG12	1.99	0.43
17:i:17:THR:HG23	17:i:36:ASN:HD21	1.83	0.43
19:k:21:MET:O	20:m:23:LYS:NZ	2.51	0.43
25:r:100:LEU:HD23	25:r:160:TYR:HB2	2.01	0.43
26:B:339:PHE:CZ	26:B:349:LEU:HD23	2.54	0.43
35:L:192:GLU:CD	35:L:192:GLU:H	2.27	0.43
35:L:254:LYS:HD2	35:L:254:LYS:C	2.43	0.43
40:R:88:ASP:O	40:R:92:GLU:HG3	2.19	0.43
41:S:63:THR:HG23	49:s:98:SER:HB3	2.01	0.43
51:u:170:GLN:O	51:u:174:GLU:HG3	2.19	0.43
51:u:335:ARG:HB2	51:u:337:LEU:HG	1.99	0.43
6:w:141:TRP:CD2	6:w:264:THR:HG22	2.54	0.43
6:w:173:ALA:O	6:w:177:ARG:CG	2.65	0.43
6:w:334:THR:O	6:w:338:ILE:HG13	2.18	0.43
53:G:82:ILE:HD13	53:G:100:TRP:CE3	2.54	0.43
53:G:319:TRP:CZ2	53:G:585:PRO:HG2	2.53	0.43
3:Af:47:GLY:C	3:Af:66:PRO:HA	2.43	0.43
1:0:28:ASP:O	1:0:31:THR:OG1	2.37	0.43
5:6:341:ILE:HG22	3:Ae:72:ARG:HE	1.84	0.43
6:7:325:PHE:O	6:7:329:VAL:HG23	2.18	0.43
6:7:328:LEU:HD11	6:7:358:TYR:CD1	2.54	0.43
7:8:142:THR:HG22	7:8:145:GLU:HB2	1.99	0.43
8:9:46:GLU:O	8:9:50:ARG:HG3	2.18	0.43
25:r:120:GLY:HA2	25:r:128:ALA:HB1	2.00	0.43
26:B:115:VAL:HG22	26:B:248:VAL:HG21	2.00	0.43
27:C:163:LYS:CE	27:C:404:THR:HG22	2.49	0.43
32:I:66:THR:OG1	32:I:95:ALA:HA	2.19	0.43
35:L:196:ILE:HD12	35:L:244:ILE:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:l:293:ILE:CD1	48:l:418:LEU:HD22	2.47	0.43
53:G:197:THR:HB	53:G:204:MET:HE3	2.01	0.43
5:6:338:ILE:HD12	5:6:354:ALA:HB3	2.00	0.43
6:7:141:TRP:HB3	6:7:268:ILE:HD13	2.01	0.43
9:a:52:LYS:HE2	9:a:52:LYS:HB3	1.88	0.43
9:a:131:LYS:HA	21:n:58:LYS:CA	2.45	0.43
11:c:34:LYS:HG2	11:c:36:MET:H	1.83	0.43
15:g:19:GLU:H	15:g:19:GLU:HG3	1.52	0.43
15:g:32:ARG:CG	17:i:339:MET:HE1	2.49	0.43
21:n:21:PHE:CD1	24:q:37:ILE:HD13	2.54	0.43
24:q:88:THR:O	24:q:92:LYS:HG3	2.18	0.43
25:r:61:LEU:HD12	25:r:216:ALA:HB3	2.00	0.43
27:C:380:SER:OG	27:C:383:SER:HB2	2.18	0.43
28:D:98:THR:HG21	36:N:93:LYS:CE	2.49	0.43
31:H:98:ARG:HD2	31:H:156:GLY:HA3	2.00	0.43
31:H:179:THR:HG1	31:H:182:GLU:HG3	1.82	0.43
44:V:9:TYR:CZ	44:V:21:LYS:HE3	2.53	0.43
37:X:87:LEU:O	37:X:90:TYR:HB3	2.19	0.43
48:l:247:LEU:O	48:l:252:MET:HB3	2.18	0.43
49:s:86:THR:N	49:s:89:ASP:OD2	2.52	0.43
6:w:90:PHE:O	6:w:94:LEU:HD12	2.19	0.43
7:x:223:PRO:HD3	7:x:234:PHE:CZ	2.54	0.43
52:Aa:47:LEU:HD22	52:Aa:47:LEU:HA	1.90	0.43
3:2:262:SER:HA	3:2:273:GLY:HA3	2.01	0.43
3:4:166:ASP:O	3:4:170:MET:HG2	2.19	0.43
3:4:230:GLU:H	3:4:230:GLU:HG2	1.58	0.43
5:6:55:TYR:HA	5:6:127:ARG:NH1	2.23	0.43
5:6:276:ALA:O	5:6:334:GLY:HA3	2.19	0.43
9:a:98:LEU:HD12	12:d:63:TYR:O	2.19	0.43
17:i:28:LEU:HD11	20:m:152:TRP:HD1	1.84	0.43
17:i:89:MET:HB2	17:i:95:MET:CG	2.47	0.43
17:i:150:ASN:OD1	17:i:151:PRO:HD2	2.19	0.43
17:i:174:GLN:O	17:i:178:ILE:HG13	2.19	0.43
20:m:82:VAL:HG12	20:m:83:TRP:H	1.84	0.43
24:q:418:LYS:HE2	24:q:421:HIS:NE2	2.34	0.43
24:q:444:LEU:HD23	24:q:444:LEU:C	2.44	0.43
25:r:138:GLN:HG3	25:r:285:LEU:HD21	2.00	0.43
25:r:196:ALA:HB3	25:r:274:ARG:HA	2.01	0.43
26:B:251:SER:N	26:B:252:PRO:HD2	2.34	0.43
26:B:314:LEU:HD12	26:B:315:LEU:N	2.34	0.43
27:C:101:LEU:HD13	27:C:464:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:416:TYR:HB3	27:C:429:LYS:HB3	2.00	0.43
35:L:300:PHE:CD2	35:L:309:THR:HG22	2.53	0.43
35:L:353:THR:O	35:L:357:LEU:HG	2.18	0.43
36:N:35:LEU:HD22	36:N:45:ARG:HA	2.01	0.43
48:l:347:ILE:CD1	48:l:354:GLN:HG2	2.48	0.43
5:v:47:LEU:CD1	5:v:238:LEU:HD13	2.49	0.43
6:w:8:HIS:HB3	6:w:11:MET:HB2	2.00	0.43
6:w:40:CYS:O	6:w:44:GLN:HG2	2.19	0.43
7:x:203:ARG:HG3	7:x:279:SER:CB	2.36	0.43
2:Ac:30:LEU:HD23	4:Ad:34:TRP:HD1	1.84	0.43
51:5:75:ILE:HG23	51:5:229:MET:HG2	2.01	0.43
51:5:390:ARG:O	51:5:394:ILE:HG13	2.19	0.43
53:G:145:MET:HA	54:M:61:ARG:HH22	1.84	0.43
3:2:134:PHE:O	3:2:138:ILE:HG13	2.19	0.42
6:7:24:PRO:HB2	6:7:27:ILE:CG2	2.46	0.42
6:7:332:LEU:HD21	6:7:358:TYR:CE1	2.53	0.42
7:8:108:HIS:HA	7:8:111:ILE:HB	2.00	0.42
10:b:24:LYS:HG3	10:b:25:ASP:N	2.34	0.42
12:d:153:ARG:NH1	24:q:182:TRP:O	2.52	0.42
15:g:117:GLU:OE1	15:g:117:GLU:HA	2.19	0.42
18:j:98:LEU:HD23	18:j:98:LEU:C	2.44	0.42
19:k:61:ILE:O	19:k:65:VAL:HG23	2.19	0.42
23:p:144:TRP:HH2	24:q:426:ILE:HB	1.84	0.42
24:q:14:MET:SD	24:q:26:ASN:HB3	2.59	0.42
25:r:157:ASN:ND2	25:r:165:LEU:HD12	2.34	0.42
26:B:35:LEU:HD11	26:B:39:ASP:HB2	2.00	0.42
27:C:90:PHE:HB3	27:C:103:LEU:HB3	2.01	0.42
32:I:65:MET:HA	32:I:94:ARG:O	2.19	0.42
36:N:54:GLU:O	36:N:58:MET:HG3	2.19	0.42
5:v:278:THR:HG22	5:v:331:SER:HA	2.01	0.42
5:v:438:MET:HB3	5:v:450:VAL:HG22	2.01	0.42
56:w:401:HEM:CMB	56:w:401:HEM:HBB2	2.50	0.42
7:x:223:PRO:HG2	7:x:226:VAL:HG21	2.00	0.42
1:Ab:85:LYS:HB3	1:Ab:85:LYS:HZ3	1.84	0.42
2:Ac:5:THR:O	2:Ac:9:ARG:HG3	2.19	0.42
51:5:96:LEU:HA	51:5:99:LYS:HG2	2.01	0.42
53:G:275:PRO:HB3	53:G:286:ILE:HG23	2.01	0.42
1:0:53:CYS:SG	1:0:56:ARG:NH1	2.90	0.42
5:6:320:PRO:HB2	3:Ae:72:ARG:NH1	2.35	0.42
6:7:337:TRP:HZ3	6:7:350:ILE:HG21	1.83	0.42
8:9:97:GLU:O	8:9:101:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:106:VAL:O	21:n:50:ARG:NH2	2.52	0.42
9:a:152:LYS:O	9:a:156:VAL:HG23	2.19	0.42
15:g:23:LEU:CD1	15:g:83:TYR:HA	2.49	0.42
16:h:22:SER:OG	16:h:37:GLU:HB3	2.19	0.42
17:i:294:MET:HE2	24:q:130:LEU:HD21	1.99	0.42
22:o:65:LEU:O	22:o:69:THR:HG23	2.19	0.42
24:q:1:MET:HG2	24:q:52:PHE:CD2	2.54	0.42
24:q:44:GLN:OE1	24:q:50:LEU:HG	2.19	0.42
26:B:292:MET:O	26:B:293:SER:HB2	2.19	0.42
27:C:81:THR:O	27:C:81:THR:HG22	2.19	0.42
27:C:139:LEU:HD13	27:C:139:LEU:C	2.43	0.42
31:H:102:ALA:O	31:H:167:ILE:HD12	2.19	0.42
31:H:158:CYS:O	31:H:167:ILE:CG2	2.67	0.42
32:I:84:TYR:CE1	32:I:171:GLU:HG3	2.55	0.42
35:L:199:SER:HB3	35:L:235:VAL:HG23	2.01	0.42
39:Q:88:LYS:O	39:Q:92:MET:HG2	2.19	0.42
51:u:71:VAL:O	51:u:147:LEU:HD11	2.20	0.42
51:u:327:THR:O	51:u:331:VAL:HG23	2.19	0.42
5:v:259:ARG:HB3	5:v:444:LEU:HD13	2.01	0.42
7:x:223:PRO:HG2	7:x:226:VAL:CG2	2.49	0.42
1:0:42:LYS:O	1:0:45:LYS:HG2	2.19	0.42
3:4:156:GLN:HE22	7:8:289:MET:HE3	1.84	0.42
5:6:131:GLU:HA	5:6:134:MET:HE3	2.00	0.42
5:6:136:PHE:O	5:6:140:VAL:HG23	2.18	0.42
5:6:319:GLN:CB	5:6:320:PRO:HD2	2.49	0.42
5:6:444:LEU:HD23	5:6:444:LEU:HA	1.81	0.42
7:8:268:ALA:O	7:8:271:VAL:HG12	2.20	0.42
16:h:16:ARG:HA	16:h:19:THR:CG2	2.50	0.42
16:h:83:ARG:O	16:h:87:ILE:HG12	2.18	0.42
16:h:105:ARG:HH22	49:s:91:LYS:HA	1.84	0.42
22:o:50:GLN:O	22:o:56:ARG:HD3	2.19	0.42
23:p:182:LEU:HD11	23:p:208:LEU:HG	2.00	0.42
27:C:102:ARG:HH12	39:Q:123:TRP:HA	1.84	0.42
27:C:331:ASP:OD2	27:C:333:TYR:HB3	2.19	0.42
28:D:71:LYS:O	36:N:103:LEU:HD12	2.19	0.42
28:D:152:PRO:HD2	39:Q:44:LYS:HG3	2.01	0.42
30:F:67:ALA:CB	31:H:111:GLU:HG2	2.49	0.42
31:H:200:GLU:OE2	34:K:88:ARG:N	2.52	0.42
35:L:165:LEU:CD2	35:L:324:LEU:HD12	2.49	0.42
48:l:528:TYR:O	48:l:532:ILE:HG23	2.20	0.42
49:s:161:GLU:O	49:s:164:THR:OG1	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:30:GLY:O	50:t:31:PHE:C	2.61	0.42
50:t:108:LEU:HD23	50:t:111:ARG:HH11	1.84	0.42
51:u:276:ARG:NH2	51:u:466:PRO:O	2.35	0.42
7:x:99:HIS:CG	7:x:106:LEU:HD23	2.55	0.42
51:5:315:ASP:OD1	51:5:340:SER:HB2	2.19	0.42
53:G:358:LEU:HA	53:G:361:VAL:HG23	2.01	0.42
53:G:381:LEU:HD13	53:G:664:TYR:HB3	2.01	0.42
53:G:512:VAL:O	53:G:512:VAL:HG12	2.20	0.42
3:Af:75:LEU:N	3:Af:75:LEU:HD22	2.34	0.42
4:3:47:TYR:O	4:3:47:TYR:CG	2.72	0.42
3:4:156:GLN:HE22	7:8:289:MET:CE	2.33	0.42
3:4:172:LYS:HB2	3:4:172:LYS:NZ	2.35	0.42
3:4:259:CYS:SG	55:4:301:FES:S2	3.04	0.42
5:6:266:LEU:HD22	3:Ae:72:ARG:CZ	2.49	0.42
7:8:113:ARG:NH1	7:8:270:ASP:OD2	2.53	0.42
9:a:60:SER:HB2	23:p:149:TRP:HA	2.02	0.42
16:h:65:GLU:HG3	45:W:111:PHE:CZ	2.54	0.42
16:h:94:PRO:HA	16:h:95:PRO:HD3	1.95	0.42
17:i:27:LEU:O	17:i:31:ILE:HG13	2.20	0.42
17:i:204:ASN:HD22	17:i:204:ASN:C	2.24	0.42
17:i:263:LYS:O	17:i:267:ILE:HG13	2.20	0.42
17:i:309:ASN:ND2	43:U:132:ARG:HD2	2.35	0.42
23:p:97:LYS:HZ3	23:p:97:LYS:HA	1.84	0.42
24:q:95:TYR:OH	24:q:226:ALA:HB3	2.19	0.42
27:C:144:ARG:HA	27:C:229:HIS:CE1	2.54	0.42
27:C:245:GLY:HA2	27:C:248:ASP:OD2	2.20	0.42
31:H:197:TRP:O	31:H:201:ILE:HG13	2.19	0.42
35:L:203:GLY:C	35:L:347:VAL:HG22	2.45	0.42
35:L:288:LEU:CD1	35:L:289:PRO:HD2	2.42	0.42
42:T:111:GLY:O	42:T:115:ILE:HG13	2.20	0.42
43:U:67:ASN:HB3	43:U:216:ILE:CD1	2.49	0.42
37:X:83:VAL:HG13	37:X:122:MET:HE3	2.00	0.42
48:l:66:TRP:O	48:l:77:SER:HB2	2.19	0.42
51:u:275:ILE:HG23	51:u:275:ILE:O	2.19	0.42
5:v:59:SER:HB2	5:v:130:ILE:CG1	2.50	0.42
5:v:300:LYS:HG2	5:v:301:ARG:HG3	2.00	0.42
51:5:92:PHE:HZ	51:5:165:ARG:HB2	1.84	0.42
53:G:171:THR:O	53:G:172:ILE:HD13	2.19	0.42
1:0:37:CYS:O	1:0:40:ILE:HB	2.19	0.42
2:1:14:LEU:O	2:1:20:THR:OG1	2.28	0.42
5:6:292:VAL:HG13	5:6:370:ASP:OD2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:202:VAL:O	7:8:208:GLY:HA2	2.20	0.42
16:h:65:GLU:OE2	45:W:110:VAL:HG11	2.19	0.42
18:j:69:ILE:CD1	25:r:148:ILE:HG13	2.49	0.42
24:q:201:MET:HE1	24:q:212:LEU:HD11	2.02	0.42
27:C:246:LEU:O	27:C:250:ILE:HG13	2.19	0.42
29:E:195:ASP:OD2	29:E:222:ARG:HD3	2.20	0.42
31:H:124:PRO:HD2	59:H:301:SF4:S1	2.59	0.42
32:I:47:VAL:HG11	32:I:191:ARG:HA	2.01	0.42
35:L:45:SER:O	35:L:72:GLY:HA3	2.18	0.42
35:L:289:PRO:HG2	35:L:292:ALA:CB	2.50	0.42
48:l:169:LEU:HA	48:l:169:LEU:HD13	1.82	0.42
48:l:285:THR:HG22	48:l:308:SER:O	2.20	0.42
49:s:229:PRO:O	49:s:230:GLU:HG3	2.20	0.42
51:u:123:TYR:CD2	51:u:130:ALA:HB3	2.55	0.42
51:u:172:LEU:HD21	51:u:202:GLU:HB3	2.01	0.42
6:w:90:PHE:HE1	56:w:401:HEM:HBB1	1.83	0.42
7:x:253:VAL:HG13	7:x:254:LEU:CD2	2.50	0.42
6:7:48:GLY:HA3	56:7:401:HEM:C4C	2.54	0.42
8:9:75:ILE:HG23	8:9:76:LEU:O	2.19	0.42
10:b:18:LEU:HD21	23:p:205:LEU:HD22	2.02	0.42
12:d:148:ALA:HB1	24:q:458:LEU:HD21	2.00	0.42
13:e:99:LEU:O	13:e:103:SER:CB	2.67	0.42
19:k:35:GLY:HA3	20:m:20:PHE:CZ	2.55	0.42
19:k:45:THR:O	19:k:49:LEU:HG	2.20	0.42
19:k:48:ILE:HG23	19:k:53:PHE:HB3	2.01	0.42
23:p:101:LYS:O	23:p:105:LEU:HG	2.19	0.42
24:q:11:LEU:HD22	24:q:11:LEU:HA	1.86	0.42
25:r:155:LEU:O	25:r:315:PRO:HG3	2.18	0.42
25:r:169:GLN:NE2	25:r:241:LEU:O	2.53	0.42
25:r:307:LEU:HB3	25:r:308:PRO:HD3	2.02	0.42
26:B:216:ILE:O	29:E:77:ALA:HB1	2.18	0.42
28:D:72:TYR:HB3	28:D:88:ILE:HG23	2.02	0.42
28:D:86:ILE:HG13	28:D:86:ILE:O	2.19	0.42
32:I:64:PRO:CD	32:I:91:VAL:HG13	2.44	0.42
41:S:69:ILE:HD11	49:s:97:VAL:HG11	2.02	0.42
43:U:137:LEU:HD23	43:U:137:LEU:HA	1.88	0.42
48:l:120:TYR:HB3	48:l:154:LEU:HD21	2.01	0.42
6:w:141:TRP:CE3	6:w:264:THR:HG22	2.55	0.42
52:Aa:20:SER:HB2	51:5:468:TYR:CE1	2.55	0.42
3:Af:45:PRO:CB	3:Af:48:PRO:HB3	2.50	0.42
1:0:57:VAL:HG22	1:0:65:GLU:CD	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:114:ARG:NH1	3:2:131:ARG:HB3	2.35	0.42
3:2:191:ARG:O	3:2:193:LYS:HD3	2.20	0.42
3:4:254:GLY:HA3	3:4:265:ASP:C	2.44	0.42
3:4:258:PRO:C	3:4:260:HIS:N	2.76	0.42
5:6:351:ILE:HD12	5:6:448:PRO:HD2	2.02	0.42
5:6:407:VAL:HG12	5:6:411:THR:HB	2.02	0.42
5:6:451:ASP:OD2	5:v:183:ARG:NH2	2.53	0.42
6:7:17:ALA:HA	6:7:201:HIS:CE1	2.54	0.42
6:7:176:THR:HB	6:w:53:MET:O	2.18	0.42
6:7:183:PHE:CE2	56:7:401:HEM:HBC1	2.55	0.42
7:8:157:ASP:HB3	7:8:166:PHE:CZ	2.55	0.42
10:b:75:VAL:C	10:b:78:PRO:HD2	2.45	0.42
11:c:125:SER:O	11:c:129:MET:HG3	2.19	0.42
13:e:137:MET:HE3	13:e:137:MET:HB2	1.93	0.42
17:i:48:PHE:HB3	20:m:175:ASN:HB2	2.00	0.42
17:i:55:ALA:HB2	19:k:96:LEU:HD11	2.01	0.42
17:i:86:ILE:HD12	17:i:86:ILE:N	2.35	0.42
17:i:158:ALA:HB1	17:i:188:GLY:O	2.20	0.42
20:m:33:LEU:HD23	20:m:33:LEU:HA	1.79	0.42
23:p:107:ARG:HG2	23:p:111:GLU:OE2	2.19	0.42
24:q:106:LEU:O	24:q:109:THR:OG1	2.32	0.42
26:B:54:LYS:H	26:B:54:LYS:NZ	2.16	0.42
26:B:319:PRO:CG	26:B:347:THR:HB	2.44	0.42
27:C:204:THR:HG22	27:C:208:TRP:NE1	2.35	0.42
27:C:368:LYS:NZ	53:G:147:GLY:O	2.37	0.42
29:E:197:THR:H	29:E:200:ASP:HB2	1.84	0.42
39:Q:46:ILE:HD13	39:Q:107:LEU:CD1	2.40	0.42
40:R:87:LEU:O	40:R:91:VAL:HG23	2.20	0.42
43:U:319:ILE:H	43:U:319:ILE:HG13	1.72	0.42
44:V:61:PHE:HD2	44:V:104:ARG:NH1	2.18	0.42
46:Y:42:PRO:HB2	47:Z:30:MET:HE2	2.02	0.42
48:l:413:LEU:O	48:l:493:VAL:HG11	2.19	0.42
49:s:196:ARG:HG2	49:s:197:PRO:HD2	2.01	0.42
51:u:373:GLN:O	51:u:377:MET:HG2	2.19	0.42
5:v:106:VAL:HG21	5:v:133:LEU:HD11	2.01	0.42
5:v:194:ASP:HA	5:v:197:ILE:HG12	2.02	0.42
5:v:290:GLN:HB2	5:v:336:PHE:HE1	1.84	0.42
7:x:216:LEU:HD21	57:x:401:HEC:HMB1	2.02	0.42
53:G:80:VAL:HG22	53:G:81:GLU:N	2.35	0.42
3:Ae:47:GLY:O	3:Ae:65:SER:O	2.37	0.42
2:1:29:ALA:HA	3:2:144:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:94:PRO:HB3	12:d:5:TRP:CD1	2.55	0.42
17:i:5:ILE:HD12	17:i:5:ILE:N	2.35	0.42
17:i:118:VAL:O	17:i:122:ILE:HG12	2.20	0.42
20:m:20:PHE:CD1	20:m:20:PHE:C	2.97	0.42
20:m:41:CYS:O	20:m:45:LEU:HG	2.20	0.42
26:B:222:LYS:HG2	26:B:379:CYS:HG	1.83	0.42
27:C:162:GLU:CD	27:C:169:PRO:HG3	2.44	0.42
35:L:165:LEU:HA	35:L:197:LYS:HB3	2.01	0.42
35:L:310:THR:HG22	35:L:311:ARG:N	2.35	0.42
37:O:128:PHE:HZ	37:O:148:ILE:HG12	1.85	0.42
38:P:36:PHE:CZ	38:P:91:LEU:HD22	2.55	0.42
43:U:244:LYS:O	43:U:249:PRO:HD3	2.18	0.42
46:Y:44:TYR:HD1	48:l:440:LEU:HD22	1.85	0.42
48:l:80:PHE:HB3	48:l:82:MET:HE2	2.01	0.42
50:t:110:GLN:O	50:t:114:ARG:HG2	2.19	0.42
51:u:118:ALA:HB2	51:u:135:ALA:HB2	2.01	0.42
5:v:142:ALA:HA	5:v:241:ARG:HH22	1.84	0.42
5:v:277:ALA:HB1	5:v:331:SER:O	2.20	0.42
5:v:295:ALA:HB1	3:Af:46:LEU:HB3	2.01	0.42
51:5:87:ASN:OD1	51:5:204:PRO:HD3	2.19	0.42
53:G:236:TYR:O	53:G:236:TYR:CG	2.72	0.42
1:0:56:ARG:O	1:0:60:ARG:HD3	2.19	0.42
5:6:359:LYS:O	5:6:363:GLN:HG3	2.19	0.42
9:a:98:LEU:HA	12:d:63:TYR:O	2.20	0.42
11:c:113:ILE:CD1	11:c:116:ARG:HG3	2.47	0.42
17:i:53:THR:O	17:i:57:THR:HG23	2.20	0.42
17:i:259:GLY:C	17:i:262:PRO:HD2	2.45	0.42
18:j:82:ASN:OD1	18:j:82:ASN:N	2.52	0.42
19:k:55:LEU:HD12	19:k:55:LEU:HA	1.81	0.42
24:q:196:TRP:CD1	24:q:250:LEU:HB3	2.53	0.42
24:q:339:SER:HB3	24:q:344:LEU:HD23	2.01	0.42
24:q:377:GLY:O	24:q:381:ILE:HG13	2.20	0.42
25:r:113:VAL:CG1	25:r:139:THR:HG21	2.40	0.42
25:r:227:GLU:O	25:r:231:ILE:HG13	2.20	0.42
26:B:120:GLY:HA2	26:B:159:ARG:NH2	2.33	0.42
29:E:149:LEU:HG	29:E:153:GLN:HE21	1.85	0.42
35:L:130:GLU:HG3	35:L:136:PHE:CD1	2.55	0.42
35:L:235:VAL:CG2	35:L:261:VAL:HA	2.49	0.42
45:W:134:LEU:HD23	45:W:134:LEU:HA	1.88	0.42
46:Y:50:LEU:HD11	48:l:364:LYS:O	2.19	0.42
48:l:249:SER:O	48:l:332:HIS:HE1	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:123:TYR:CE2	51:u:130:ALA:HB3	2.55	0.42
5:v:173:VAL:HG21	5:v:268:HIS:CB	2.50	0.42
53:G:53:CYS:O	53:G:56:VAL:HG22	2.20	0.42
53:G:217:GLU:HG2	53:G:412:PRO:CG	2.50	0.42
3:Af:48:PRO:HA	3:Af:65:SER:C	2.44	0.42
1:0:24:GLU:HB3	1:0:25:GLU:H	1.63	0.42
5:6:300:LYS:HD3	5:6:301:ARG:NH2	2.35	0.42
5:6:380:ALA:O	5:6:384:MET:HG3	2.19	0.42
10:b:22:TRP:O	10:b:26:GLN:HG2	2.19	0.42
10:b:83:HIS:HB3	12:d:45:VAL:HG21	2.01	0.42
11:c:144:PHE:HE2	48:l:283:ILE:CG1	2.33	0.42
12:d:77:CYS:SG	12:d:84:CYS:HB3	2.60	0.42
17:i:158:ALA:O	17:i:162:ILE:HG13	2.19	0.42
17:i:159:MET:HE2	17:i:281:LEU:HB3	2.02	0.42
17:i:275:SER:O	17:i:279:PRO:HG2	2.20	0.42
18:j:38:GLU:OE2	27:C:88:LEU:HD12	2.19	0.42
20:m:6:ALA:HB3	20:m:124:ASP:OD2	2.20	0.42
20:m:31:LEU:O	20:m:35:VAL:HG23	2.19	0.42
20:m:125:TRP:CH2	45:W:126:GLY:HA2	2.52	0.42
26:B:318:ILE:CG1	26:B:357:MET:HE1	2.35	0.42
27:C:146:ASP:HB2	27:C:466:GLU:HG3	2.02	0.42
27:C:157:TYR:O	27:C:161:VAL:HG23	2.20	0.42
27:C:163:LYS:HE3	27:C:404:THR:HG22	2.02	0.42
27:C:226:ALA:HB2	31:H:98:ARG:NH2	2.35	0.42
27:C:385:ILE:HG23	53:G:140:GLN:HG2	2.02	0.42
28:D:93:VAL:HG23	28:D:94:ILE:N	2.35	0.42
29:E:108:PRO:HA	29:E:109:PRO:HD3	1.98	0.42
34:K:49:TYR:HB2	34:K:61:TRP:CE2	2.55	0.42
35:L:159:LEU:HD23	35:L:159:LEU:C	2.44	0.42
35:L:190:PHE:HB3	35:L:193:ALA:HB2	2.01	0.42
46:Y:52:ARG:O	46:Y:56:ILE:HG13	2.20	0.42
46:Y:55:LEU:HD12	46:Y:55:LEU:N	2.35	0.42
48:l:412:THR:O	48:l:416:THR:HG23	2.20	0.42
50:t:62:TYR:CD2	50:t:90:CYS:HB2	2.55	0.42
51:5:112:GLU:O	51:5:116:MET:HG3	2.20	0.42
51:5:192:PHE:HB3	51:5:195:THR:OG1	2.20	0.42
51:5:373:GLN:NE2	51:5:471:ILE:HG23	2.34	0.42
53:G:266:ARG:O	53:G:267:THR:OG1	2.36	0.42
7:8:245:MET:HB2	57:8:401:HEC:ND	2.35	0.41
13:e:73:SER:O	13:e:74:HIS:HB2	2.20	0.41
16:h:13:ASP:OD1	16:h:16:ARG:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:55:ALA:HB2	19:k:96:LEU:CD1	2.50	0.41
22:o:25:ILE:HG12	22:o:30:ARG:HE	1.84	0.41
23:p:47:ALA:HB1	23:p:194:GLU:HB2	2.02	0.41
24:q:23:ILE:HG13	24:q:24:TRP:N	2.35	0.41
26:B:113:LEU:HD13	26:B:149:MET:HE1	2.02	0.41
26:B:424:ILE:HG22	53:G:76:ARG:CZ	2.50	0.41
28:D:44:ARG:NH2	54:M:62:GLU:OE1	2.51	0.41
29:E:134:VAL:HG22	29:E:186:VAL:CG1	2.50	0.41
29:E:140:CYS:HA	29:E:183:ALA:CB	2.50	0.41
37:O:104:PHE:CB	37:O:110:LEU:HD21	2.45	0.41
42:T:151:VAL:HB	49:s:207:LYS:HD3	2.02	0.41
5:v:138:LEU:CD1	5:v:233:VAL:HG22	2.44	0.41
5:v:173:VAL:HG21	5:v:268:HIS:HB2	2.01	0.41
52:z:51:PRO:N	52:z:52:PRO:CD	2.83	0.41
51:5:437:ASP:OD1	51:5:440:VAL:HG23	2.20	0.41
53:G:124:HIS:CG	53:G:125:PRO:HD2	2.55	0.41
53:G:262:VAL:HG23	53:G:276:ARG:HB2	2.01	0.41
3:Ae:68:LEU:HA	3:Ae:68:LEU:HD23	1.76	0.41
3:Ae:71:LYS:O	3:Ae:71:LYS:HD3	2.20	0.41
1:0:75:LEU:HD23	1:0:79:ASP:OD1	2.19	0.41
3:4:230:GLU:HG3	3:4:231:TRP:HD1	1.84	0.41
6:7:150:LEU:CD1	6:7:164:ILE:HD12	2.50	0.41
8:9:29:LYS:HB3	8:9:75:ILE:HG12	2.02	0.41
8:9:29:LYS:HB3	8:9:75:ILE:CG1	2.50	0.41
14:f:36:HIS:CD2	43:U:345:TYR:HE2	2.38	0.41
14:f:72:ARG:NH1	15:g:21:ARG:HB2	2.35	0.41
25:r:207:LEU:O	25:r:208:VAL:C	2.63	0.41
26:B:77:LEU:HB3	26:B:81:LYS:NZ	2.34	0.41
26:B:126:LYS:HG3	26:B:127:ASP:H	1.84	0.41
27:C:107:LEU:HD23	27:C:112:VAL:HA	2.02	0.41
35:L:34:ALA:C	35:L:35:LEU:HD22	2.45	0.41
37:O:103:HIS:HA	37:O:139:MET:O	2.20	0.41
47:Z:82:ALA:O	48:l:374:ILE:HD13	2.20	0.41
48:l:190:LEU:O	48:l:194:ASN:HA	2.20	0.41
48:l:387:THR:HG23	48:l:461:SER:O	2.19	0.41
50:t:111:ARG:O	50:t:115:ARG:HG2	2.20	0.41
5:v:138:LEU:HB3	5:v:237:PHE:CG	2.55	0.41
6:w:244:LEU:HD12	7:x:293:MET:HG2	2.02	0.41
7:x:172:LEU:HD12	7:x:172:LEU:C	2.45	0.41
53:G:35:PHE:HA	53:G:39:GLN:O	2.21	0.41
3:2:245:PRO:HA	3:2:256:TYR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:185:ASN:HD22	3:4:247:ALA:HB2	1.84	0.41
6:7:374:ASN:O	6:7:379:TRP:HB2	2.21	0.41
7:8:212:VAL:O	7:8:216:LEU:HG	2.19	0.41
8:9:57:ASN:C	8:9:60:VAL:HG22	2.46	0.41
10:b:86:LEU:HD13	10:b:89:HIS:CE1	2.55	0.41
11:c:81:ARG:HD2	11:c:85:GLU:OE1	2.20	0.41
13:e:95:PHE:O	13:e:100:VAL:HG23	2.20	0.41
16:h:82:GLN:NE2	16:h:82:GLN:HA	2.35	0.41
18:j:108:GLN:HB2	20:m:169:MET:HE2	2.03	0.41
23:p:106:LEU:HD23	23:p:106:LEU:HA	1.83	0.41
26:B:153:ALA:HB1	26:B:196:PHE:HE1	1.84	0.41
27:C:326:ILE:O	31:H:41:VAL:HG22	2.20	0.41
31:H:119:CYS:O	31:H:158:CYS:SG	2.77	0.41
32:I:62:LEU:HD22	32:I:102:VAL:CG2	2.50	0.41
35:L:59:PHE:HZ	35:L:203:GLY:HA3	1.85	0.41
35:L:240:VAL:O	35:L:244:ILE:HG13	2.20	0.41
39:Q:67:ARG:HG2	39:Q:67:ARG:H	1.65	0.41
43:U:291:ARG:HH21	43:U:295:ARG:HG3	1.85	0.41
43:U:356:LEU:HD23	43:U:356:LEU:HA	1.88	0.41
37:X:131:PRO:HD2	37:X:147:TYR:OH	2.20	0.41
46:Y:40:ILE:HG23	46:Y:49:GLN:HB3	2.02	0.41
47:Z:68:ARG:HE	48:l:436:ARG:HA	1.86	0.41
48:l:359:MET:O	48:l:436:ARG:NH2	2.54	0.41
6:w:37:LEU:HD13	56:w:401:HEM:C4B	2.56	0.41
53:G:591:GLU:HA	53:G:610:VAL:O	2.20	0.41
3:2:216:LEU:CD1	3:2:269:ARG:HD2	2.50	0.41
3:2:269:ARG:HA	3:2:278:ASN:CG	2.46	0.41
5:6:160:ILE:O	5:6:164:VAL:HG23	2.19	0.41
7:8:140:CYS:HG	7:8:141:TYR:HD1	1.68	0.41
8:9:72:ARG:H	8:9:72:ARG:HG2	1.60	0.41
13:e:61:PRO:O	13:e:62:GLU:C	2.63	0.41
13:e:77:ASP:HB3	13:e:83:ASP:OD1	2.21	0.41
18:j:5:LEU:O	18:j:5:LEU:HD23	2.21	0.41
18:j:37:TYR:HD1	32:I:123:GLN:HE22	1.68	0.41
20:m:58:LEU:C	20:m:58:LEU:HD23	2.45	0.41
22:o:100:PHE:O	22:o:104:VAL:HG23	2.20	0.41
23:p:54:HIS:O	23:p:58:VAL:HG23	2.20	0.41
23:p:80:ARG:HD2	47:Z:59:ASP:OD1	2.20	0.41
24:q:154:LEU:HA	24:q:157:SER:OG	2.20	0.41
24:q:204:MET:O	24:q:207:MET:O	2.38	0.41
24:q:225:ILE:HD13	24:q:331:ASN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:32:GLN:CG	27:C:204:THR:HG23	2.44	0.41
25:r:256:THR:O	25:r:260:VAL:HG23	2.20	0.41
25:r:267:THR:O	25:r:271:LEU:HG	2.20	0.41
26:B:63:TYR:CE2	29:E:245:VAL:HG21	2.55	0.41
26:B:112:TYR:CD1	26:B:155:TYR:HE1	2.37	0.41
26:B:364:VAL:HB	26:B:449:ARG:NH1	2.33	0.41
28:D:88:ILE:HD13	28:D:96:VAL:HG11	2.01	0.41
29:E:55:PHE:CZ	29:E:86:ALA:HB2	2.56	0.41
29:E:78:ALA:O	29:E:82:VAL:HG23	2.20	0.41
35:L:301:GLU:OE2	35:L:310:THR:HG23	2.20	0.41
43:U:216:ILE:HA	43:U:219:ARG:HD2	2.02	0.41
46:Y:80:VAL:C	46:Y:81:LEU:HD22	2.46	0.41
47:Z:92:ALA:O	47:Z:96:VAL:HG23	2.20	0.41
48:l:117:PHE:CE1	48:l:243:VAL:HG23	2.54	0.41
48:l:155:ILE:HD13	48:l:155:ILE:HA	1.86	0.41
48:l:562:LEU:HD23	48:l:562:LEU:HA	1.79	0.41
5:v:47:LEU:HD12	5:v:218:MET:HB2	2.02	0.41
6:w:120:LEU:HB2	56:w:401:HEM:CMC	2.49	0.41
6:w:323:CYS:O	6:w:327:MET:HG3	2.21	0.41
8:y:76:LEU:HD12	8:y:76:LEU:HA	1.89	0.41
53:G:179:CYS:SG	53:G:181:ARG:HB2	2.61	0.41
5:6:343:GLN:NE2	3:Ae:72:ARG:HH22	2.17	0.41
5:6:444:LEU:O	5:6:445:GLY:C	2.63	0.41
6:7:92:ILE:HG13	6:7:272:TRP:CZ2	2.55	0.41
6:7:129:MET:CE	6:7:185:LEU:HD12	2.50	0.41
6:7:218:ILE:HD12	6:7:219:PRO:O	2.20	0.41
7:8:246:ALA:O	7:8:247:PRO:C	2.63	0.41
17:i:109:SER:HA	17:i:111:PHE:H	1.86	0.41
22:o:75:ASN:C	22:o:78:PRO:HD2	2.46	0.41
24:q:86:LYS:HE2	24:q:86:LYS:HB3	1.83	0.41
24:q:216:LEU:HD22	24:q:291:VAL:CG2	2.51	0.41
26:B:193:PHE:N	40:R:98:MET:HE1	2.36	0.41
27:C:362:ILE:H	27:C:362:ILE:HG13	1.75	0.41
28:D:114:LEU:HD13	28:D:130:TYR:CE2	2.55	0.41
29:E:201:ILE:O	29:E:205:ILE:HG13	2.21	0.41
31:H:168:VAL:HG21	31:H:205:ILE:HD11	2.01	0.41
35:L:165:LEU:HA	35:L:165:LEU:HD23	1.77	0.41
39:Q:69:VAL:HG11	39:Q:86:ARG:HG3	2.01	0.41
39:Q:90:ARG:HH21	39:Q:94:MET:HE2	1.85	0.41
43:U:325:GLN:O	43:U:329:VAL:HG23	2.20	0.41
48:l:4:PHE:O	48:l:8:THR:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:29:TYR:HD1	50:t:29:TYR:HA	1.77	0.41
50:t:113:LYS:HG3	50:t:114:ARG:HH21	1.85	0.41
51:u:429:TRP:O	51:u:433:ILE:HG13	2.20	0.41
5:v:271:LEU:O	5:v:337:GLY:HA3	2.20	0.41
6:w:27:ILE:HD11	6:w:224:TYR:CE1	2.55	0.41
6:w:221:HIS:HA	6:w:225:THR:HG23	2.02	0.41
6:w:366:MET:HB3	6:w:367:PRO:HD3	2.03	0.41
52:Aa:55:VAL:O	52:Aa:59:VAL:HG23	2.20	0.41
53:G:75:CYS:SG	53:G:76:ARG:N	2.94	0.41
3:4:265:ASP:OD1	3:4:269:ARG:N	2.53	0.41
5:6:184:ASN:O	5:6:185:ALA:HB3	2.20	0.41
6:7:186:PRO:HG2	56:7:401:HEM:CMC	2.49	0.41
7:8:266:GLN:HE22	1:Ab:91:LYS:H	1.69	0.41
9:a:156:VAL:HG22	15:g:103:PHE:CZ	2.55	0.41
11:c:113:ILE:CG1	11:c:116:ARG:HG3	2.50	0.41
12:d:79:GLU:CD	15:g:114:ILE:HD13	2.46	0.41
18:j:75:LEU:HD13	25:r:305:ILE:CD1	2.49	0.41
19:k:10:MET:HE2	19:k:10:MET:HB2	1.97	0.41
23:p:67:ARG:HD3	23:p:67:ARG:HA	1.79	0.41
26:B:226:LYS:O	26:B:227:PRO:C	2.63	0.41
27:C:284:VAL:CG2	27:C:335:ARG:HH21	2.34	0.41
28:D:177:PHE:CE1	39:Q:110:ILE:HD13	2.55	0.41
28:D:184:LEU:HD23	28:D:184:LEU:HA	1.86	0.41
30:F:64:GLU:H	30:F:64:GLU:HG2	1.60	0.41
43:U:67:ASN:HD21	43:U:236:LEU:HB3	1.86	0.41
43:U:171:PHE:O	43:U:175:MET:HG3	2.21	0.41
43:U:201:LEU:CD1	43:U:288:GLN:HG3	2.50	0.41
43:U:260:TYR:CE2	43:U:271:VAL:HG13	2.54	0.41
43:U:280:CYS:SG	43:U:282:LYS:O	2.79	0.41
45:W:84:LEU:HD13	49:s:85:PRO:HG3	2.02	0.41
50:t:74:PHE:CG	50:t:75:PRO:HA	2.56	0.41
51:u:118:ALA:HA	51:u:134:LYS:O	2.21	0.41
6:w:253:PRO:HB2	7:x:204:ALA:O	2.20	0.41
51:5:328:LEU:HB2	51:5:375:GLN:HG3	2.02	0.41
53:G:398:ASP:C	53:G:427:LEU:HD12	2.46	0.41
54:M:8:ILE:O	54:M:12:ARG:HG2	2.20	0.41
3:2:190:TRP:HZ3	3:2:235:ILE:HD13	1.86	0.41
5:6:69:SER:O	5:6:72:GLU:HB2	2.21	0.41
9:a:74:TYR:CG	13:e:91:PHE:HB3	2.55	0.41
10:b:71:ALA:O	10:b:75:VAL:HG13	2.21	0.41
10:b:84:TYR:OH	12:d:52:ILE:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:49:ARG:HD2	12:d:53:GLU:CD	2.45	0.41
16:h:37:GLU:O	16:h:41:ILE:HG13	2.20	0.41
18:j:13:LEU:C	18:j:13:LEU:HD23	2.45	0.41
18:j:67:LEU:CG	19:k:68:ALA:HB3	2.50	0.41
22:o:3:PHE:CE1	23:p:112:GLU:HA	2.56	0.41
26:B:387:GLU:OE2	53:G:158:ARG:NH2	2.54	0.41
26:B:412:LEU:HG	26:B:435:VAL:HG11	2.02	0.41
26:B:430:GLY:O	26:B:434:PRO:CD	2.68	0.41
29:E:138:THR:HB	29:E:139:PRO:HD3	2.02	0.41
31:H:89:GLU:HG2	34:K:61:TRP:HB3	2.02	0.41
32:I:50:LEU:O	32:I:54:VAL:HG13	2.21	0.41
32:I:86:MET:CE	32:I:93:PHE:CD2	3.02	0.41
32:I:126:GLU:HA	32:I:127:PRO:C	2.46	0.41
36:N:55:LYS:HD3	36:N:72:LEU:HD22	2.01	0.41
39:Q:69:VAL:N	39:Q:70:PRO:HD2	2.35	0.41
43:U:66:GLY:O	43:U:163:ARG:NH2	2.46	0.41
48:l:135:ASN:HA	48:l:198:LEU:HD12	2.03	0.41
48:l:260:LEU:HD23	48:l:260:LEU:HA	1.90	0.41
48:l:292:ALA:HB2	48:l:304:PHE:HB2	2.01	0.41
48:l:327:LEU:O	48:l:331:MET:HG2	2.20	0.41
5:v:61:ILE:CD1	5:v:130:ILE:HD12	2.49	0.41
5:v:125:CYS:SG	5:v:133:LEU:HD22	2.61	0.41
5:v:130:ILE:HD13	5:v:130:ILE:HA	1.79	0.41
6:w:37:LEU:HB3	56:w:401:HEM:C2B	2.56	0.41
53:G:64:CYS:SG	53:G:64:CYS:O	2.79	0.41
1:0:34:ARG:HG2	1:0:82:VAL:HG21	2.02	0.41
1:0:48:GLU:O	1:0:52:LEU:HG	2.20	0.41
5:6:364:GLY:HA2	5:6:425:ILE:HD13	2.02	0.41
7:8:263:THR:O	7:8:267:VAL:HG23	2.21	0.41
8:9:57:ASN:O	8:9:60:VAL:CG2	2.68	0.41
9:a:106:VAL:HB	21:n:50:ARG:NH2	2.36	0.41
9:a:152:LYS:HD3	15:g:96:VAL:HG21	2.03	0.41
15:g:110:THR:O	15:g:114:ILE:HG23	2.20	0.41
16:h:17:TRP:CZ3	16:h:18:MET:HB2	2.55	0.41
17:i:22:ILE:O	17:i:22:ILE:HG23	2.21	0.41
17:i:141:VAL:O	17:i:145:ILE:HG12	2.21	0.41
17:i:249:LEU:HD13	24:q:127:VAL:HG13	2.03	0.41
17:i:291:TYR:HE1	24:q:147:LEU:HD13	1.86	0.41
17:i:343:LEU:C	17:i:343:LEU:HD12	2.45	0.41
18:j:67:LEU:HD13	19:k:65:VAL:HG13	2.03	0.41
19:k:97:GLN:O	19:k:98:CYS:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:m:7:PHE:CE2	20:m:104:VAL:HG13	2.55	0.41
22:o:114:LYS:HE2	22:o:114:LYS:HB3	1.80	0.41
25:r:37:PRO:HD3	32:I:87:ASP:OD2	2.20	0.41
25:r:139:THR:HA	25:r:142:TYR:CD2	2.55	0.41
26:B:36:LYS:HE3	26:B:36:LYS:HB3	1.95	0.41
26:B:146:GLY:HA3	26:B:193:PHE:CE1	2.55	0.41
27:C:292:TYR:CE2	27:C:443:LYS:HD2	2.55	0.41
29:E:193:TYR:CE1	29:E:214:PRO:HB2	2.56	0.41
31:H:149:MET:HB2	31:H:183:LEU:O	2.21	0.41
35:L:279:ALA:C	35:L:352:ARG:HG3	2.45	0.41
37:O:120:MET:HE3	39:Q:67:ARG:CZ	2.51	0.41
43:U:88:PHE:HB2	43:U:161:LEU:CD2	2.46	0.41
44:V:26:THR:OG1	44:V:68:ALA:HB2	2.20	0.41
48:l:559:GLU:HG2	48:l:564:LYS:HE2	2.03	0.41
50:t:66:LEU:O	50:t:69:CYS:SG	2.79	0.41
51:u:119:HIS:ND1	5:v:384:MET:HE1	2.36	0.41
5:v:292:VAL:HG23	5:v:374:ALA:CB	2.51	0.41
53:G:600:GLU:OE1	53:G:602:ARG:NH2	2.53	0.41
3:2:263:HIS:N	3:2:272:LYS:O	2.42	0.41
5:6:36:GLN:HB3	5:6:37:ASP:H	1.56	0.41
5:6:438:MET:HB3	5:6:450:VAL:HG13	2.03	0.41
5:6:447:THR:HA	5:6:448:PRO:HD3	1.95	0.41
6:7:107:TYR:HB2	6:7:305:PRO:HG3	2.03	0.41
7:8:125:CYS:HB2	57:8:401:HEC:HBC2	1.98	0.41
7:8:144:GLU:CD	7:8:144:GLU:H	2.26	0.41
9:a:144:ALA:HB2	12:d:82:ILE:HG12	2.02	0.41
10:b:23:LEU:HD12	10:b:23:LEU:HA	1.84	0.41
16:h:77:SER:CB	20:m:122:LEU:HD11	2.46	0.41
20:m:17:PHE:HA	20:m:20:PHE:CD2	2.56	0.41
20:m:112:GLU:OE2	20:m:118:LYS:HB3	2.21	0.41
20:m:114:GLU:HA	20:m:117:PHE:O	2.21	0.41
22:o:5:LYS:HD3	22:o:5:LYS:O	2.21	0.41
22:o:57:LEU:C	22:o:57:LEU:HD23	2.46	0.41
23:p:66:LEU:HD23	23:p:66:LEU:HA	1.88	0.41
23:p:206:PRO:HA	23:p:207:PRO:HD3	1.96	0.41
24:q:4:ILE:H	24:q:4:ILE:HG12	1.64	0.41
24:q:253:LEU:HD12	24:q:253:LEU:HA	1.84	0.41
24:q:282:LEU:HG	24:q:342:MET:HG3	2.03	0.41
26:B:36:LYS:HG3	26:B:38:GLU:HG3	2.03	0.41
26:B:41:ILE:HG12	26:B:289:GLU:OE2	2.21	0.41
26:B:157:TYR:CB	26:B:212:LEU:HD21	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:192:ASP:HB3	40:R:98:MET:CE	2.51	0.41
26:B:381:GLN:O	53:G:74:ASN:HB2	2.21	0.41
26:B:430:GLY:O	26:B:434:PRO:HD3	2.21	0.41
27:C:120:GLY:HA3	28:D:188:LEU:HA	2.03	0.41
27:C:194:THR:CG2	27:C:206:PHE:HA	2.51	0.41
27:C:194:THR:CG2	27:C:206:PHE:HD2	2.34	0.41
27:C:240:GLN:OE1	31:H:212:ARG:HG2	2.20	0.41
27:C:368:LYS:HE2	27:C:386:HIS:HE1	1.86	0.41
27:C:392:THR:CG2	31:H:118:LEU:HB2	2.51	0.41
28:D:230:PHE:O	33:J:123:ASN:ND2	2.54	0.41
29:E:41:HIS:CD2	29:E:95:ILE:HD12	2.55	0.41
31:H:62:LEU:HD13	45:W:35:MET:HE2	2.03	0.41
32:I:113:MET:O	32:I:113:MET:HG3	2.20	0.41
32:I:134:GLY:HA2	32:I:165:GLY:O	2.20	0.41
35:L:207:ARG:O	35:L:211:TYR:HB2	2.21	0.41
35:L:221:VAL:HG11	35:L:272:VAL:HG11	2.03	0.41
35:L:275:ILE:HG23	35:L:348:LEU:HD13	2.02	0.41
36:N:65:VAL:O	36:N:69:GLU:HG3	2.21	0.41
37:O:138:LEU:O	37:O:139:MET:SD	2.78	0.41
39:Q:76:PHE:HE2	39:Q:124:LYS:O	2.03	0.41
43:U:297:ARG:CA	43:U:300:VAL:HG22	2.50	0.41
44:V:69:ILE:CG1	44:V:100:THR:HG21	2.43	0.41
45:W:129:THR:O	45:W:133:ILE:HG13	2.21	0.41
46:Y:81:LEU:HD13	46:Y:81:LEU:HA	1.85	0.41
47:Z:41:GLU:H	47:Z:41:GLU:HG3	1.63	0.41
48:l:60:GLU:OE1	48:l:84:TYR:N	2.54	0.41
51:u:319:GLY:CA	3:Af:58:ALA:HB3	2.51	0.41
5:v:170:GLN:HB3	3:Af:67:VAL:CG1	2.51	0.41
6:w:196:HIS:CE1	56:w:401:HEM:ND	2.86	0.41
6:w:215:MET:HE3	6:w:215:MET:HB3	2.00	0.41
6:w:364:VAL:O	6:w:367:PRO:HD2	2.21	0.41
51:5:195:THR:HG21	51:5:269:ARG:H	1.86	0.41
53:G:75:CYS:O	53:G:76:ARG:HB2	2.21	0.41
53:G:128:CYS:HB2	53:G:129:PRO:HD3	2.02	0.41
53:G:307:ILE:HG22	53:G:317:THR:HB	2.02	0.41
53:G:323:LEU:HA	53:G:326:VAL:CG2	2.51	0.41
5:6:50:ALA:HB3	5:6:221:ILE:HG13	2.02	0.41
5:6:173:VAL:HG21	5:6:268:HIS:HB2	2.02	0.41
5:6:377:LYS:HG2	51:5:117:GLY:HA2	2.03	0.41
12:d:115:GLN:HB2	48:l:199:GLN:NE2	2.36	0.41
17:i:28:LEU:HD23	17:i:31:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:2:ASN:HB3	25:r:96:ILE:CD1	2.50	0.41
24:q:359:TRP:HZ3	24:q:410:MET:SD	2.44	0.41
26:B:192:ASP:C	40:R:98:MET:HE1	2.46	0.41
27:C:255:LYS:HG3	27:C:256:ASN:OD1	2.21	0.41
34:K:44:TYR:CE2	34:K:83:PRO:HB3	2.54	0.41
35:L:339:PRO:HD2	35:L:342:LEU:HD12	2.03	0.41
35:L:365:LYS:HA	35:L:365:LYS:HD3	1.94	0.41
38:P:57:GLU:O	53:G:651:PRO:HB2	2.20	0.41
40:R:93:LEU:O	40:R:97:ARG:HD3	2.21	0.41
41:S:63:THR:HG21	49:s:163:TRP:CZ3	2.56	0.41
42:T:138:TYR:CG	42:T:139:PRO:HD2	2.56	0.41
43:U:170:VAL:HG13	43:U:242:ALA:HB3	2.03	0.41
45:W:82:ARG:HG2	45:W:86:MET:HE2	2.03	0.41
48:l:587:TYR:O	48:l:590:SER:OG	2.31	0.41
49:s:127:GLU:O	49:s:128:LYS:HB2	2.20	0.41
51:u:253:LEU:HD12	51:u:253:LEU:HA	1.88	0.41
5:v:60:ARG:CD	5:v:393:LEU:HD22	2.51	0.41
5:v:383:LEU:HD21	5:v:413:LEU:HD11	2.04	0.41
6:w:373:GLU:HG2	8:y:21:TYR:CE2	2.56	0.41
7:x:245:MET:HE3	7:x:245:MET:HB3	1.85	0.41
7:x:311:LYS:HD3	7:x:311:LYS:HA	1.85	0.41
8:y:14:LEU:HA	8:y:17:ILE:HG12	2.03	0.41
4:Ad:42:LEU:HD23	4:Ad:42:LEU:HA	1.93	0.41
51:5:234:ALA:HB3	51:5:410:CYS:SG	2.61	0.41
51:5:327:THR:O	51:5:331:VAL:HG23	2.21	0.41
53:G:569:GLN:HE21	53:G:619:ASP:CB	2.34	0.41
6:7:200:LEU:HD13	56:7:402:HEM:HAD2	2.03	0.40
6:7:345:HIS:N	6:7:346:PRO:HD2	2.36	0.40
10:b:112:GLU:O	10:b:113:THR:OG1	2.33	0.40
22:o:28:GLU:H	22:o:28:GLU:CD	2.27	0.40
23:p:82:PHE:CE1	48:l:513:PHE:HB2	2.56	0.40
23:p:91:ASP:HA	23:p:94:LYS:HB2	2.02	0.40
24:q:315:LEU:HD12	24:q:381:ILE:HD12	2.03	0.40
25:r:29:GLY:O	25:r:34:ARG:N	2.40	0.40
26:B:132:ARG:HB2	26:B:165:GLU:CG	2.51	0.40
26:B:132:ARG:HB2	26:B:165:GLU:HG3	2.03	0.40
26:B:373:PHE:HD1	29:E:175:GLU:HB3	1.85	0.40
27:C:180:PHE:CE2	27:C:223:VAL:HG11	2.57	0.40
28:D:171:TRP:O	28:D:174:PHE:O	2.38	0.40
28:D:173:MET:O	28:D:197:PRO:O	2.39	0.40
29:E:177:LEU:HB3	29:E:192:TYR:HE1	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:L:244:ILE:O	35:L:248:ILE:HG13	2.21	0.40
37:O:76:LEU:HB2	37:O:155:TYR:HE2	1.85	0.40
39:Q:76:PHE:HB2	39:Q:78:LEU:HG	2.02	0.40
44:V:18:CYS:SG	44:V:72:LEU:HD22	2.61	0.40
48:l:62:ILE:C	48:l:62:ILE:HD13	2.46	0.40
48:l:367:PRO:HD2	48:l:445:GLU:OE1	2.21	0.40
5:v:352:LYS:HA	5:v:352:LYS:HD2	1.89	0.40
6:w:27:ILE:HG12	6:w:224:TYR:OH	2.21	0.40
6:w:122:THR:HG23	6:w:185:LEU:HD22	2.03	0.40
6:w:130:GLY:O	6:w:134:PRO:HD3	2.20	0.40
6:w:183:PHE:O	6:w:186:PRO:HD2	2.21	0.40
53:G:307:ILE:CD1	53:G:582:VAL:HG22	2.47	0.40
53:G:574:ASP:OD1	53:G:575:VAL:HG23	2.20	0.40
5:6:163:ALA:O	5:6:167:GLN:HG3	2.22	0.40
6:7:25:SER:HB2	6:7:218:ILE:CG2	2.51	0.40
6:7:69:ILE:HA	6:7:73:VAL:HG21	2.03	0.40
7:8:215:LEU:HD12	7:8:235:ASN:CG	2.46	0.40
11:c:101:TRP:CD1	11:c:101:TRP:C	2.99	0.40
11:c:143:MET:HB3	48:l:407:TRP:CD2	2.55	0.40
16:h:85:LYS:O	16:h:85:LYS:HD2	2.22	0.40
19:k:8:ILE:CD1	19:k:42:ILE:HG22	2.49	0.40
25:r:102:VAL:HG12	25:r:150:LEU:HD21	2.02	0.40
26:B:63:TYR:O	26:B:256:ARG:HD3	2.21	0.40
26:B:411:SER:O	26:B:415:ILE:HG12	2.21	0.40
27:C:168:GLN:N	28:D:46:THR:O	2.47	0.40
39:Q:71:ASN:O	39:Q:75:LEU:HG	2.21	0.40
46:Y:97:LEU:H	50:t:111:ARG:HH21	1.68	0.40
48:l:580:GLN:O	48:l:580:GLN:HG2	2.22	0.40
49:s:102:LEU:HD23	49:s:148:PHE:CZ	2.56	0.40
51:u:104:ARG:HB2	51:u:108:ALA:HB3	2.03	0.40
5:v:330:TYR:HB2	5:v:333:SER:O	2.21	0.40
6:w:27:ILE:HG12	6:w:224:TYR:CE1	2.56	0.40
51:5:373:GLN:HE22	51:5:471:ILE:HG23	1.86	0.40
53:G:194:ASP:O	53:G:208:THR:HG22	2.20	0.40
53:G:217:GLU:OE2	53:G:409:PHE:HA	2.21	0.40
53:G:382:ARG:HA	53:G:385:TYR:CE1	2.57	0.40
3:2:225:ARG:NH1	3:2:269:ARG:HG3	2.36	0.40
3:4:225:ARG:HG3	3:4:281:VAL:HG11	2.04	0.40
5:6:347:ALA:O	5:6:351:ILE:HG13	2.22	0.40
6:7:186:PRO:HB3	56:7:401:HEM:HBB2	2.03	0.40
6:7:307:LEU:HD11	6:7:363:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:320:LEU:HD21	8:9:20:TRP:HH2	1.85	0.40
7:8:92:ALA:HA	7:8:237:TYR:CE1	2.56	0.40
10:b:14:GLN:HA	10:b:17:GLU:CD	2.46	0.40
10:b:119:LEU:HD23	10:b:119:LEU:HA	1.89	0.40
12:d:149:HIS:ND1	24:q:248:THR:HG22	2.35	0.40
16:h:7:GLN:HB3	16:h:12:LEU:O	2.20	0.40
16:h:17:TRP:CE3	16:h:18:MET:HB2	2.57	0.40
18:j:98:LEU:HD22	25:r:298:LEU:HD11	2.02	0.40
19:k:43:MET:HA	19:k:43:MET:CE	2.52	0.40
23:p:150:HIS:CD2	23:p:151:PRO:HD2	2.56	0.40
24:q:318:ALA:HB1	24:q:374:ASN:CG	2.47	0.40
26:B:141:GLY:CA	26:B:252:PRO:HD3	2.49	0.40
26:B:320:GLY:HA3	26:B:349:LEU:O	2.21	0.40
27:C:339:ARG:O	27:C:343:MET:HG3	2.21	0.40
27:C:381:MET:HE3	27:C:381:MET:CA	2.48	0.40
28:D:199:ARG:C	28:D:201:ASP:H	2.28	0.40
30:F:109:GLY:O	30:F:117:GLN:HA	2.21	0.40
31:H:178:GLU:HG2	32:I:161:ILE:CD1	2.51	0.40
35:L:59:PHE:CZ	35:L:237:ILE:HB	2.57	0.40
35:L:103:TRP:CZ3	35:L:105:GLY:HA2	2.57	0.40
37:O:87:LEU:HG	37:O:122:MET:CE	2.52	0.40
37:O:128:PHE:CZ	37:O:148:ILE:HG12	2.56	0.40
43:U:248:LEU:HB2	43:U:249:PRO:HD3	2.03	0.40
45:W:53:TRP:HA	45:W:53:TRP:CE3	2.56	0.40
51:u:192:PHE:O	51:u:198:ALA:HB2	2.21	0.40
51:u:226:ALA:HB3	51:u:227:PRO:HD3	2.03	0.40
51:u:229:MET:HE1	51:u:253:LEU:CD2	2.43	0.40
51:u:392:LYS:HD2	51:u:433:ILE:O	2.21	0.40
5:v:60:ARG:CZ	5:v:124:GLU:HG2	2.51	0.40
7:x:293:MET:HG3	7:x:294:LEU:N	2.37	0.40
51:5:453:CYS:HA	51:5:454:PRO:HD3	1.92	0.40
53:G:456:ALA:O	53:G:499:ASN:ND2	2.55	0.40
53:G:476:LEU:CD2	53:G:481:LEU:HD21	2.51	0.40
2:1:44:TYR:OH	7:x:105:SER:HB3	2.22	0.40
3:4:200:ARG:HD2	3:4:204:GLU:HB3	2.04	0.40
7:8:195:PRO:HA	7:8:196:PRO:HD3	1.86	0.40
15:g:33:LEU:HD12	15:g:33:LEU:HA	1.94	0.40
18:j:18:VAL:HA	25:r:222:MET:HE1	2.03	0.40
18:j:35:SER:HB2	18:j:36:PRO:HD2	2.02	0.40
20:m:34:ILE:HD11	25:r:114:TYR:CE1	2.57	0.40
23:p:62:TYR:CZ	23:p:66:LEU:HD11	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:340:ASP:OD1	26:B:341:ALA:N	2.55	0.40
27:C:58:MET:HE2	27:C:58:MET:HB2	1.79	0.40
27:C:86:LEU:HD13	27:C:86:LEU:C	2.46	0.40
27:C:309:ARG:HD2	27:C:317:TYR:CE1	2.57	0.40
29:E:63:ILE:O	29:E:67:VAL:HG23	2.21	0.40
29:E:146:ASP:OD1	29:E:146:ASP:N	2.53	0.40
31:H:135:ARG:HG3	31:H:136:ALA:N	2.29	0.40
35:L:51:ALA:HA	35:L:120:VAL:O	2.21	0.40
35:L:166:ASN:HB3	35:L:319:MET:CE	2.52	0.40
35:L:174:ARG:HG2	35:L:177:ARG:NH2	2.37	0.40
43:U:292:THR:HG22	43:U:295:ARG:HH21	1.86	0.40
44:V:9:TYR:CE2	44:V:21:LYS:HE3	2.56	0.40
37:X:136:GLU:O	37:X:139:MET:HE2	2.21	0.40
51:u:119:HIS:CD2	5:v:298:HIS:HA	2.56	0.40
5:v:304:ASN:HD21	3:Af:71:LYS:HG3	1.87	0.40
5:v:328:ALA:HB2	3:Af:65:SER:CB	2.51	0.40
6:w:90:PHE:HD1	6:w:94:LEU:HD11	1.85	0.40
6:w:303:LEU:CB	6:w:306:MET:HE2	2.47	0.40
6:w:312:GLN:HG3	6:w:379:TRP:HZ3	1.86	0.40
7:x:202:VAL:HG23	7:x:275:LEU:HB3	2.02	0.40
52:z:26:ALA:O	52:z:28:PRO:HD3	2.21	0.40
3:Ae:59:LEU:HG	3:Ae:59:LEU:O	2.22	0.40
3:4:218:ASP:HB2	3:4:278:ASN:ND2	2.36	0.40
5:6:112:VAL:HA	5:6:120:ALA:O	2.21	0.40
5:6:401:LEU:HD12	5:6:401:LEU:HA	1.89	0.40
6:7:181:PHE:CE1	6:w:53:MET:HE2	2.57	0.40
7:8:294:LEU:HA	7:8:294:LEU:HD23	1.85	0.40
7:8:309:ARG:HH12	52:Aa:30:TYR:HE1	1.70	0.40
9:a:179:ILE:HD13	16:h:38:LYS:HA	2.02	0.40
10:b:77:ILE:HB	10:b:78:PRO:HD3	2.03	0.40
10:b:111:LEU:HD13	10:b:111:LEU:HA	1.92	0.40
13:e:100:VAL:O	13:e:104:THR:HG23	2.21	0.40
16:h:83:ARG:HD2	16:h:83:ARG:C	2.46	0.40
17:i:68:MET:HE3	19:k:40:LEU:HD12	2.02	0.40
18:j:79:SER:HA	18:j:87:MET:HE2	2.04	0.40
22:o:11:LEU:HD13	48:l:535:ARG:HB3	2.02	0.40
22:o:41:SER:OG	23:p:191:PRO:O	2.36	0.40
24:q:325:MET:HE1	24:q:441:ILE:HD11	2.02	0.40
25:r:272:TRP:CE2	31:H:70:LEU:HG	2.57	0.40
25:r:310:MET:HA	42:T:124:THR:HG22	2.04	0.40
26:B:311:TRP:HE1	26:B:333:GLU:CD	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:J:98:LYS:HG3	33:J:125:VAL:HG22	2.02	0.40
34:K:37:THR:O	34:K:49:TYR:HA	2.22	0.40
35:L:32:HIS:HD1	35:L:32:HIS:N	2.19	0.40
36:N:22:GLU:O	36:N:26:ILE:HG13	2.22	0.40
38:P:42:VAL:HG13	53:G:671:LEU:HD22	2.04	0.40
39:Q:47:PHE:HB3	39:Q:57:ARG:CZ	2.52	0.40
45:W:86:MET:HE3	45:W:124:LEU:HD22	2.03	0.40
48:l:90:ILE:HB	48:l:91:PRO:HD3	2.03	0.40
48:l:140:LEU:HD23	48:l:140:LEU:O	2.22	0.40
51:u:287:VAL:HB	51:u:358:PHE:CE1	2.57	0.40
52:Aa:27:PHE:N	52:Aa:28:PRO:HD3	2.37	0.40
52:Aa:50:ALA:N	52:Aa:51:PRO:CD	2.84	0.40
53:G:203:ASP:O	53:G:205:GLN:HG3	2.22	0.40
53:G:634:LEU:HD13	53:G:636:TYR:OH	2.21	0.40
3:Af:46:LEU:HG	3:Af:47:GLY:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	66/91 (72%)	64 (97%)	2 (3%)	0	100	100
1	Ab	64/91 (70%)	64 (100%)	0	0	100	100
2	1	58/64 (91%)	58 (100%)	0	0	100	100
2	Ac	57/64 (89%)	57 (100%)	0	0	100	100
3	2	193/299 (64%)	193 (100%)	0	0	100	100
3	4	194/299 (65%)	185 (95%)	9 (5%)	0	100	100
3	Ae	37/299 (12%)	27 (73%)	9 (24%)	1 (3%)	4	16
3	Af	32/299 (11%)	27 (84%)	5 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
4	Ad	49/56 (88%)	46 (94%)	3 (6%)	0	100	100
5	6	416/453 (92%)	410 (99%)	5 (1%)	1 (0%)	43	72
5	v	416/453 (92%)	413 (99%)	3 (1%)	0	100	100
6	7	377/379 (100%)	370 (98%)	7 (2%)	0	100	100
6	w	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
7	8	236/326 (72%)	233 (99%)	3 (1%)	0	100	100
7	x	236/326 (72%)	234 (99%)	2 (1%)	0	100	100
8	9	97/111 (87%)	97 (100%)	0	0	100	100
8	y	99/111 (89%)	99 (100%)	0	0	100	100
9	a	136/189 (72%)	136 (100%)	0	0	100	100
10	b	102/128 (80%)	94 (92%)	8 (8%)	0	100	100
11	c	151/186 (81%)	149 (99%)	2 (1%)	0	100	100
12	d	166/176 (94%)	166 (100%)	0	0	100	100
13	e	97/154 (63%)	91 (94%)	6 (6%)	0	100	100
14	f	44/76 (58%)	44 (100%)	0	0	100	100
15	g	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
16	h	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
17	i	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
18	j	112/115 (97%)	112 (100%)	0	0	100	100
19	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
20	m	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
21	n	54/58 (93%)	50 (93%)	4 (7%)	0	100	100
22	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
23	p	176/221 (80%)	175 (99%)	1 (1%)	0	100	100
24	q	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
25	r	316/318 (99%)	312 (99%)	4 (1%)	0	100	100
26	B	429/464 (92%)	422 (98%)	7 (2%)	0	100	100
27	C	428/469 (91%)	417 (97%)	11 (3%)	0	100	100
28	D	206/264 (78%)	199 (97%)	7 (3%)	0	100	100
29	E	212/249 (85%)	203 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	F	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
31	H	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
32	I	154/196 (79%)	152 (99%)	2 (1%)	0	100	100
33	J	116/175 (66%)	116 (100%)	0	0	100	100
34	K	142/145 (98%)	142 (100%)	0	0	100	100
35	L	338/372 (91%)	335 (99%)	3 (1%)	0	100	100
36	N	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
37	O	82/156 (53%)	80 (98%)	1 (1%)	1 (1%)	10	34
37	X	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
38	P	81/99 (82%)	81 (100%)	0	0	100	100
39	Q	110/154 (71%)	109 (99%)	1 (1%)	0	100	100
40	R	33/110 (30%)	33 (100%)	0	0	100	100
41	S	68/70 (97%)	68 (100%)	0	0	100	100
42	T	80/169 (47%)	78 (98%)	2 (2%)	0	100	100
43	U	316/357 (88%)	308 (98%)	8 (2%)	0	100	100
44	V	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
45	W	138/144 (96%)	138 (100%)	0	0	100	100
46	Y	60/105 (57%)	57 (95%)	3 (5%)	0	100	100
47	Z	76/114 (67%)	76 (100%)	0	0	100	100
48	l	601/606 (99%)	584 (97%)	16 (3%)	1 (0%)	43	72
49	s	169/249 (68%)	167 (99%)	2 (1%)	0	100	100
50	t	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
51	5	431/480 (90%)	426 (99%)	5 (1%)	0	100	100
51	u	444/480 (92%)	440 (99%)	4 (1%)	0	100	100
52	Aa	76/82 (93%)	76 (100%)	0	0	100	100
52	z	77/82 (94%)	76 (99%)	1 (1%)	0	100	100
53	G	680/727 (94%)	666 (98%)	14 (2%)	0	100	100
54	M	92/113 (81%)	90 (98%)	2 (2%)	0	100	100
All	All	12178/14729 (83%)	11950 (98%)	224 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Ae	50	CYS
37	O	139	MET
5	6	185	ALA
48	l	563	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	0	64/85 (75%)	55 (86%)	9 (14%)	3	11
1	Ab	63/85 (74%)	51 (81%)	12 (19%)	1	5
2	1	49/52 (94%)	47 (96%)	2 (4%)	27	61
2	Ac	48/52 (92%)	44 (92%)	4 (8%)	10	32
3	2	166/245 (68%)	152 (92%)	14 (8%)	10	31
3	4	166/245 (68%)	148 (89%)	18 (11%)	6	21
3	Ae	27/245 (11%)	20 (74%)	7 (26%)	0	2
3	Af	25/245 (10%)	22 (88%)	3 (12%)	5	16
4	3	40/46 (87%)	38 (95%)	2 (5%)	22	53
4	Ad	41/46 (89%)	40 (98%)	1 (2%)	43	75
5	6	329/355 (93%)	309 (94%)	20 (6%)	17	46
5	v	329/355 (93%)	306 (93%)	23 (7%)	14	40
6	7	332/332 (100%)	319 (96%)	13 (4%)	28	63
6	w	332/332 (100%)	320 (96%)	12 (4%)	31	65
7	8	203/259 (78%)	184 (91%)	19 (9%)	8	26
7	x	203/259 (78%)	190 (94%)	13 (6%)	16	44
8	9	91/99 (92%)	81 (89%)	10 (11%)	6	20
8	y	93/99 (94%)	85 (91%)	8 (9%)	10	30
9	a	121/158 (77%)	116 (96%)	5 (4%)	27	61
10	b	97/121 (80%)	85 (88%)	12 (12%)	4	15
11	c	138/160 (86%)	126 (91%)	12 (9%)	9	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	d	152/156 (97%)	141 (93%)	11 (7%)	13	39
13	e	91/129 (70%)	73 (80%)	18 (20%)	1	5
14	f	42/66 (64%)	39 (93%)	3 (7%)	13	40
15	g	108/109 (99%)	100 (93%)	8 (7%)	13	38
16	h	93/94 (99%)	90 (97%)	3 (3%)	34	68
17	i	311/311 (100%)	291 (94%)	20 (6%)	16	44
18	j	99/100 (99%)	92 (93%)	7 (7%)	13	40
19	k	85/85 (100%)	79 (93%)	6 (7%)	13	40
20	m	141/141 (100%)	132 (94%)	9 (6%)	16	44
21	n	52/55 (94%)	48 (92%)	4 (8%)	12	35
22	o	113/114 (99%)	109 (96%)	4 (4%)	32	66
23	p	159/190 (84%)	145 (91%)	14 (9%)	9	29
24	q	409/409 (100%)	389 (95%)	20 (5%)	22	54
25	r	275/275 (100%)	258 (94%)	17 (6%)	16	46
26	B	345/368 (94%)	328 (95%)	17 (5%)	22	54
27	C	370/398 (93%)	331 (90%)	39 (10%)	6	22
28	D	188/228 (82%)	171 (91%)	17 (9%)	9	28
29	E	183/207 (88%)	172 (94%)	11 (6%)	17	47
30	F	78/97 (80%)	73 (94%)	5 (6%)	16	44
31	H	151/176 (86%)	140 (93%)	11 (7%)	13	38
32	I	132/163 (81%)	129 (98%)	3 (2%)	44	76
33	J	107/152 (70%)	101 (94%)	6 (6%)	19	50
34	K	130/131 (99%)	127 (98%)	3 (2%)	44	76
35	L	294/320 (92%)	278 (95%)	16 (5%)	20	51
36	N	99/101 (98%)	94 (95%)	5 (5%)	21	53
37	O	78/132 (59%)	68 (87%)	10 (13%)	4	14
37	X	79/132 (60%)	75 (95%)	4 (5%)	21	53
38	P	74/82 (90%)	68 (92%)	6 (8%)	11	33
39	Q	105/134 (78%)	99 (94%)	6 (6%)	18	49
40	R	34/92 (37%)	32 (94%)	2 (6%)	18	48
41	S	58/58 (100%)	56 (97%)	2 (3%)	32	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	T	69/134 (52%)	67 (97%)	2 (3%)	37	71
43	U	281/307 (92%)	259 (92%)	22 (8%)	11	35
44	V	101/102 (99%)	94 (93%)	7 (7%)	14	41
45	W	122/124 (98%)	117 (96%)	5 (4%)	27	61
46	Y	54/84 (64%)	45 (83%)	9 (17%)	2	7
47	Z	60/90 (67%)	55 (92%)	5 (8%)	10	32
48	l	537/540 (99%)	506 (94%)	31 (6%)	18	49
49	s	153/206 (74%)	144 (94%)	9 (6%)	18	48
50	t	107/120 (89%)	97 (91%)	10 (9%)	8	27
51	5	363/397 (91%)	347 (96%)	16 (4%)	25	59
51	u	372/397 (94%)	351 (94%)	21 (6%)	19	50
52	Aa	70/73 (96%)	64 (91%)	6 (9%)	10	30
52	z	70/73 (96%)	64 (91%)	6 (9%)	10	30
53	G	576/610 (94%)	534 (93%)	42 (7%)	13	38
54	M	86/98 (88%)	81 (94%)	5 (6%)	18	49
All	All	10613/12435 (85%)	9891 (93%)	722 (7%)	16	42

All (722) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	26	LEU
1	0	31	THR
1	0	42	LYS
1	0	48	GLU
1	0	64	GLU
1	0	69	GLU
1	0	70	GLU
1	0	75	LEU
1	0	81	CYS
2	1	37	ASP
2	1	41	ASP
3	2	104	ILE
3	2	126	GLU
3	2	158	VAL
3	2	172	LYS
3	2	204	GLU
3	2	205	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2	207	GLN
3	2	212	GLU
3	2	230	GLU
3	2	240	HIS
3	2	251	ASP
3	2	280	GLU
3	2	287	THR
3	2	290	ASP
4	3	6	LEU
4	3	39	ARG
3	4	103	ASP
3	4	104	ILE
3	4	119	ASP
3	4	143	THR
3	4	172	LYS
3	4	174	GLU
3	4	179	ASP
3	4	182	GLU
3	4	184	LYS
3	4	186	MET
3	4	230	GLU
3	4	237	VAL
3	4	241	LEU
3	4	251	ASP
3	4	259	CYS
3	4	281	VAL
3	4	290	ASP
3	4	294	VAL
5	6	39	GLU
5	6	49	ILE
5	6	101	ARG
5	6	122	THR
5	6	124	GLU
5	6	129	ASP
5	6	203	ASP
5	6	233	VAL
5	6	244	LEU
5	6	319	GLN
5	6	329	SER
5	6	370	ASP
5	6	378	LEU
5	6	393	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	6	401	LEU
5	6	421	ASP
5	6	435	ARG
5	6	450	VAL
5	6	451	ASP
5	6	453	LEU
6	7	10	LEU
6	7	27	ILE
6	7	111	GLU
6	7	112	THR
6	7	202	GLU
6	7	207	ASN
6	7	211	ILE
6	7	252	ASP
6	7	254	ASP
6	7	273	TYR
6	7	311	LYS
6	7	341	GLN
6	7	379	TRP
7	8	103	LEU
7	8	106	LEU
7	8	107	ASP
7	8	109	THR
7	8	120	GLN
7	8	125	CYS
7	8	126	HIS
7	8	144	GLU
7	8	161	GLU
7	8	164	GLU
7	8	184	GLU
7	8	190	ASN
7	8	198	LEU
7	8	226	VAL
7	8	230	GLU
7	8	251	ASN
7	8	276	ARG
7	8	293	MET
7	8	310	HIS
8	9	14	LEU
8	9	15	GLU
8	9	40	GLU
8	9	41	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	9	53	GLU
8	9	72	ARG
8	9	75	ILE
8	9	83	LYS
8	9	85	GLU
8	9	92	GLU
9	a	58	LYS
9	a	82	VAL
9	a	130	GLU
9	a	143	GLU
9	a	153	GLU
10	b	17	GLU
10	b	23	LEU
10	b	53	ASP
10	b	75	VAL
10	b	86	LEU
10	b	89	HIS
10	b	97	VAL
10	b	99	GLU
10	b	111	LEU
10	b	112	GLU
10	b	117	ILE
10	b	119	LEU
11	c	68	ASP
11	c	70	MET
11	c	74	ASP
11	c	77	LYS
11	c	98	ARG
11	c	101	TRP
11	c	110	ASP
11	c	116	ARG
11	c	124	VAL
11	c	165	ASP
11	c	182	VAL
11	c	185	GLU
12	d	6	ASP
12	d	8	ASP
12	d	49	ARG
12	d	50	GLU
12	d	59	ASN
12	d	61	TYR
12	d	69	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	d	71	VAL
12	d	78	GLU
12	d	82	ILE
12	d	156	LEU
13	e	54	ARG
13	e	55	LEU
13	e	58	ASP
13	e	62	GLU
13	e	63	ASP
13	e	64	GLU
13	e	70	ASN
13	e	72	ASP
13	e	77	ASP
13	e	82	VAL
13	e	84	LEU
13	e	87	MET
13	e	89	VAL
13	e	96	SER
13	e	99	LEU
13	e	116	GLU
13	e	138	GLU
13	e	149	LEU
14	f	31	ILE
14	f	33	GLU
14	f	70	LYS
15	g	3	MET
15	g	16	LEU
15	g	19	GLU
15	g	29	THR
15	g	64	LEU
15	g	84	MET
15	g	101	GLU
15	g	114	ILE
16	h	74	LYS
16	h	91	LYS
16	h	101	LYS
17	i	22	ILE
17	i	36	ASN
17	i	140	SER
17	i	159	MET
17	i	183	SER
17	i	193	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	i	194	LEU
17	i	201	THR
17	i	258	SER
17	i	290	LEU
17	i	296	LEU
17	i	303	THR
17	i	311	MET
17	i	318	GLU
17	i	319	HIS
17	i	321	LYS
17	i	323	MET
17	i	328	THR
17	i	336	VAL
17	i	346	LEU
18	j	1	MET
18	j	16	LEU
18	j	49	LEU
18	j	57	LEU
18	j	82	ASN
18	j	86	THR
18	j	109	LYS
19	k	3	LEU
19	k	26	LEU
19	k	43	MET
19	k	55	LEU
19	k	59	MET
19	k	73	LEU
20	m	45	LEU
20	m	56	VAL
20	m	61	LEU
20	m	66	VAL
20	m	74	MET
20	m	76	THR
20	m	103	MET
20	m	136	PHE
20	m	151	THR
21	n	17	VAL
21	n	39	ARG
21	n	44	LEU
21	n	57	TRP
22	o	3	PHE
22	o	5	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	o	111	LYS
22	o	120	LYS
23	p	76	ARG
23	p	77	ASP
23	p	97	LYS
23	p	101	LYS
23	p	106	LEU
23	p	110	GLU
23	p	123	ILE
23	p	126	GLU
23	p	137	GLU
23	p	165	GLU
23	p	176	GLU
23	p	192	ARG
23	p	202	GLU
23	p	218	GLU
24	q	4	ILE
24	q	11	LEU
24	q	14	MET
24	q	36	LEU
24	q	61	LEU
24	q	87	GLU
24	q	114	GLU
24	q	116	ILE
24	q	200	ILE
24	q	230	VAL
24	q	250	LEU
24	q	253	LEU
24	q	263	MET
24	q	282	LEU
24	q	315	LEU
24	q	343	ILE
24	q	369	LEU
24	q	426	ILE
24	q	441	ILE
24	q	454	ILE
25	r	13	ILE
25	r	33	LEU
25	r	61	LEU
25	r	62	ARG
25	r	108	MET
25	r	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	r	117	LEU
25	r	170	GLU
25	r	204	GLU
25	r	214	GLU
25	r	224	PHE
25	r	227	GLU
25	r	241	LEU
25	r	253	GLU
25	r	282	TYR
25	r	285	LEU
25	r	314	ILE
26	B	38	GLU
26	B	41	ILE
26	B	54	LYS
26	B	71	LYS
26	B	83	SER
26	B	102	MET
26	B	119	GLU
26	B	134	ASP
26	B	210	THR
26	B	226	LYS
26	B	302	LYS
26	B	317	VAL
26	B	327	ILE
26	B	338	ASP
26	B	390	ASP
26	B	424	ILE
26	B	445	GLU
27	C	57	VAL
27	C	58	MET
27	C	63	GLU
27	C	75	VAL
27	C	80	ASP
27	C	83	VAL
27	C	100	VAL
27	C	115	CYS
27	C	124	ARG
27	C	134	THR
27	C	143	ASP
27	C	147	TYR
27	C	148	VAL
27	C	150	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	C	159	LEU
27	C	164	LEU
27	C	165	LEU
27	C	167	ILE
27	C	191	MET
27	C	194	THR
27	C	203	MET
27	C	221	GLU
27	C	238	VAL
27	C	240	GLN
27	C	249	ASP
27	C	264	LEU
27	C	266	GLU
27	C	280	ASP
27	C	281	ILE
27	C	284	VAL
27	C	304	ILE
27	C	314	TYR
27	C	318	ASP
27	C	337	LEU
27	C	361	GLU
27	C	365	ASP
27	C	377	MET
27	C	418	VAL
27	C	462	ILE
28	D	68	ILE
28	D	81	PHE
28	D	94	ILE
28	D	111	LEU
28	D	113	ASP
28	D	119	VAL
28	D	136	ARG
28	D	143	VAL
28	D	145	THR
28	D	149	GLU
28	D	154	GLU
28	D	187	ILE
28	D	201	ASP
28	D	204	LEU
28	D	215	GLU
28	D	219	VAL
28	D	250	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	E	42	ARG
29	E	58	GLU
29	E	85	LEU
29	E	137	THR
29	E	172	ILE
29	E	185	MET
29	E	201	ILE
29	E	203	GLU
29	E	209	LYS
29	E	235	THR
29	E	249	LEU
30	F	37	LYS
30	F	46	ASP
30	F	57	ASP
30	F	79	VAL
30	F	85	SER
31	H	70	LEU
31	H	73	THR
31	H	111	GLU
31	H	114	ILE
31	H	118	LEU
31	H	119	CYS
31	H	135	ARG
31	H	150	THR
31	H	162	CYS
31	H	174	GLU
31	H	181	GLU
32	I	71	CYS
32	I	86	MET
32	I	169	THR
33	J	70	GLU
33	J	86	ASN
33	J	124	LEU
33	J	125	VAL
33	J	146	ASP
33	J	175	LYS
34	K	129	THR
34	K	136	GLU
34	K	144	TYR
35	L	73	SER
35	L	74	GLN
35	L	119	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	L	129	TRP
35	L	165	LEU
35	L	168	ASP
35	L	170	LYS
35	L	175	TYR
35	L	177	ARG
35	L	179	LYS
35	L	205	GLU
35	L	254	LYS
35	L	295	TRP
35	L	305	PHE
35	L	341	GLU
35	L	352	ARG
36	N	5	LEU
36	N	40	LYS
36	N	87	GLU
36	N	88	LEU
36	N	94	MET
37	O	96	GLU
37	O	98	LEU
37	O	99	SER
37	O	106	LYS
37	O	112	SER
37	O	114	ASP
37	O	115	GLN
37	O	118	ILE
37	O	124	ASP
37	O	133	ILE
38	P	19	ILE
38	P	45	LYS
38	P	50	ASP
38	P	53	ILE
38	P	85	ASP
38	P	92	GLU
39	Q	56	ARG
39	Q	67	ARG
39	Q	88	LYS
39	Q	107	LEU
39	Q	108	LEU
39	Q	127	THR
40	R	76	LEU
40	R	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	S	3	PHE
41	S	64	LYS
42	T	100	LYS
42	T	166	LEU
43	U	43	LEU
43	U	49	GLU
43	U	54	LYS
43	U	69	CYS
43	U	74	ARG
43	U	97	ASP
43	U	215	GLU
43	U	228	GLU
43	U	232	THR
43	U	240	GLU
43	U	245	LYS
43	U	250	GLU
43	U	253	GLU
43	U	255	CYS
43	U	256	GLU
43	U	263	ARG
43	U	276	GLU
43	U	281	ASP
43	U	291	ARG
43	U	335	GLU
43	U	347	GLU
43	U	352	LYS
44	V	3	LYS
44	V	6	LEU
44	V	82	GLU
44	V	99	LEU
44	V	104	ARG
44	V	140	LYS
44	V	141	VAL
45	W	80	ASP
45	W	99	LYS
45	W	110	VAL
45	W	113	THR
45	W	131	GLU
37	X	76	LEU
37	X	129	GLU
37	X	133	ILE
37	X	138	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	Y	39	HIS
46	Y	46	GLN
46	Y	62	SER
46	Y	72	ARG
46	Y	76	ASP
46	Y	80	VAL
46	Y	81	LEU
46	Y	88	ASP
46	Y	92	TRP
47	Z	29	LYS
47	Z	41	GLU
47	Z	59	ASP
47	Z	67	TRP
47	Z	101	GLU
48	1	1	MET
48	1	34	ASN
48	1	59	GLN
48	1	60	GLU
48	1	62	ILE
48	1	65	ASN
48	1	102	GLU
48	1	122	VAL
48	1	169	LEU
48	1	246	LEU
48	1	247	LEU
48	1	268	GLU
48	1	271	LYS
48	1	314	MET
48	1	321	GLN
48	1	364	LYS
48	1	373	LEU
48	1	383	MET
48	1	387	THR
48	1	397	GLU
48	1	407	TRP
48	1	411	MET
48	1	434	LYS
48	1	440	LEU
48	1	445	GLU
48	1	470	ASN
48	1	486	MET
48	1	502	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	l	559	GLU
48	l	589	LEU
48	l	598	SER
49	s	83	GLU
49	s	88	GLU
49	s	129	ASP
49	s	135	GLU
49	s	175	ARG
49	s	188	VAL
49	s	191	LYS
49	s	214	LEU
49	s	216	GLU
50	t	21	ARG
50	t	29	TYR
50	t	31	PHE
50	t	33	GLU
50	t	48	ASP
50	t	57	ASP
50	t	65	GLN
50	t	83	GLU
50	t	88	ASP
50	t	91	GLU
51	u	84	GLU
51	u	94	GLU
51	u	138	LYS
51	u	157	GLU
51	u	181	ASP
51	u	190	THR
51	u	201	VAL
51	u	206	GLU
51	u	256	THR
51	u	274	GLU
51	u	341	PHE
51	u	342	GLN
51	u	350	GLU
51	u	363	MET
51	u	368	MET
51	u	375	GLN
51	u	384	THR
51	u	411	GLU
51	u	435	GLU
51	u	443	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	u	467	ASP
5	v	47	LEU
5	v	83	LEU
5	v	115	THR
5	v	122	THR
5	v	124	GLU
5	v	129	ASP
5	v	130	ILE
5	v	147	ARG
5	v	154	LEU
5	v	158	LEU
5	v	161	ASP
5	v	175	GLU
5	v	203	ASP
5	v	225	VAL
5	v	230	LEU
5	v	231	LYS
5	v	233	VAL
5	v	250	LYS
5	v	390	GLU
5	v	401	LEU
5	v	407	VAL
5	v	421	ASP
5	v	451	ASP
6	w	83	HIS
6	w	94	LEU
6	w	97	HIS
6	w	171	ASP
6	w	216	ASP
6	w	233	LEU
6	w	255	ASN
6	w	273	TYR
6	w	306	MET
6	w	311	LYS
6	w	366	MET
6	w	379	TRP
7	x	107	ASP
7	x	129	ASP
7	x	136	LEU
7	x	152	GLU
7	x	154	GLU
7	x	164	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	x	221	GLU
7	x	243	ILE
7	x	245	MET
7	x	249	ILE
7	x	252	GLU
7	x	293	MET
7	x	320	LEU
8	y	15	GLU
8	y	68	ASP
8	y	72	ARG
8	y	75	ILE
8	y	79	GLU
8	y	83	LYS
8	y	85	GLU
8	y	97	GLU
52	z	16	THR
52	z	19	LEU
52	z	32	THR
52	z	40	ARG
52	z	47	LEU
52	z	68	GLU
52	Aa	5	PHE
52	Aa	17	TYR
52	Aa	32	THR
52	Aa	47	LEU
52	Aa	48	ARG
52	Aa	79	GLU
1	Ab	26	LEU
1	Ab	35	GLU
1	Ab	37	CYS
1	Ab	38	GLU
1	Ab	42	LYS
1	Ab	51	GLU
1	Ab	54	ASP
1	Ab	66	ASP
1	Ab	69	GLU
1	Ab	81	CYS
1	Ab	85	LYS
1	Ab	91	LYS
2	Ac	13	LEU
2	Ac	14	LEU
2	Ac	45	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ac	54	LYS
4	Ad	13	LEU
51	5	47	GLU
51	5	84	GLU
51	5	98	PHE
51	5	101	THR
51	5	142	LYS
51	5	164	GLU
51	5	183	VAL
51	5	218	GLU
51	5	244	ASP
51	5	284	LEU
51	5	327	THR
51	5	341	PHE
51	5	350	GLU
51	5	363	MET
51	5	368	MET
51	5	411	GLU
53	G	41	VAL
53	G	44	GLU
53	G	64	CYS
53	G	75	CYS
53	G	94	MET
53	G	107	GLU
53	G	158	ARG
53	G	194	ASP
53	G	197	THR
53	G	217	GLU
53	G	225	ILE
53	G	241	ARG
53	G	247	LYS
53	G	252	ASP
53	G	310	GLU
53	G	325	ARG
53	G	329	MET
53	G	338	VAL
53	G	347	ASP
53	G	349	GLU
53	G	361	VAL
53	G	370	GLU
53	G	426	ASP
53	G	429	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	G	447	ASP
53	G	450	LYS
53	G	470	LYS
53	G	493	VAL
53	G	511	LYS
53	G	519	ILE
53	G	571	HIS
53	G	592	LYS
53	G	617	ARG
53	G	632	MET
53	G	636	TYR
53	G	652	ASN
53	G	657	ASP
53	G	659	VAL
53	G	660	GLU
53	G	671	LEU
53	G	679	LEU
53	G	680	LEU
54	M	10	LEU
54	M	25	GLN
54	M	69	VAL
54	M	91	GLU
54	M	95	VAL
3	Ae	62	THR
3	Ae	63	SER
3	Ae	65	SER
3	Ae	67	VAL
3	Ae	68	LEU
3	Ae	71	LYS
3	Ae	75	LEU
3	Af	53	VAL
3	Af	62	THR
3	Af	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	39	GLN
1	0	62	GLN
1	0	76	HIS
2	1	38	GLN
2	1	55	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2	207	GLN
3	4	101	HIS
3	4	185	ASN
3	4	220	GLN
3	4	240	HIS
5	6	36	GLN
5	6	75	ASN
5	6	155	GLN
5	6	170	GLN
5	6	184	ASN
5	6	232	GLN
5	6	268	HIS
5	6	304	ASN
5	6	319	GLN
5	6	343	GLN
5	6	368	ASN
6	7	137	GLN
6	7	201	HIS
6	7	260	ASN
6	7	286	ASN
6	7	312	GLN
6	7	341	GLN
7	8	108	HIS
7	8	120	GLN
7	8	190	ASN
7	8	283	HIS
7	8	285	HIS
7	8	310	HIS
8	9	23	ASN
9	a	132	ASN
9	a	181	HIS
10	b	67	HIS
10	b	83	HIS
12	d	23	GLN
12	d	107	GLN
13	e	70	ASN
13	e	145	ASN
14	f	36	HIS
15	g	18	ASN
15	g	90	HIS
16	h	82	GLN
16	h	97	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	h	98	HIS
17	i	289	ASN
17	i	319	HIS
17	i	347	ASN
18	j	28	ASN
19	k	57	ASN
20	m	86	ASN
21	n	3	ASN
21	n	14	HIS
22	o	52	ASN
22	o	117	GLN
23	p	117	GLN
23	p	120	GLN
23	p	211	HIS
24	q	83	HIS
24	q	184	HIS
24	q	279	GLN
24	q	304	GLN
24	q	338	HIS
24	q	366	ASN
24	q	390	ASN
24	q	399	ASN
24	q	421	HIS
24	q	422	HIS
25	r	230	ASN
26	B	133	HIS
26	B	170	GLN
26	B	244	ASN
26	B	376	HIS
26	B	381	GLN
26	B	393	ASN
26	B	418	GLN
27	C	42	GLN
27	C	168	GLN
27	C	239	HIS
27	C	240	GLN
27	C	305	GLN
27	C	386	HIS
28	D	51	ASN
28	D	124	ASN
28	D	181	HIS
28	D	236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	E	41	HIS
29	E	74	HIS
29	E	87	GLN
29	E	123	ASN
29	E	133	GLN
29	E	144	ASN
29	E	153	GLN
30	F	120	GLN
32	I	123	GLN
33	J	86	ASN
33	J	93	ASN
35	L	67	HIS
35	L	74	GLN
35	L	117	HIS
35	L	123	ASN
35	L	133	ASN
35	L	145	HIS
35	L	210	ASN
35	L	290	HIS
35	L	318	HIS
35	L	326	HIS
36	N	21	HIS
36	N	50	GLN
36	N	73	GLN
36	N	83	GLN
39	Q	77	GLN
41	S	25	HIS
41	S	44	GLN
42	T	125	ASN
43	U	144	GLN
43	U	151	HIS
43	U	217	GLN
43	U	237	GLN
43	U	325	GLN
46	Y	54	GLN
48	l	25	ASN
48	l	56	HIS
48	l	59	GLN
48	l	65	ASN
48	l	72	GLN
48	l	136	ASN
48	l	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	l	192	HIS
48	l	194	ASN
48	l	248	HIS
48	l	309	GLN
48	l	328	HIS
48	l	354	GLN
48	l	470	ASN
48	l	603	ASN
49	s	181	GLN
50	t	44	GLN
50	t	92	HIS
51	u	103	ASN
51	u	152	GLN
51	u	153	ASN
51	u	160	GLN
51	u	323	HIS
51	u	342	GLN
5	v	212	HIS
5	v	319	GLN
5	v	372	GLN
6	w	32	ASN
6	w	44	GLN
6	w	54	HIS
6	w	196	HIS
6	w	221	HIS
6	w	255	ASN
6	w	267	HIS
7	x	120	GLN
7	x	241	GLN
7	x	283	HIS
8	y	23	ASN
52	z	29	HIS
52	Aa	13	HIS
52	Aa	24	GLN
1	Ab	76	HIS
51	5	119	HIS
51	5	128	HIS
51	5	323	HIS
51	5	397	ASN
53	G	142	GLN
53	G	278	HIS
53	G	359	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	G	425	ASN
53	G	569	GLN
53	G	604	GLN
53	G	666	GLN
53	G	678	GLN
54	M	25	GLN
54	M	52	ASN
3	Ae	39	HIS
3	Af	56	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	FES	2	301	3	0,4,4	-	-	-		
59	SF4	B	502	26	0,12,12	-	-	-		
55	FES	G	803	53	0,4,4	-	-	-		
59	SF4	H	302	31	0,12,12	-	-	-		
56	HEM	w	401	-	50,50,50	1.38	9 (18%)	67,82,82	1.14	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	FMN	B	501	-	33,33,33	1.04	2 (6%)	48,50,50	1.21	6 (12%)
59	SF4	G	801	53	0,12,12	-	-	-	-	-
57	HEC	x	401	7	46,50,50	1.85	5 (10%)	58,82,82	1.72	7 (12%)
60	NDP	L	401	-	51,52,52	0.49	0	71,80,80	0.71	1 (1%)
59	SF4	G	802	53	0,12,12	-	-	-	-	-
56	HEM	7	401	6	50,50,50	1.52	6 (12%)	67,82,82	1.10	2 (2%)
55	FES	4	301	3	0,4,4	-	-	-	-	-
59	SF4	H	301	31	0,12,12	-	-	-	-	-
56	HEM	w	402	6	50,50,50	1.38	9 (18%)	67,82,82	1.09	4 (5%)
57	HEC	8	401	7	46,50,50	1.82	7 (15%)	58,82,82	2.14	6 (10%)
55	FES	E	301	29	0,4,4	-	-	-	-	-
61	ZMP	Q	201	-	27,29,36	1.78	6 (22%)	34,38,45	1.74	7 (20%)
56	HEM	7	402	-	50,50,50	1.61	7 (14%)	67,82,82	1.05	2 (2%)
59	SF4	I	201	32	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
55	FES	2	301	3	-	-	0/1/1/1
59	SF4	B	502	26	-	-	0/6/5/5
55	FES	G	803	53	-	-	0/1/1/1
59	SF4	H	302	31	-	-	0/6/5/5
56	HEM	w	401	-	-	0/14/54/54	-
58	FMN	B	501	-	-	2/18/18/18	0/3/3/3
59	SF4	G	801	53	-	-	0/6/5/5
57	HEC	x	401	7	-	6/14/54/54	-
60	NDP	L	401	-	-	4/34/77/77	0/5/5/5
59	SF4	G	802	53	-	-	0/6/5/5
56	HEM	7	401	6	-	5/14/54/54	-
55	FES	4	301	3	-	-	0/1/1/1
59	SF4	H	301	31	-	-	0/6/5/5
56	HEM	w	402	6	-	0/14/54/54	-
57	HEC	8	401	7	-	8/14/54/54	-
55	FES	E	301	29	-	-	0/1/1/1
61	ZMP	Q	201	-	-	12/36/36/43	-
56	HEM	7	402	-	-	7/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	I	201	32	-	-	0/6/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	x	401	HEC	CAB-C3B	6.32	1.55	1.35
57	8	401	HEC	CAC-C3C	6.26	1.55	1.35
57	x	401	HEC	CAC-C3C	6.21	1.55	1.35
57	8	401	HEC	CAB-C3B	5.86	1.54	1.35
57	x	401	HEC	C3D-C2D	5.66	1.53	1.38
57	8	401	HEC	C3D-C2D	5.59	1.53	1.38
56	7	402	HEM	FE-ND	5.52	2.11	1.94
61	Q	201	ZMP	C16-N2	5.24	1.45	1.33
61	Q	201	ZMP	C13-N1	5.16	1.45	1.33
56	7	401	HEM	FE-ND	4.33	2.08	1.94
56	7	402	HEM	FE-NB	4.00	2.07	1.94
56	7	401	HEM	FE-NB	3.65	2.06	1.94
56	w	401	HEM	FE-NC	3.50	2.06	1.95
58	B	501	FMN	C4A-N5	3.38	1.38	1.30
56	7	402	HEM	FE-NA	3.37	2.06	1.95
56	7	401	HEM	FE-NC	3.36	2.06	1.95
56	7	401	HEM	FE-NA	3.33	2.06	1.95
56	w	402	HEM	FE-ND	3.26	2.04	1.94
56	w	402	HEM	FE-NB	3.18	2.04	1.94
56	w	401	HEM	FE-NA	3.16	2.05	1.95
56	w	401	HEM	CAC-C3C	3.04	1.55	1.47
56	7	402	HEM	FE-NC	2.98	2.05	1.95
56	w	402	HEM	CAB-C3B	2.98	1.55	1.47
56	7	402	HEM	CAB-C3B	2.92	1.55	1.47
56	w	401	HEM	CAB-C3B	2.89	1.55	1.47
56	7	402	HEM	CAC-C3C	2.86	1.55	1.47
56	7	401	HEM	CAB-C3B	2.83	1.54	1.47
56	w	402	HEM	CAC-C3C	2.80	1.54	1.47
56	7	401	HEM	CAC-C3C	2.80	1.54	1.47
56	w	401	HEM	FE-NB	2.75	2.03	1.94
56	w	402	HEM	FE-NA	2.73	2.04	1.95
58	B	501	FMN	C10-N1	2.52	1.38	1.33
61	Q	201	ZMP	C10-S1	2.42	1.82	1.76
56	w	402	HEM	FE-NC	2.40	2.03	1.95
57	8	401	HEC	C3B-C2B	-2.39	1.33	1.41
61	Q	201	ZMP	O3-C16	-2.37	1.18	1.23
56	w	401	HEM	FE-ND	2.37	2.02	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	Q	201	ZMP	O2-C13	-2.29	1.18	1.23
57	x	401	HEC	CMB-C2B	2.26	1.55	1.50
57	8	401	HEC	C3C-C2C	-2.26	1.33	1.41
57	x	401	HEC	CMC-C2C	2.19	1.55	1.50
61	Q	201	ZMP	C9-C10	2.18	1.53	1.50
56	w	401	HEM	CMC-C2C	2.17	1.55	1.50
56	w	402	HEM	CMC-C2C	2.13	1.55	1.50
56	w	401	HEM	CMA-C3A	2.05	1.55	1.50
56	w	402	HEM	CMB-C2B	2.05	1.55	1.50
56	w	402	HEM	CMA-C3A	2.03	1.54	1.50
57	8	401	HEC	CMD-C2D	2.03	1.54	1.50
56	7	402	HEM	C2A-C3A	-2.02	1.33	1.38
57	8	401	HEC	CMB-C2B	2.01	1.54	1.50
56	w	401	HEM	C2A-C3A	-2.00	1.33	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	8	401	HEC	CBB-CAB-C3B	-10.29	106.86	127.43
57	8	401	HEC	CBC-CAC-C3C	-8.71	110.03	127.43
57	x	401	HEC	CBC-CAC-C3C	-7.11	113.22	127.43
57	x	401	HEC	CBB-CAB-C3B	-6.39	114.67	127.43
61	Q	201	ZMP	C9-C10-S1	5.74	120.24	113.40
60	L	401	NDP	P2B-O2B-C2B	-4.13	112.42	123.43
61	Q	201	ZMP	O1-C10-C9	-3.54	119.90	123.98
57	8	401	HEC	C4D-ND-C1D	3.40	111.36	105.82
57	x	401	HEC	C4D-ND-C1D	3.21	111.06	105.82
58	B	501	FMN	C4-N3-C2	-3.20	119.97	125.64
57	x	401	HEC	CMC-C2C-C1C	-3.08	120.73	125.42
61	Q	201	ZMP	C17-C16-N2	3.02	122.21	116.48
58	B	501	FMN	C4A-C10-N10	2.73	120.39	116.48
56	7	401	HEM	C3B-C2B-C1B	2.63	108.39	106.41
58	B	501	FMN	C4A-C4-N3	2.63	119.96	113.25
56	w	401	HEM	C4D-ND-C1D	2.59	108.28	105.21
61	Q	201	ZMP	C14-C15-N2	-2.53	106.62	112.00
61	Q	201	ZMP	O3-C16-N2	-2.49	117.70	122.98
58	B	501	FMN	O4-C4-C4A	-2.48	120.00	126.53
57	8	401	HEC	CHD-C4C-NC	2.44	127.11	124.45
57	8	401	HEC	CHA-C1A-NA	2.40	127.06	124.45
56	w	402	HEM	C4D-ND-C1D	2.34	107.97	105.21
57	x	401	HEC	CAA-CBA-CGA	-2.34	107.47	113.67
58	B	501	FMN	C10-C4A-N5	-2.33	120.05	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	401	HEM	C1B-NB-C4B	2.32	107.96	105.21
56	w	401	HEM	C3B-C2B-C1B	2.28	108.13	106.41
56	w	402	HEM	CHC-C1C-NC	2.27	126.92	124.45
57	x	401	HEC	CAD-CBD-CGD	-2.25	107.69	113.67
61	Q	201	ZMP	O1-C10-S1	-2.22	119.85	122.68
56	w	402	HEM	C3B-C2B-C1B	2.22	108.08	106.41
56	7	401	HEM	C1B-NB-C4B	2.16	107.76	105.21
56	w	401	HEM	C3D-C4D-ND	-2.14	107.82	110.17
57	x	401	HEC	C2A-C1A-NA	-2.12	108.28	110.32
56	w	401	HEM	CHD-C1D-ND	2.12	126.70	124.42
61	Q	201	ZMP	C11-S1-C10	2.09	108.01	101.84
57	8	401	HEC	C2C-C1C-NC	-2.07	106.83	110.14
56	w	401	HEM	C2D-C1D-ND	-2.07	107.51	109.90
56	7	402	HEM	C1B-NB-C4B	2.06	107.65	105.21
56	7	402	HEM	CAA-CBA-CGA	-2.06	108.21	113.67
58	B	501	FMN	C4A-C10-N1	-2.04	119.59	124.59
56	w	402	HEM	C2D-C1D-ND	-2.02	107.57	109.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	7	402	HEM	C1A-C2A-CAA-CBA
57	8	401	HEC	C2B-C3B-CAB-CBB
57	8	401	HEC	C4B-C3B-CAB-CBB
57	8	401	HEC	C2C-C3C-CAC-CBC
57	8	401	HEC	C4C-C3C-CAC-CBC
57	x	401	HEC	C2C-C3C-CAC-CBC
57	x	401	HEC	C4C-C3C-CAC-CBC
61	Q	201	ZMP	N2-C16-C17-O4
61	Q	201	ZMP	C17-C16-N2-C15
61	Q	201	ZMP	S1-C11-C12-N1
61	Q	201	ZMP	C12-C11-S1-C10
61	Q	201	ZMP	O3-C16-N2-C15
60	L	401	NDP	O4D-C1D-N1N-C6N
56	7	401	HEM	C3D-CAD-CBD-CGD
60	L	401	NDP	C3B-C4B-C5B-O5B
56	7	402	HEM	C4D-C3D-CAD-CBD
61	Q	201	ZMP	O3-C16-C17-O4
60	L	401	NDP	O4B-C4B-C5B-O5B
56	7	402	HEM	C3A-C2A-CAA-CBA
61	Q	201	ZMP	O3-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
56	7	402	HEM	C2D-C3D-CAD-CBD
61	Q	201	ZMP	N2-C16-C17-C18
61	Q	201	ZMP	O1-C10-S1-C11
61	Q	201	ZMP	C9-C10-S1-C11
61	Q	201	ZMP	C4-C5-C6-C7
56	7	401	HEM	C4B-C3B-CAB-CBB
56	7	401	HEM	C4C-C3C-CAC-CBC
60	L	401	NDP	C5B-O5B-PA-O1A
57	8	401	HEC	C1A-C2A-CAA-CBA
57	8	401	HEC	C3A-C2A-CAA-CBA
57	x	401	HEC	CAD-CBD-CGD-O1D
61	Q	201	ZMP	C11-C12-N1-C13
57	x	401	HEC	CAD-CBD-CGD-O2D
56	7	402	HEM	CAD-CBD-CGD-O1D
58	B	501	FMN	O2'-C2'-C3'-C4'
57	x	401	HEC	CAA-CBA-CGA-O2A
56	7	401	HEM	CAA-CBA-CGA-O1A
56	7	401	HEM	CAA-CBA-CGA-O2A
57	x	401	HEC	CAA-CBA-CGA-O1A
58	B	501	FMN	O2'-C2'-C3'-O3'
56	7	402	HEM	CAD-CBD-CGD-O2D
56	7	402	HEM	CAA-CBA-CGA-O1A
57	8	401	HEC	C3D-CAD-CBD-CGD
57	8	401	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

16 monomers are involved in 90 short contacts:

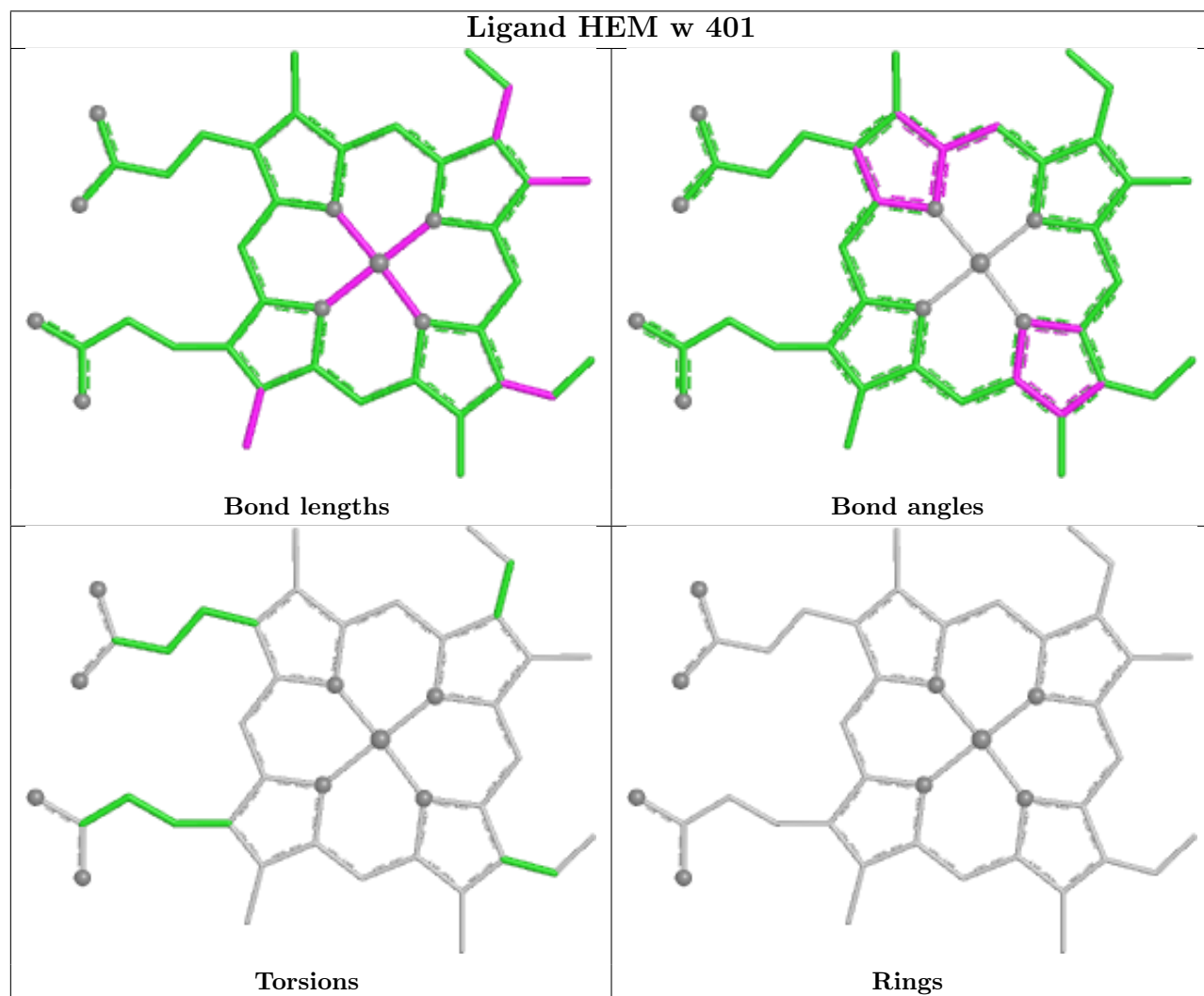
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2	301	FES	4	0
59	H	302	SF4	4	0
56	w	401	HEM	14	0
58	B	501	FMN	3	0
59	G	801	SF4	1	0
57	x	401	HEC	9	0
60	L	401	NDP	5	0
56	7	401	HEM	9	0
55	4	301	FES	2	0
59	H	301	SF4	3	0
56	w	402	HEM	5	0
57	8	401	HEC	11	0
55	E	301	FES	7	0

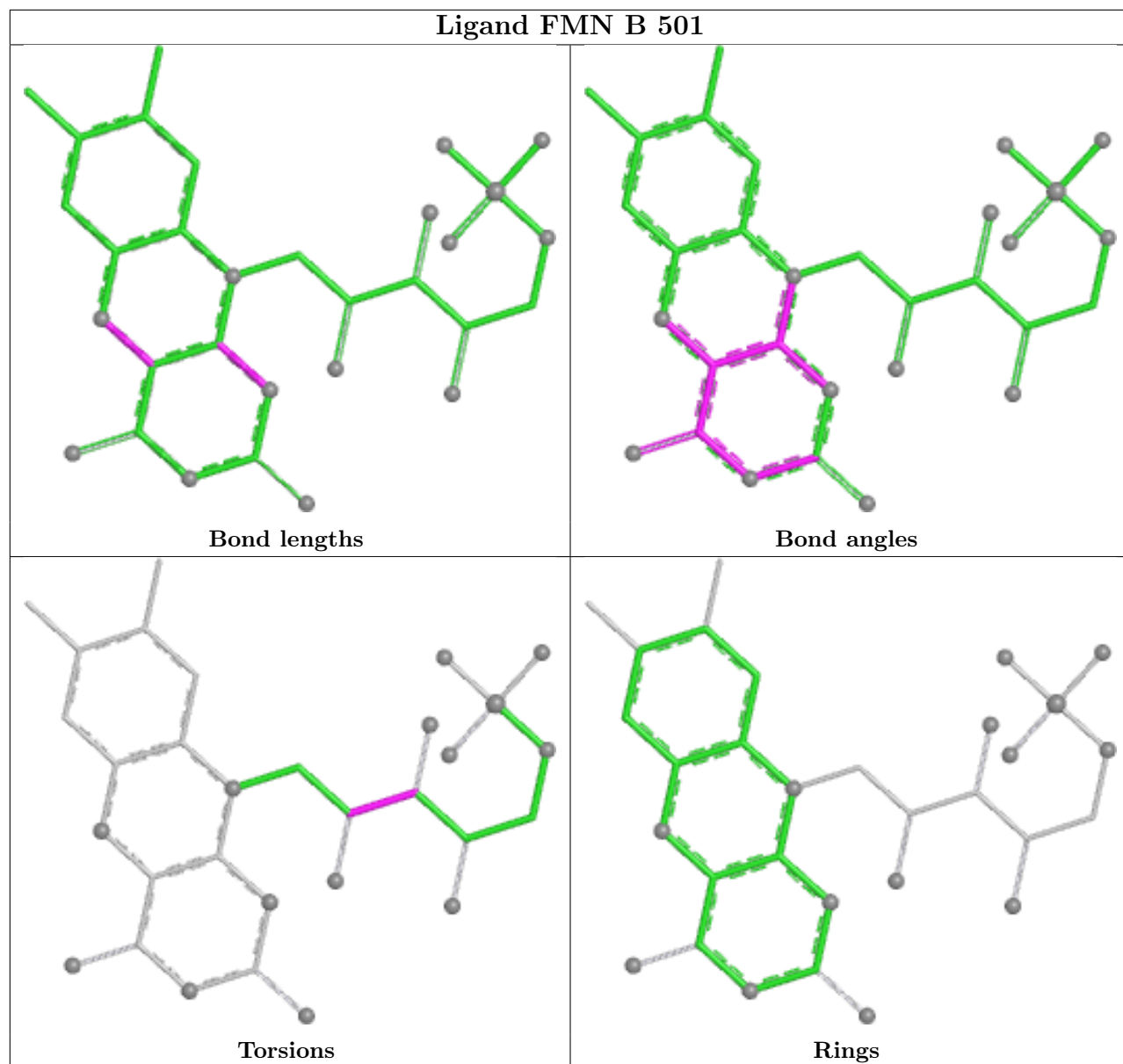
Continued on next page...

Continued from previous page...

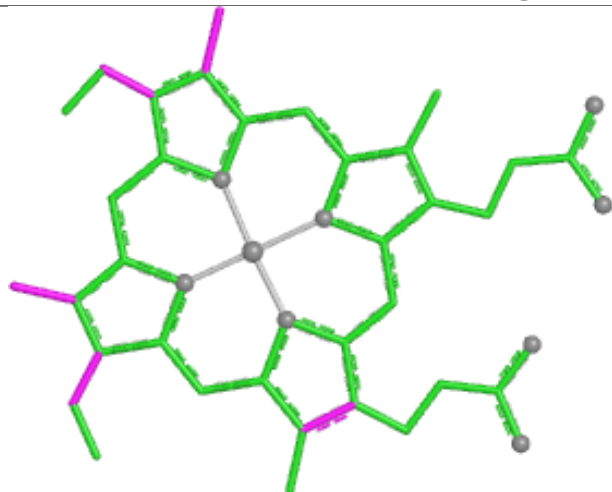
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	Q	201	ZMP	1	0
56	7	402	HEM	10	0
59	I	201	SF4	2	0

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.

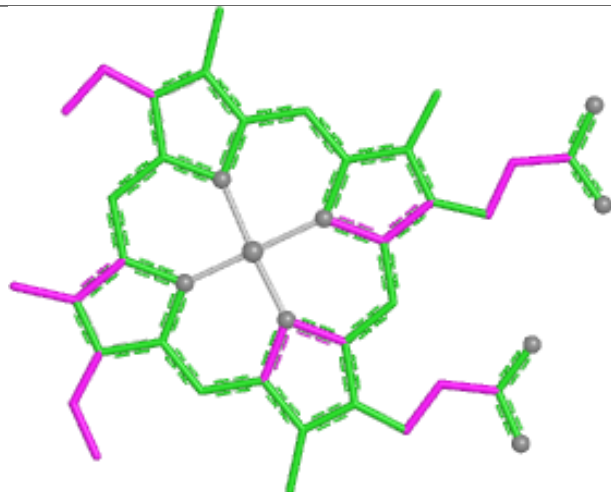




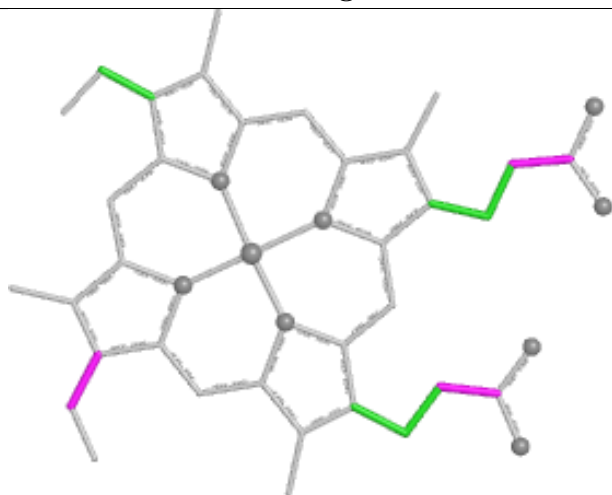
Ligand HEC x 401



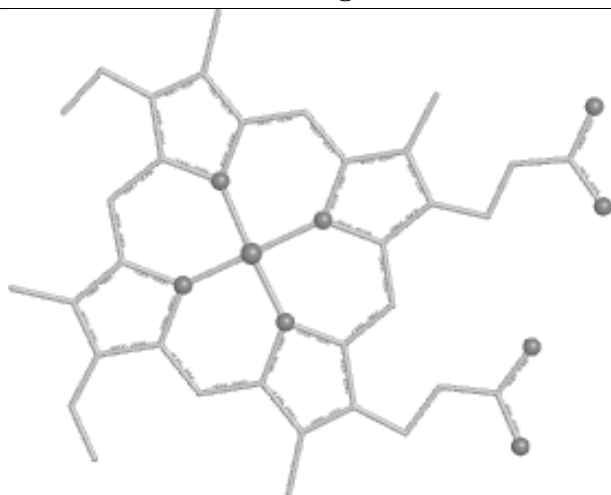
Bond lengths



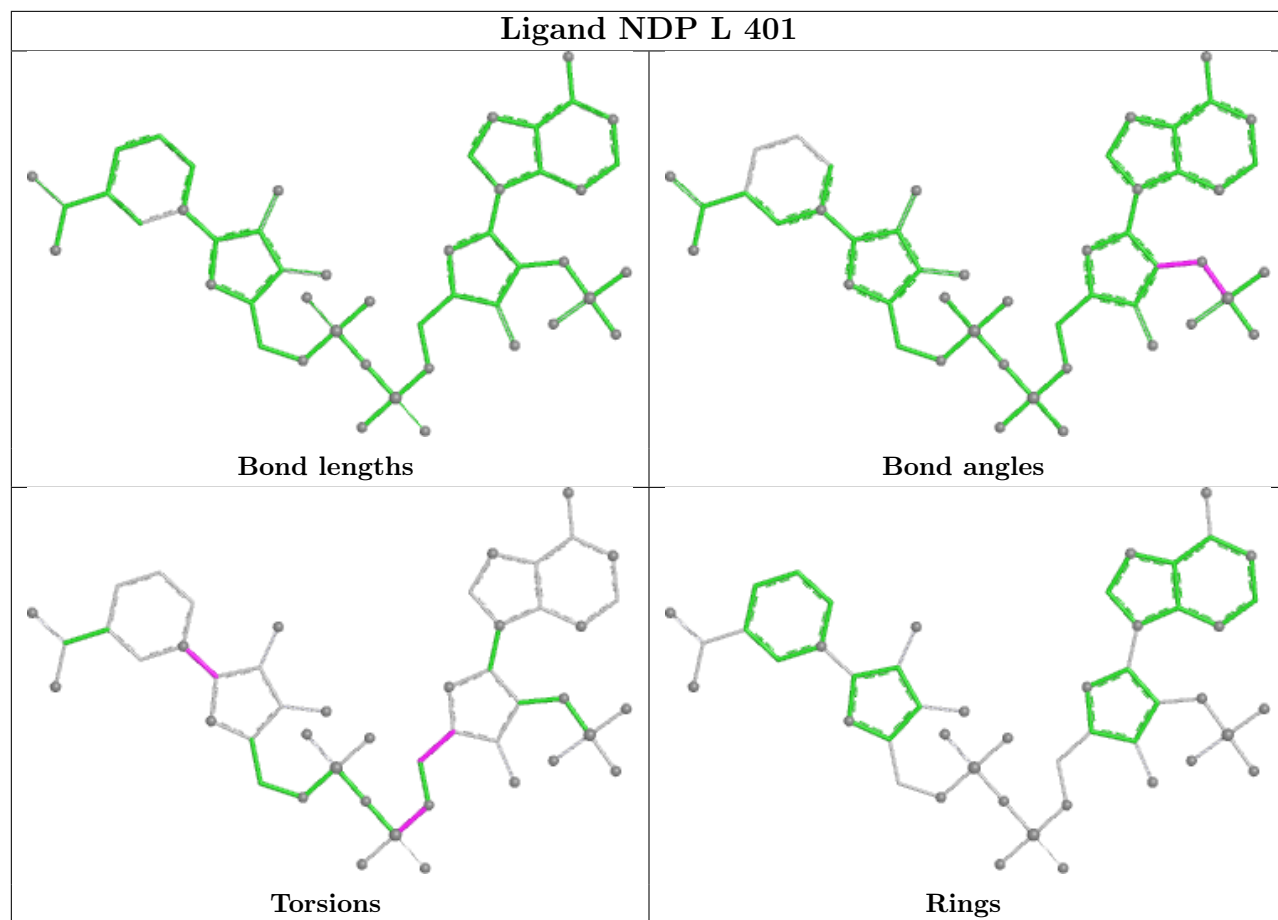
Bond angles

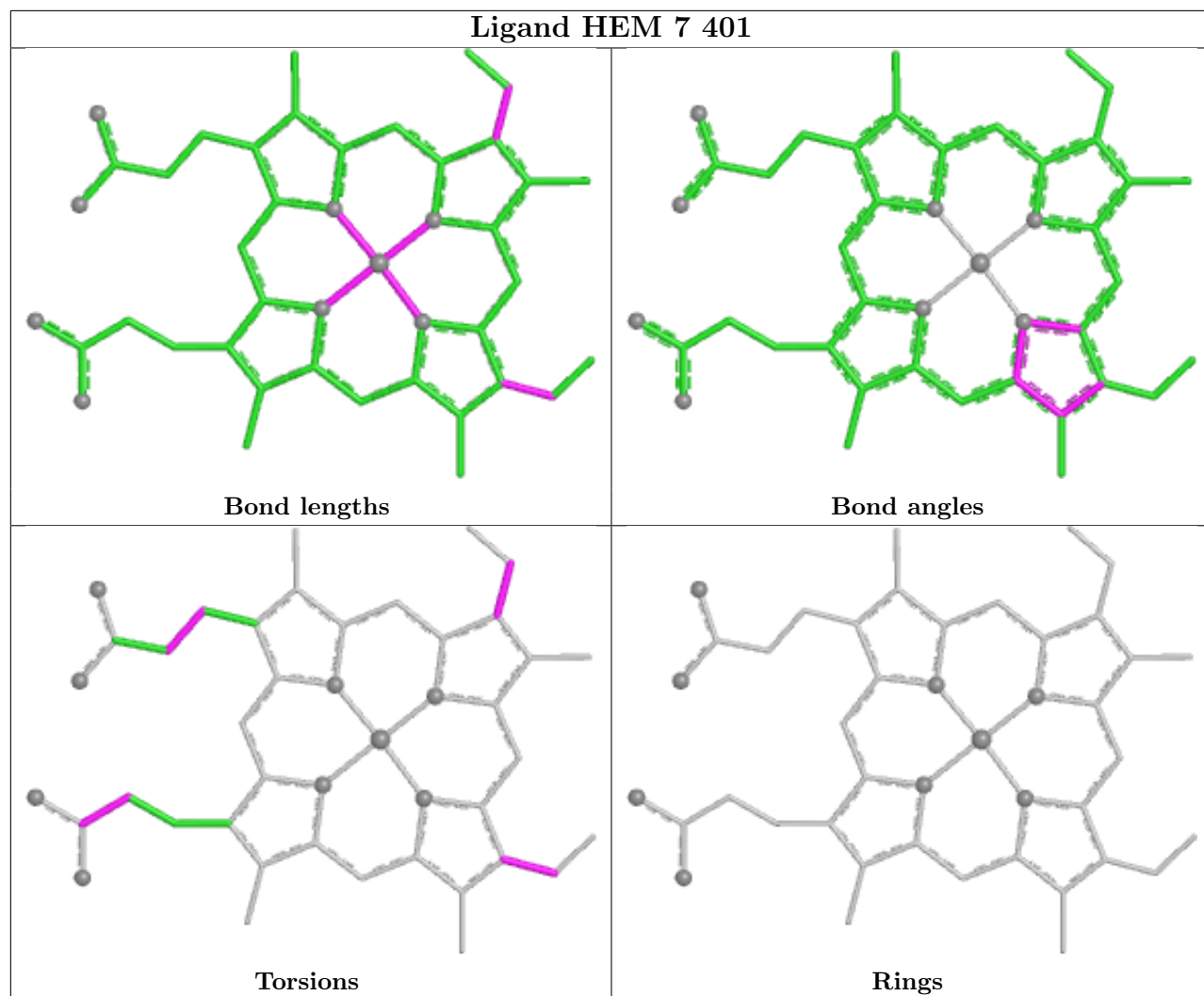


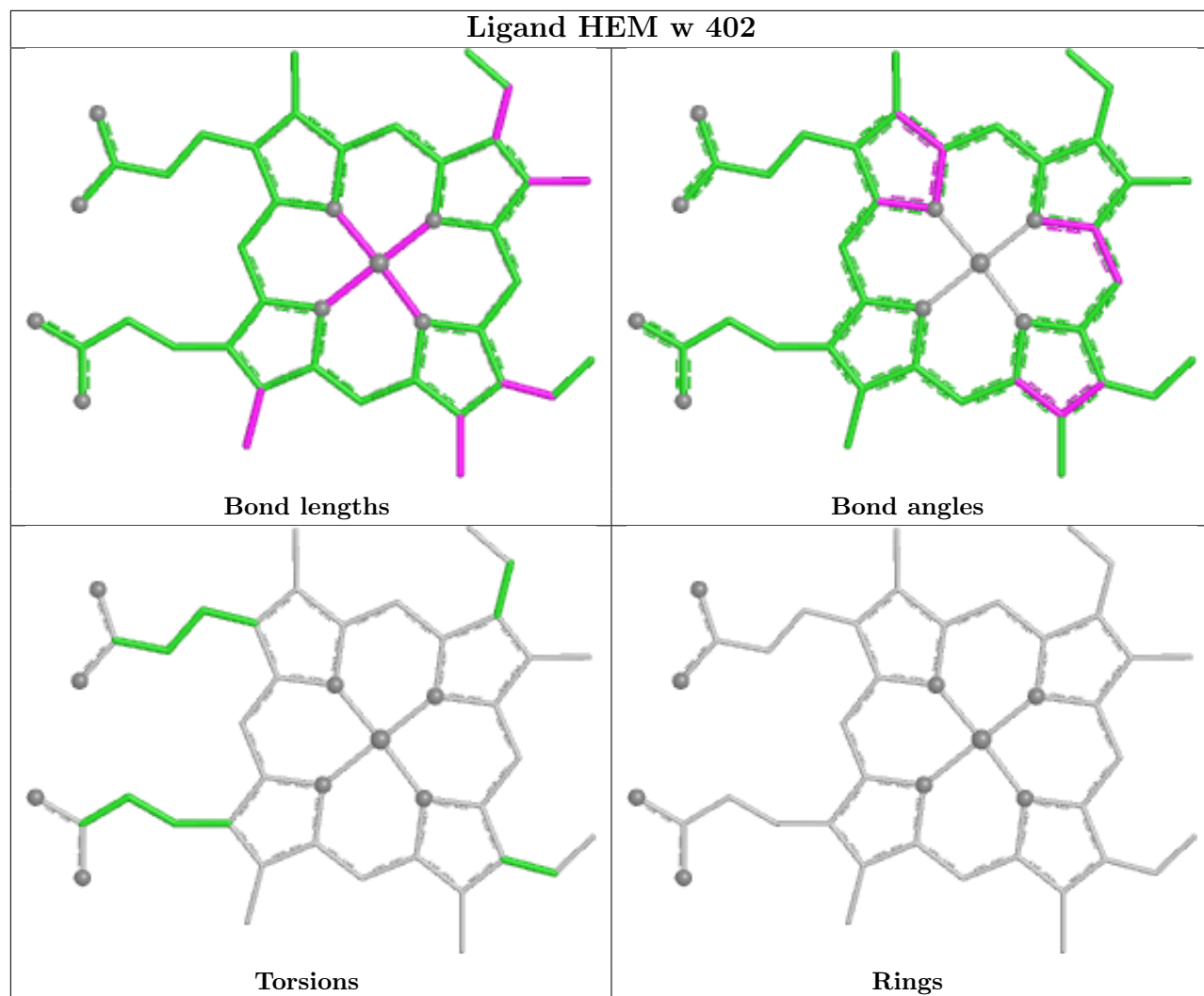
Torsions



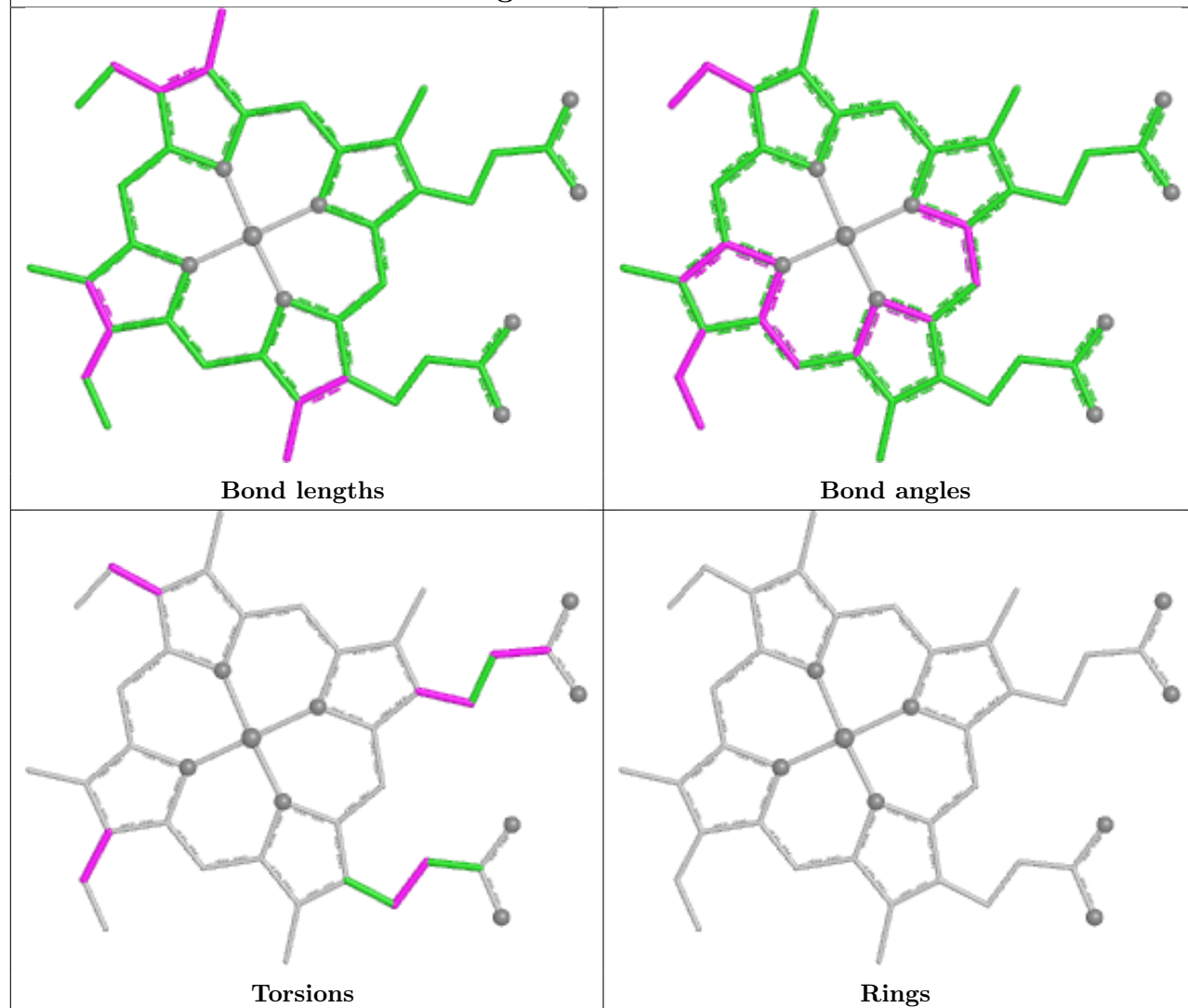
Rings



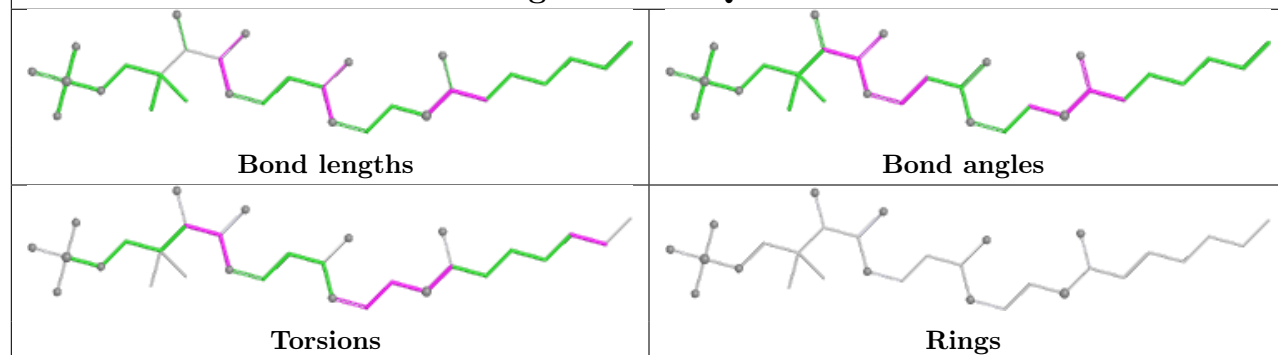


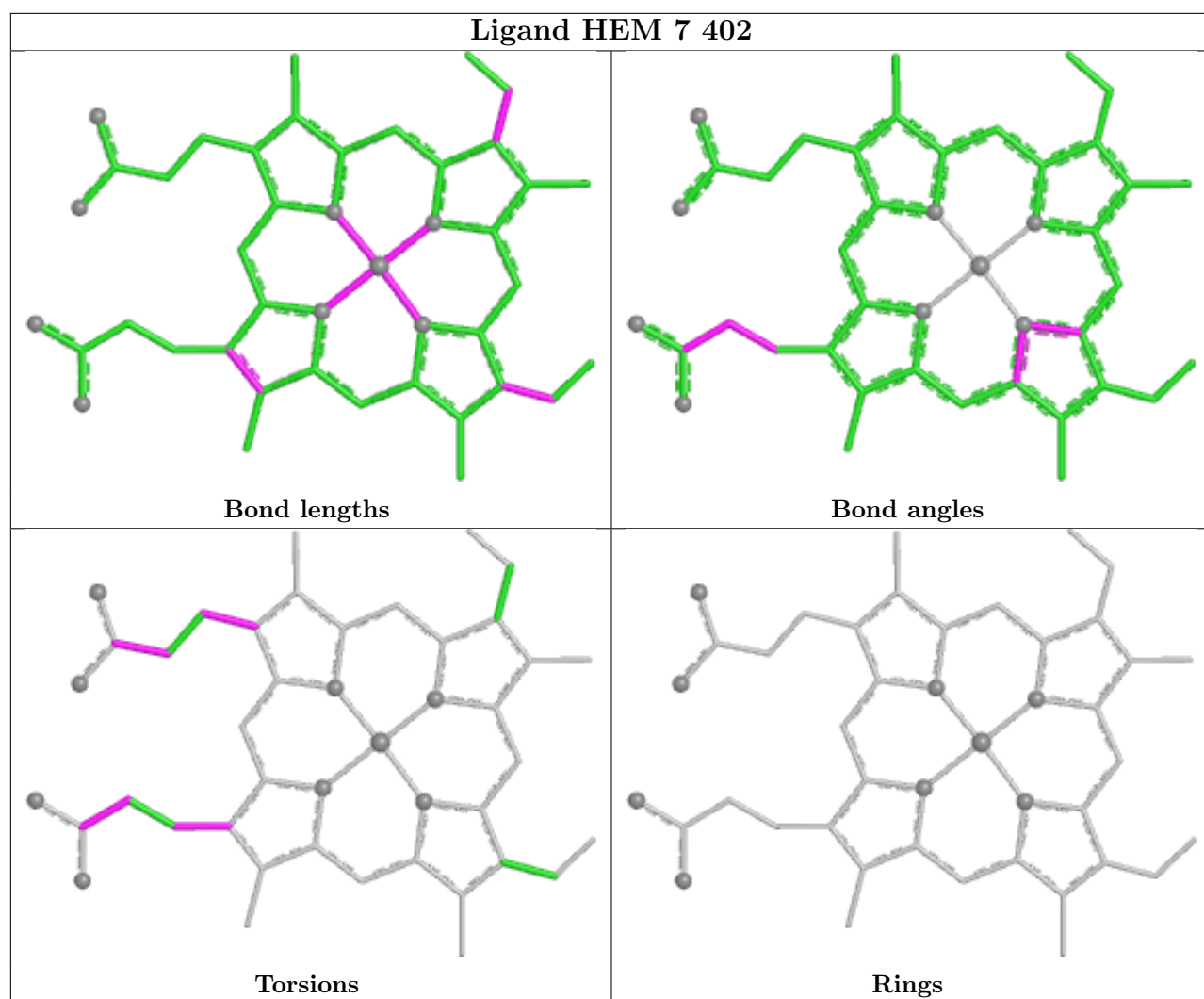


Ligand HEC 8 401



Ligand ZMP Q 201





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.

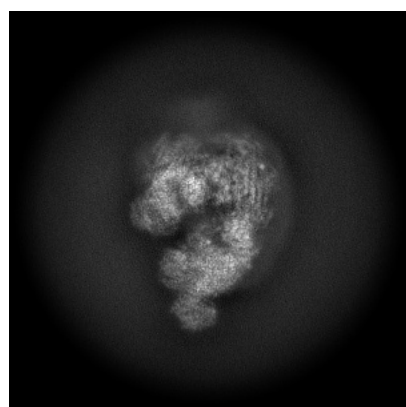
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45013. These allow visual inspection of the internal detail of the map and identification of artifacts.

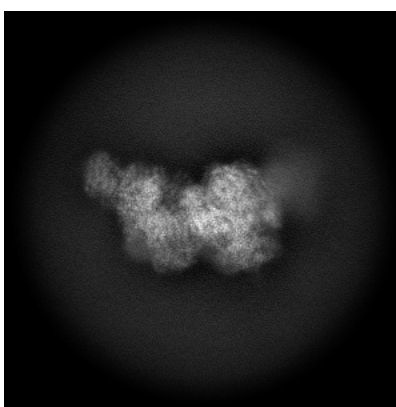
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

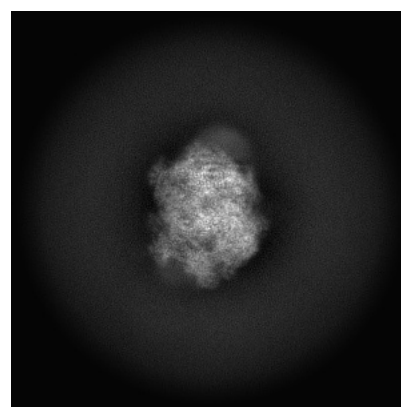
6.1.1 Primary map



X



Y

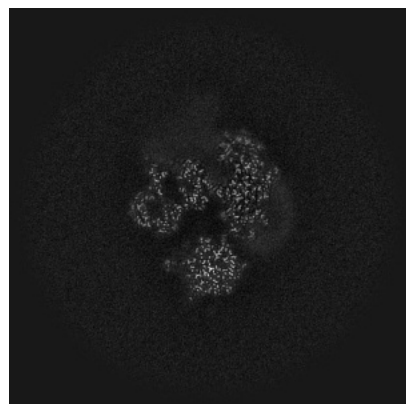


Z

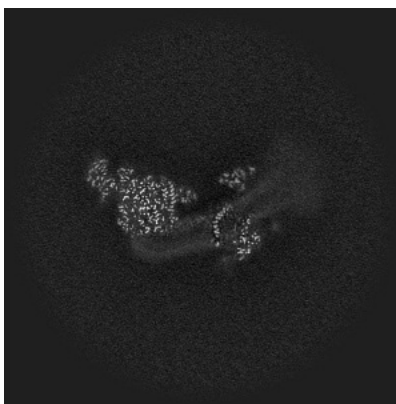
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

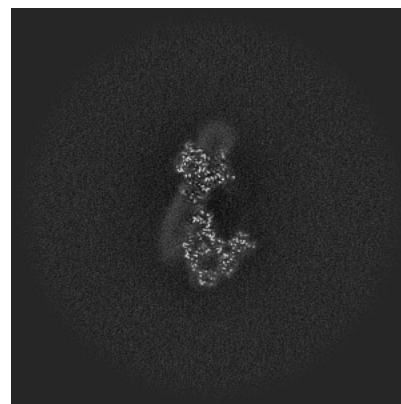
6.2.1 Primary map



X Index: 256



Y Index: 256

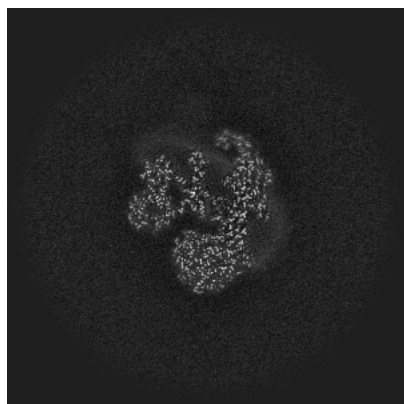


Z Index: 256

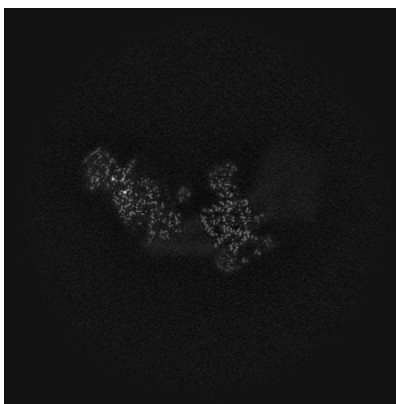
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

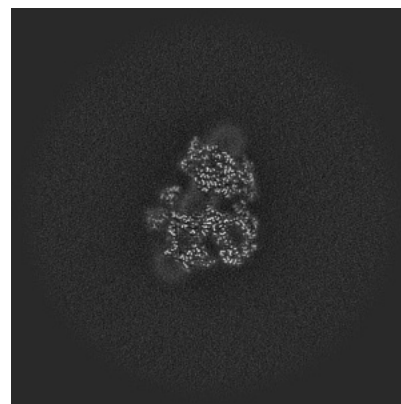
6.3.1 Primary map



X Index: 244



Y Index: 241



Z Index: 287

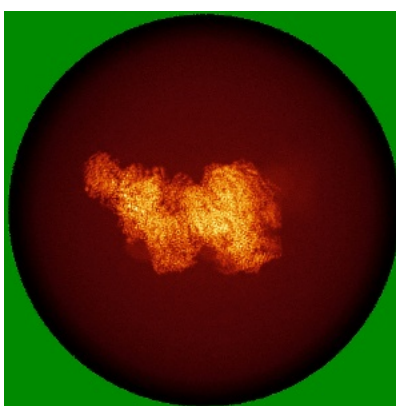
The images above show the largest variance slices of the map in three orthogonal directions.

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

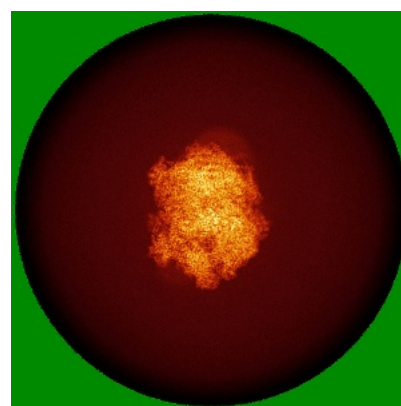
6.4.1 Primary map



X



Y

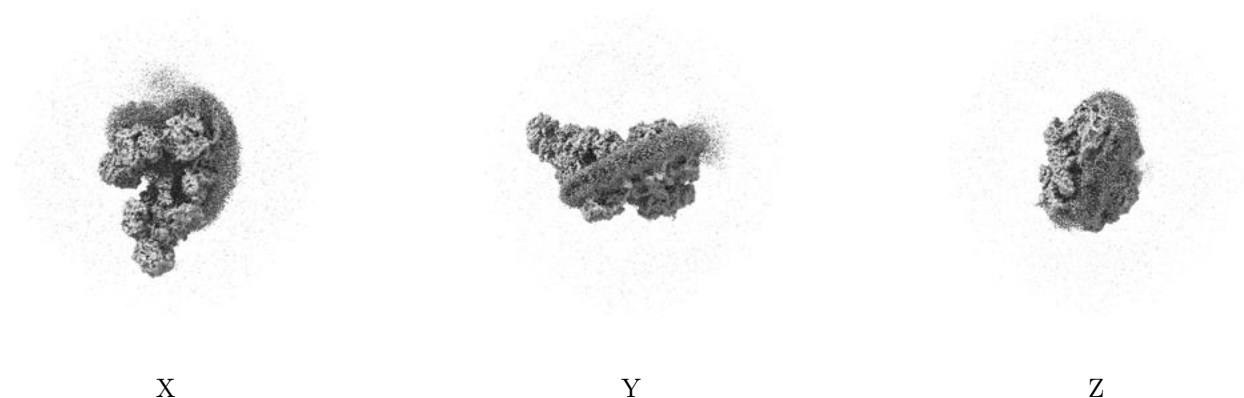


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

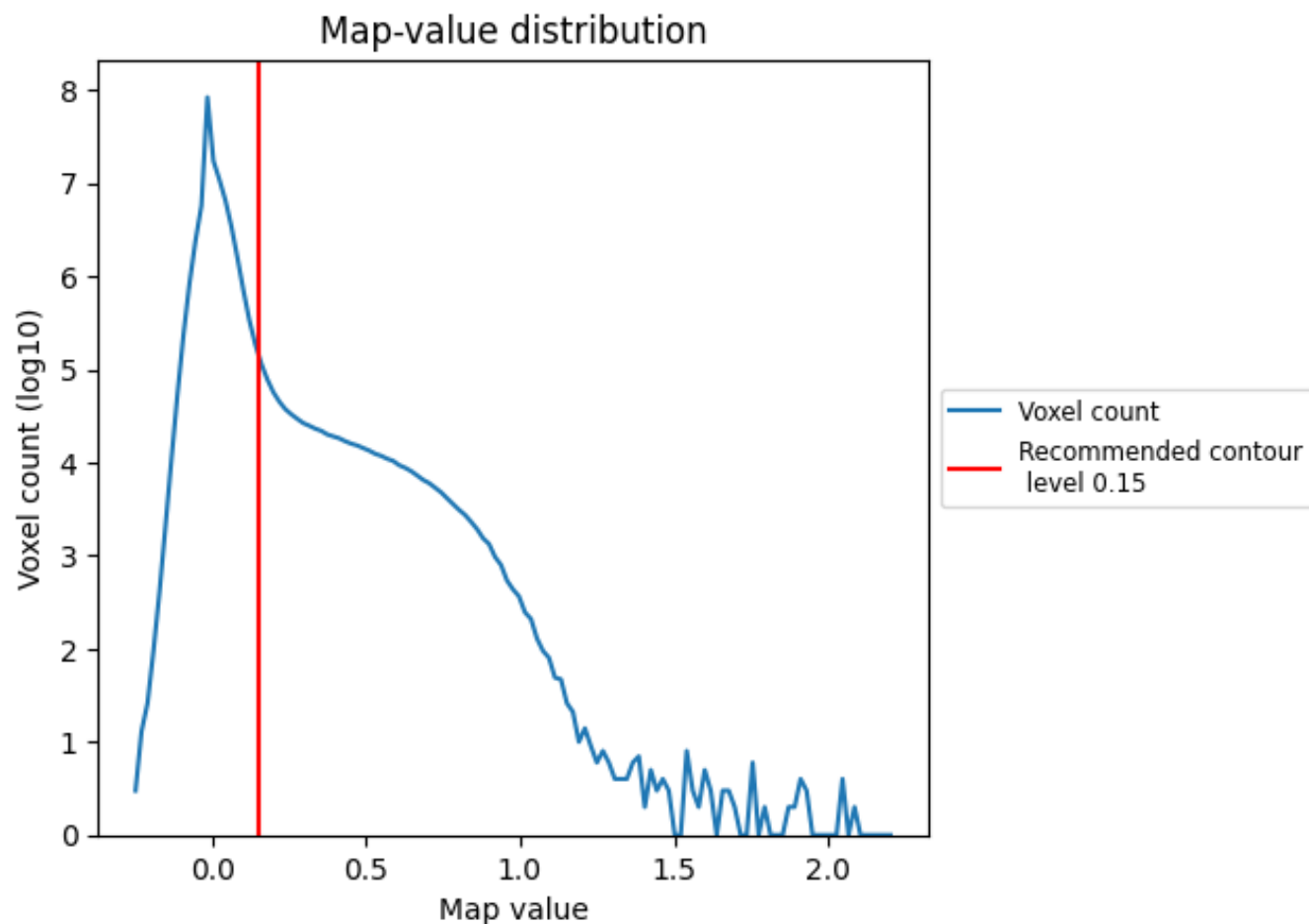
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

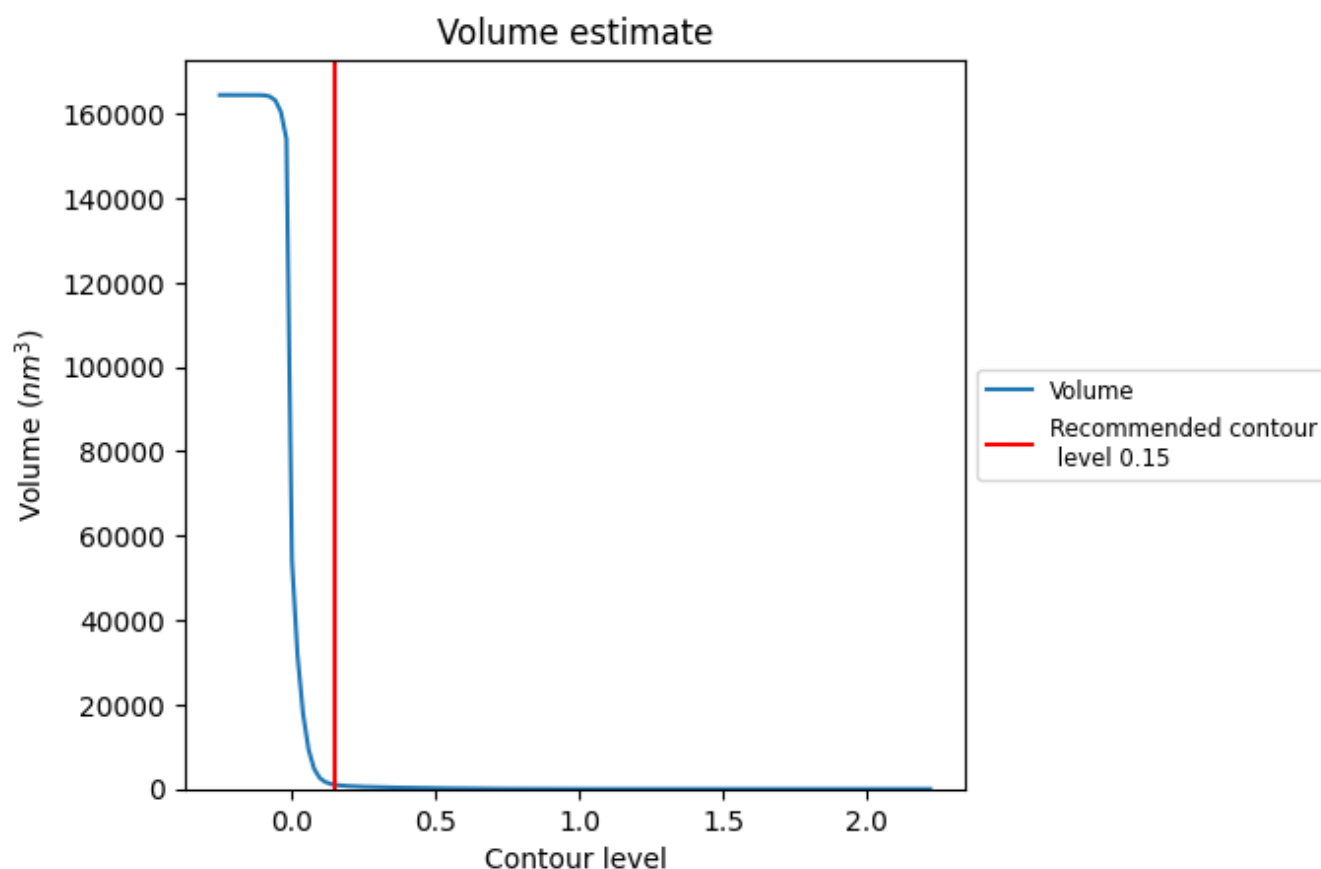
This section contains the results of statistical analysis of the map.

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.

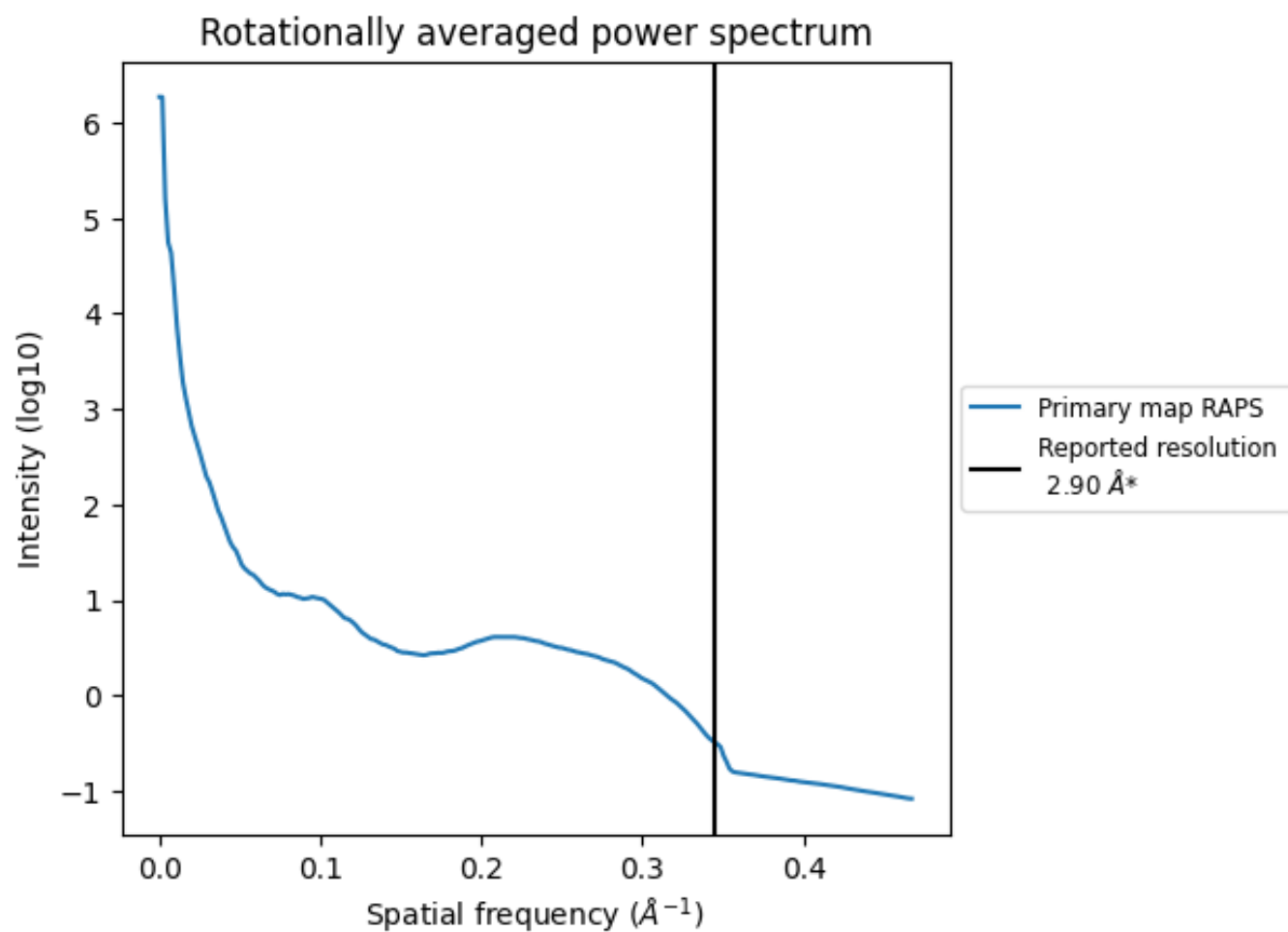
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1035 nm³; this corresponds to an approximate mass of 935 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 0.345 Å⁻¹

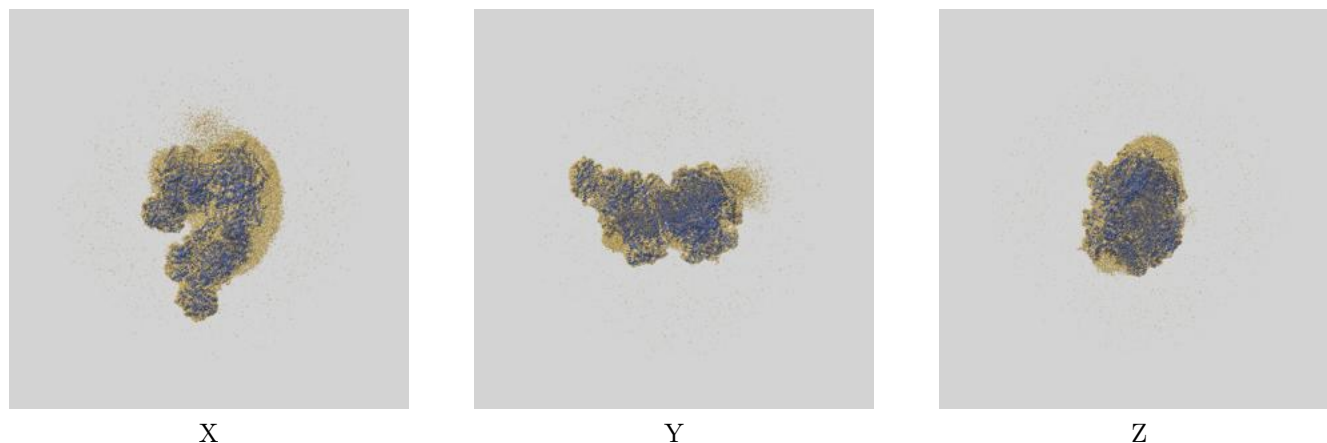
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

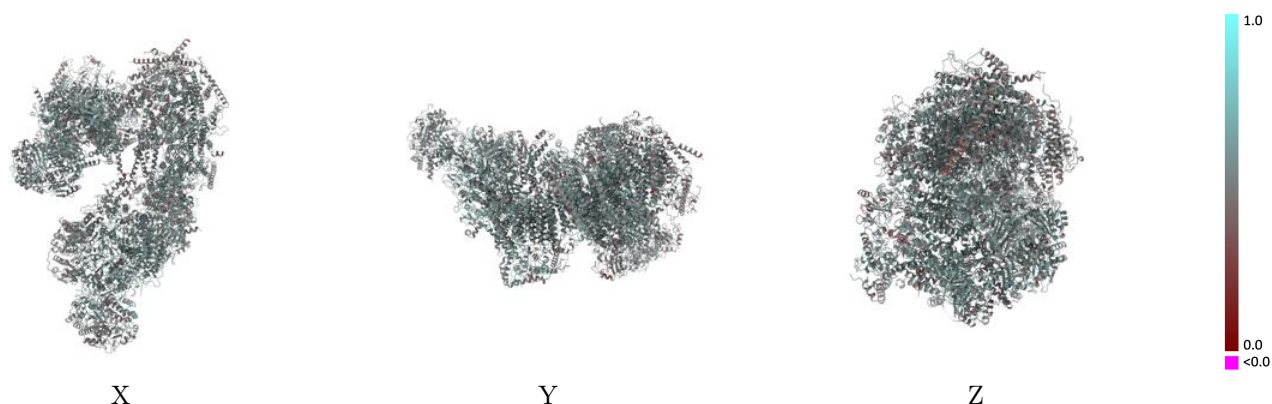
This section contains information regarding the fit between EMDB map EMD-45013 and PDB model 9BXV. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



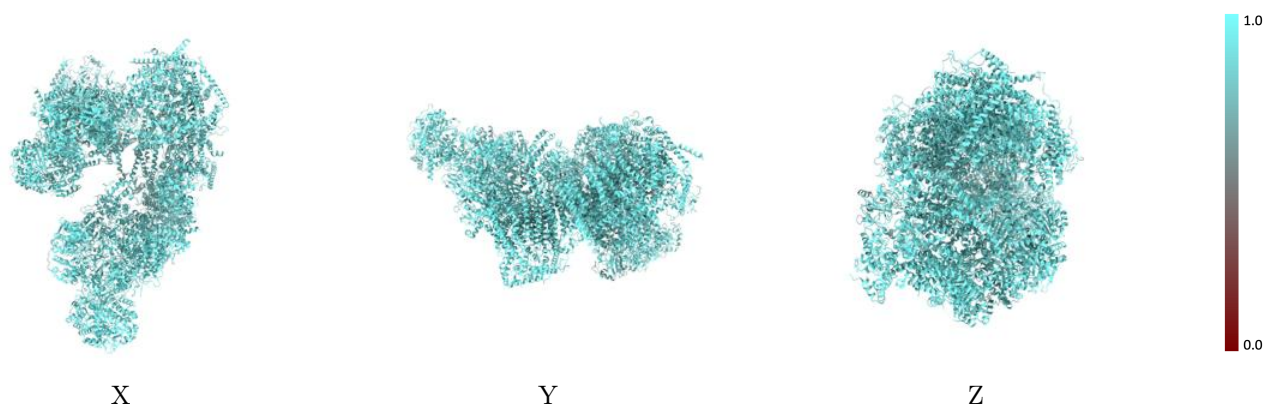
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



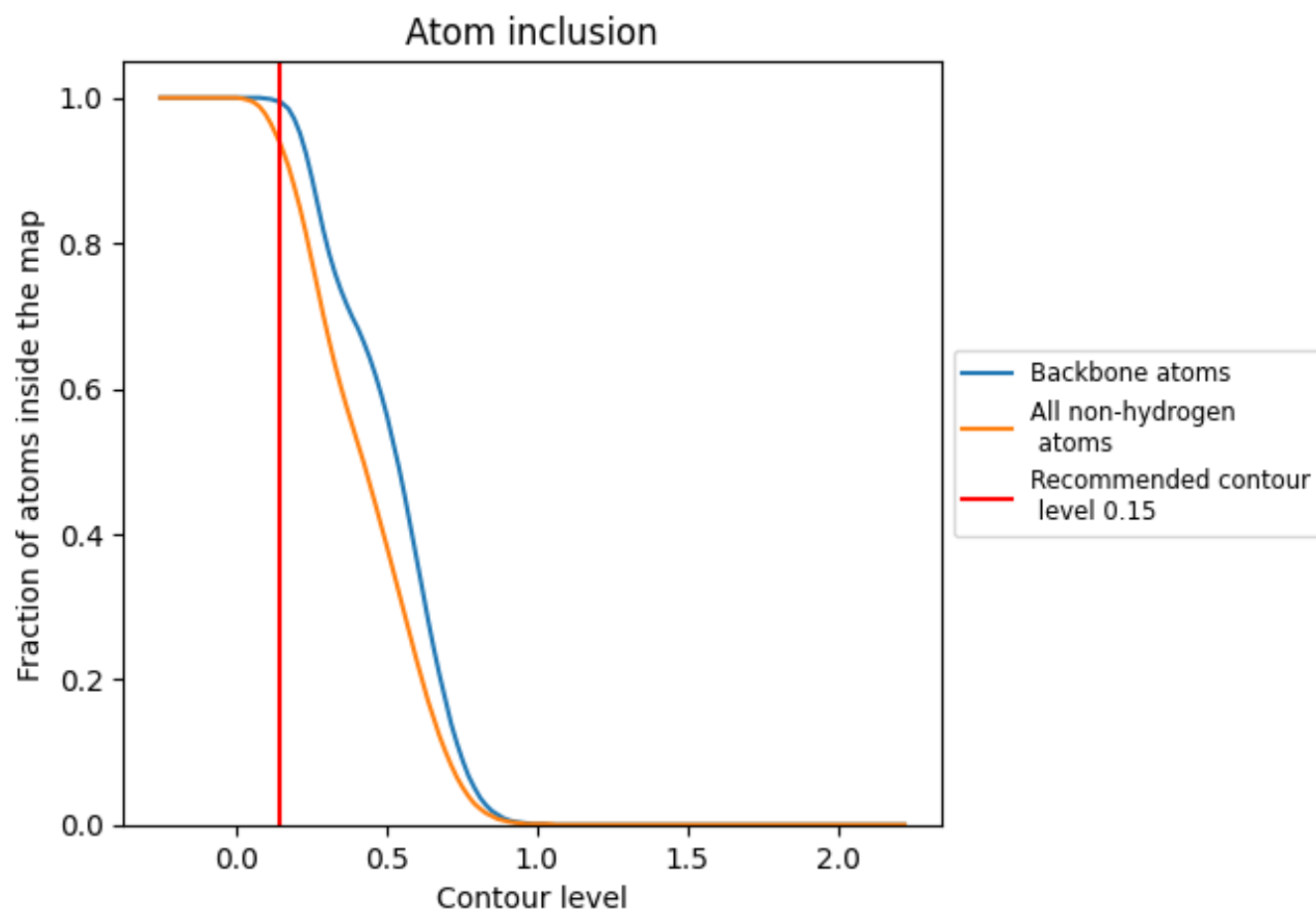
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.5280
0	 0.8770	 0.4700
1	 0.9270	 0.5170
2	 0.8750	 0.4880
3	 0.9430	 0.5290
4	 0.8420	 0.4700
5	 0.9480	 0.5410
6	 0.9400	 0.5340
7	 0.9520	 0.5550
8	 0.9480	 0.5290
9	 0.9410	 0.5380
Aa	 0.9360	 0.5280
Ab	 0.8830	 0.4620
Ac	 0.9390	 0.5280
Ad	 0.9230	 0.5250
Ae	 0.6560	 0.3400
Af	 0.7160	 0.3660
B	 0.9460	 0.5150
C	 0.9640	 0.5600
D	 0.9680	 0.5610
E	 0.9280	 0.5130
F	 0.9180	 0.5460
G	 0.9430	 0.5320
H	 0.9760	 0.5630
I	 0.9750	 0.5680
J	 0.9560	 0.5600
K	 0.9330	 0.5470
L	 0.9400	 0.5330
M	 0.9410	 0.5440
N	 0.9490	 0.5340
O	 0.8500	 0.4430
P	 0.9110	 0.4820
Q	 0.9280	 0.5330
R	 0.9020	 0.4930
S	 0.9560	 0.5500



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.9380	 0.5240
U	 0.9190	 0.5100
V	 0.9160	 0.5140
W	 0.9490	 0.5340
X	 0.8860	 0.4820
Y	 0.8970	 0.4450
Z	 0.8930	 0.4620
a	 0.9500	 0.5430
b	 0.8900	 0.4460
c	 0.9280	 0.5160
d	 0.9380	 0.5120
e	 0.9010	 0.4980
f	 0.8660	 0.4810
g	 0.9520	 0.5430
h	 0.9070	 0.4690
i	 0.9650	 0.5550
j	 0.9410	 0.5460
k	 0.9560	 0.5490
l	 0.9250	 0.5230
m	 0.9080	 0.5170
n	 0.9090	 0.4900
o	 0.9100	 0.5140
p	 0.9230	 0.5140
q	 0.9600	 0.5510
r	 0.9590	 0.5490
s	 0.9360	 0.5250
t	 0.8990	 0.4450
u	 0.9480	 0.5430
v	 0.9470	 0.5370
w	 0.9620	 0.5540
x	 0.9500	 0.5450
y	 0.9240	 0.5440
z	 0.9520	 0.5520