



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 01:15 AM EDT

PDB ID : 7LBM / pdb_00007lbm
EMDB ID : EMD-23255
Title : Structure of the human Mediator-bound transcription pre-initiation complex
Authors : Abdella, R.; Talyzina, A.; He, Y.
Deposited on : 2021-01-08
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

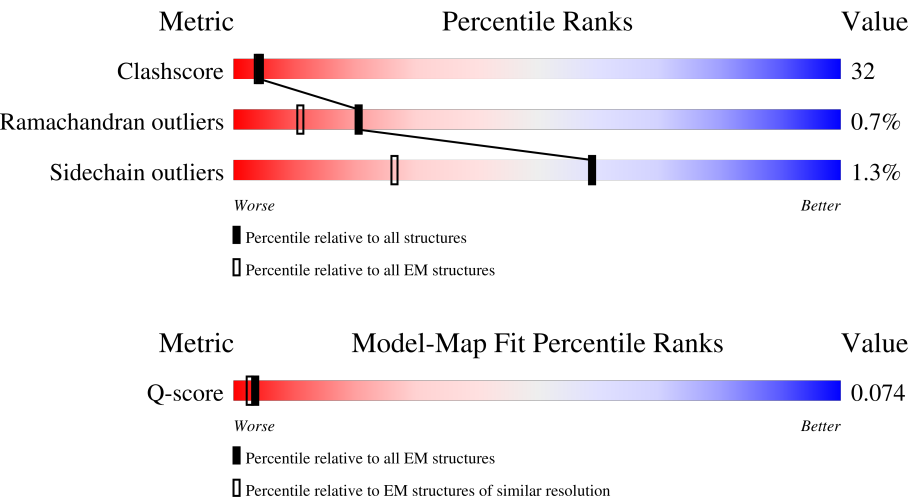
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.



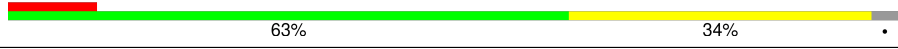
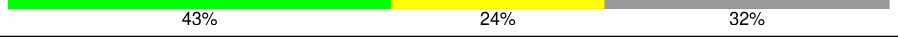
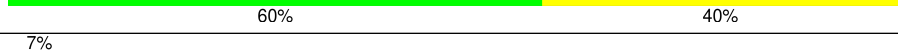
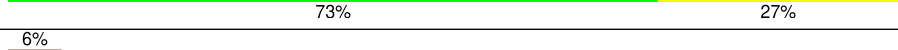
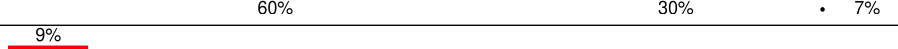
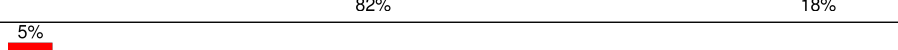
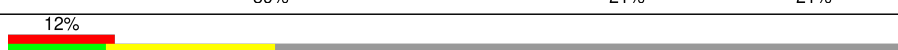
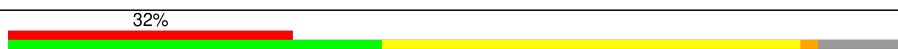
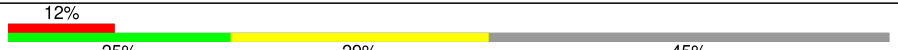
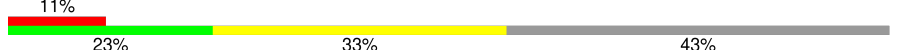
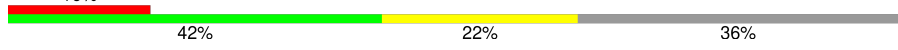
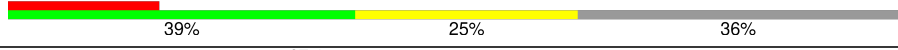
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	841	14% 46% 40% 11%
2	1	1368	48% 60% 36%
3	2	989	31% 52% 38% 9%
4	3	747	10% 12% 13% 74%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	1970	
6	B	1174	
7	C	275	
8	D	142	
9	E	210	
10	F	127	
11	G	172	
12	H	150	
13	I	125	
14	J	67	
15	K	117	
16	L	58	
17	M	376	
18	N	109	
19	O	316	
20	P	339	
21	Q	439	
22	R	291	
23	S	517	
24	T	249	
25	U	100	
26	V	100	
27	W	782	
28	X	760	
29	Y	548	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	Z	462	
31	a	395	
32	b	308	
33	c	71	
34	d	309	
35	e	346	
36	f	323	
37	g	246	
38	h	268	
39	i	117	
40	j	651	
41	k	208	
42	l	212	
43	m	200	
44	n	311	
45	o	178	
46	p	200	
47	q	178	
48	r	1454	
49	s	270	
50	t	233	
51	u	146	
52	v	135	
53	w	244	
54	x	144	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	y	131	18%5%70%14%11%
56	z	788	8%8%81%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 129277 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 Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			5864	3744	1005	1068	47		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	1317	Total	C	N	O	S	0	0
			10636	6878	1809	1880	69		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	897	Total	C	N	O	S	0	0
			7007	4487	1180	1284	56		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	195	Total	C	N	O	S	0	0
			1504	969	249	277	9		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1455	Total	C	N	O	S	0	0
			11519	7241	2052	2154	72		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1142	Total	C	N	O	S	0	0
			9129	5769	1604	1692	64		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	267	Total	C	N	O	S	0	0
			2147	1344	370	426	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	129	Total	C	N	O	S	0	0
			1062	665	179	214	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	210	Total	C	N	O	S	0	0
			1723	1088	301	325	9		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	86	Total	C	N	O	S	0	0
			689	437	120	127	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			928	599	153	174	2		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 17 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 18 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 19 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 20 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 21 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 23 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	127	Total	C	N	O	S	0	0
			1059	671	196	189	3		

- Molecule 24 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 25 is a DNA chain called super core promoter sense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	64	Total	C	N	O	P	0	0
			1321	623	256	379	63		

- Molecule 26 is a DNA chain called super core promoter antisense strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	64	Total	C	N	O	P	0	0
			1300	616	233	387	64		

- Molecule 27 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	574	Total	C	N	O	S	0	0
			4645	2973	807	835	30		

- Molecule 28 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	760	Total	C	N	O	S	0	0
			6109	3899	1066	1115	29		

- Molecule 29 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	218	Total	C	N	O	S	0	0
			1631	1028	290	305	8		

- Molecule 30 is a protein called General transcription factor IIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	436	Total	C	N	O	S	0	0
			3473	2239	609	611	14		

- Molecule 31 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	331	Total	C	N	O	S	0	0
			2580	1628	443	482	27		

- Molecule 32 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

- Molecule 33 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 34 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	275	Total	C	N	O	S	0	0
			2104	1315	368	410	11		

- Molecule 35 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	298	Total	C	N	O	S	0	0
			2376	1537	404	423	12		

- Molecule 36 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	281	Total	C	N	O	S	0	0
			2293	1465	394	416	18		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	130	Total	C	N	O	S	0	0
			1035	664	174	192	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	158	Total	C	N	O	S	0	0
			1230	767	214	246	3		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	110	Total	C	N	O	S	0	0
			863	527	160	172	4		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	504	Total	C	N	O	S	0	0
			4005	2530	719	739	17		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	185	Total	C	N	O	S	0	0
			1484	942	259	268	15		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	184	Total	C	N	O	S	0	0
			1425	907	235	267	16		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	125	Total	C	N	O	S	0	0
			1024	632	175	213	4		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	283	Total	C	N	O	S	0	0
			2279	1445	406	417	11		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	108	Total	C	N	O	S	0	0
			887	553	155	176	3		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	114	Total	C	N	O	S	0	0
			893	559	154	171	9		

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	122	Total	C	N	O	S	0	0
			1007	628	188	182	9		

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	1034	Total	C	N	O	S	0	0
			8174	5239	1427	1461	47		

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	135	Total	C	N	O	S	0	0
			1084	676	191	212	5		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	116	Total	C	N	O	S	0	0
			975	621	175	173	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	60	Total	C	N	O	S	0	0
			501	314	93	90	4		

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	131	Total	C	N	O	S	0	0
			1067	676	182	204	5		

- Molecule 53 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	39	Total	C	N	O	S	0	0
			309	198	52	57	2		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	111	Total	C	N	O	S	0	0
			852	528	142	178	4		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	116	Total	C	N	O	S	0	0
			1003	649	177	172	5		

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	149	Total	C	N	O	S	0	0
			1168	747	204	210	7		

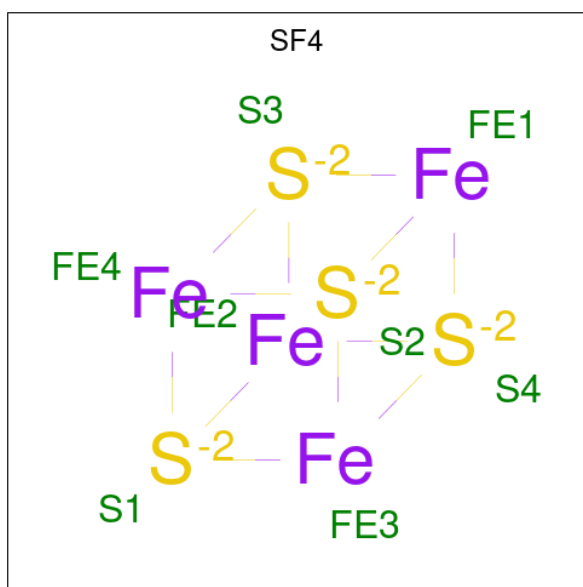
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	2	Total	Mg	0
			2	2	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	A	2	Total	Zn	0
			2	2	
58	B	1	Total	Zn	0
			1	1	
58	C	1	Total	Zn	0
			1	1	
58	I	2	Total	Zn	0
			2	2	
58	J	1	Total	Zn	0
			1	1	
58	L	1	Total	Zn	0
			1	1	
58	O	1	Total	Zn	0
			1	1	
58	Q	1	Total	Zn	0
			1	1	
58	a	3	Total	Zn	0
			3	3	
58	b	1	Total	Zn	0
			1	1	
58	d	2	Total	Zn	0
			2	2	

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

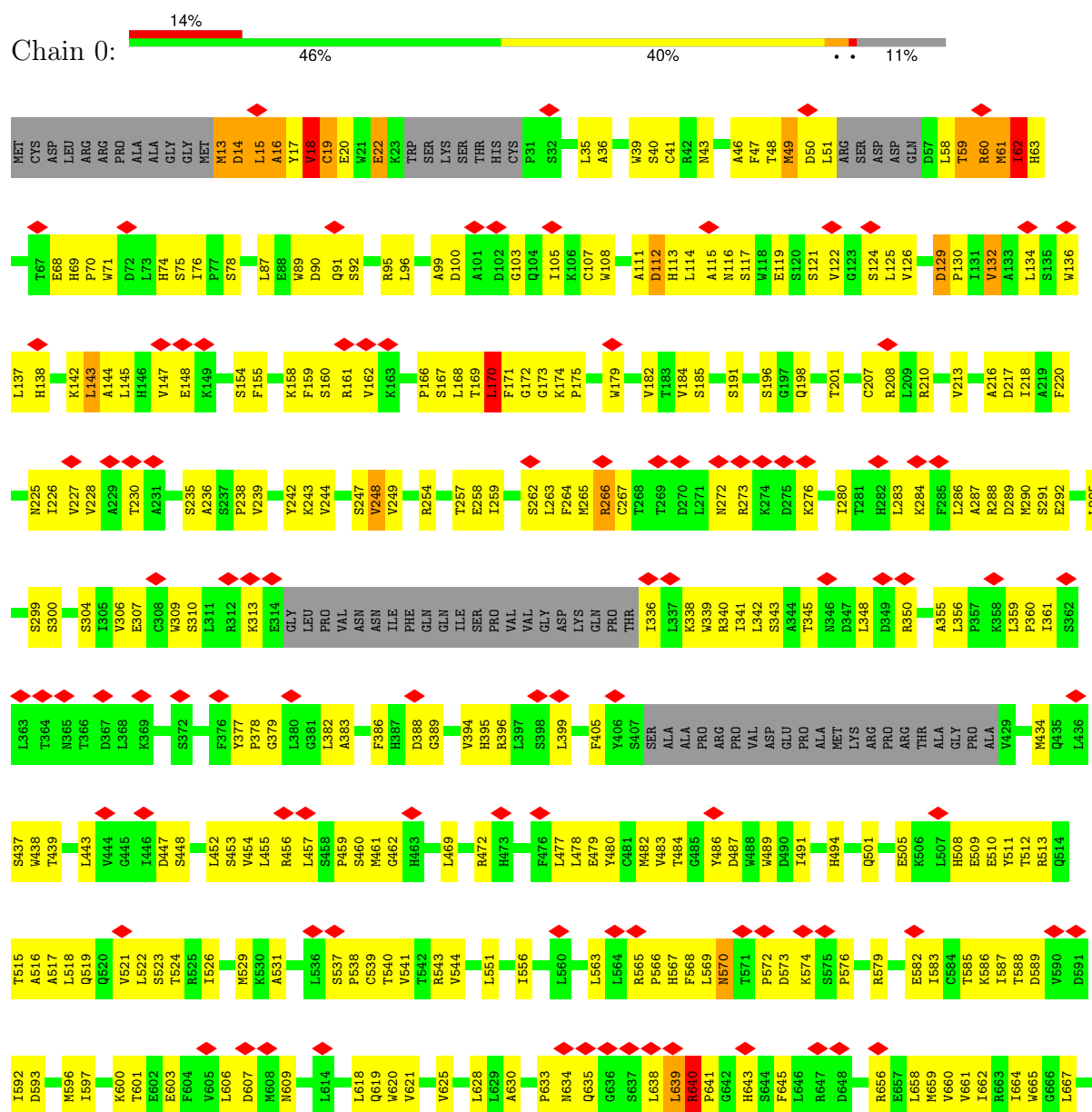


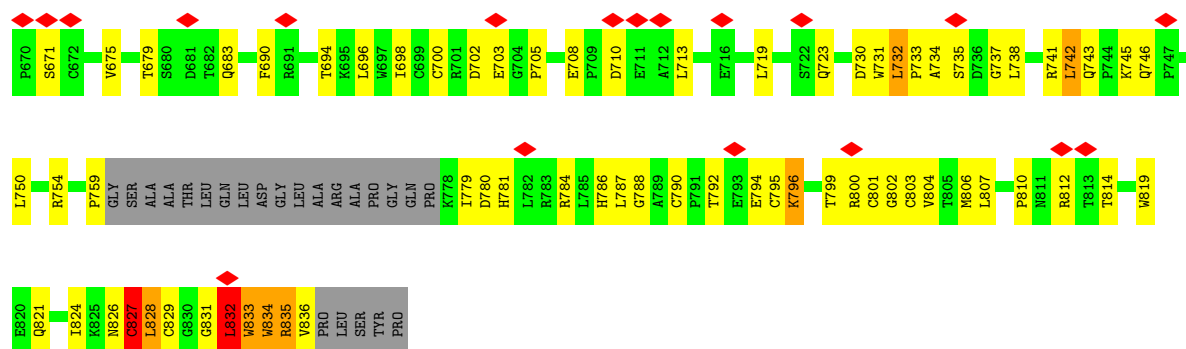
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	X	1	8	4	4	0

3 Residue-property plots

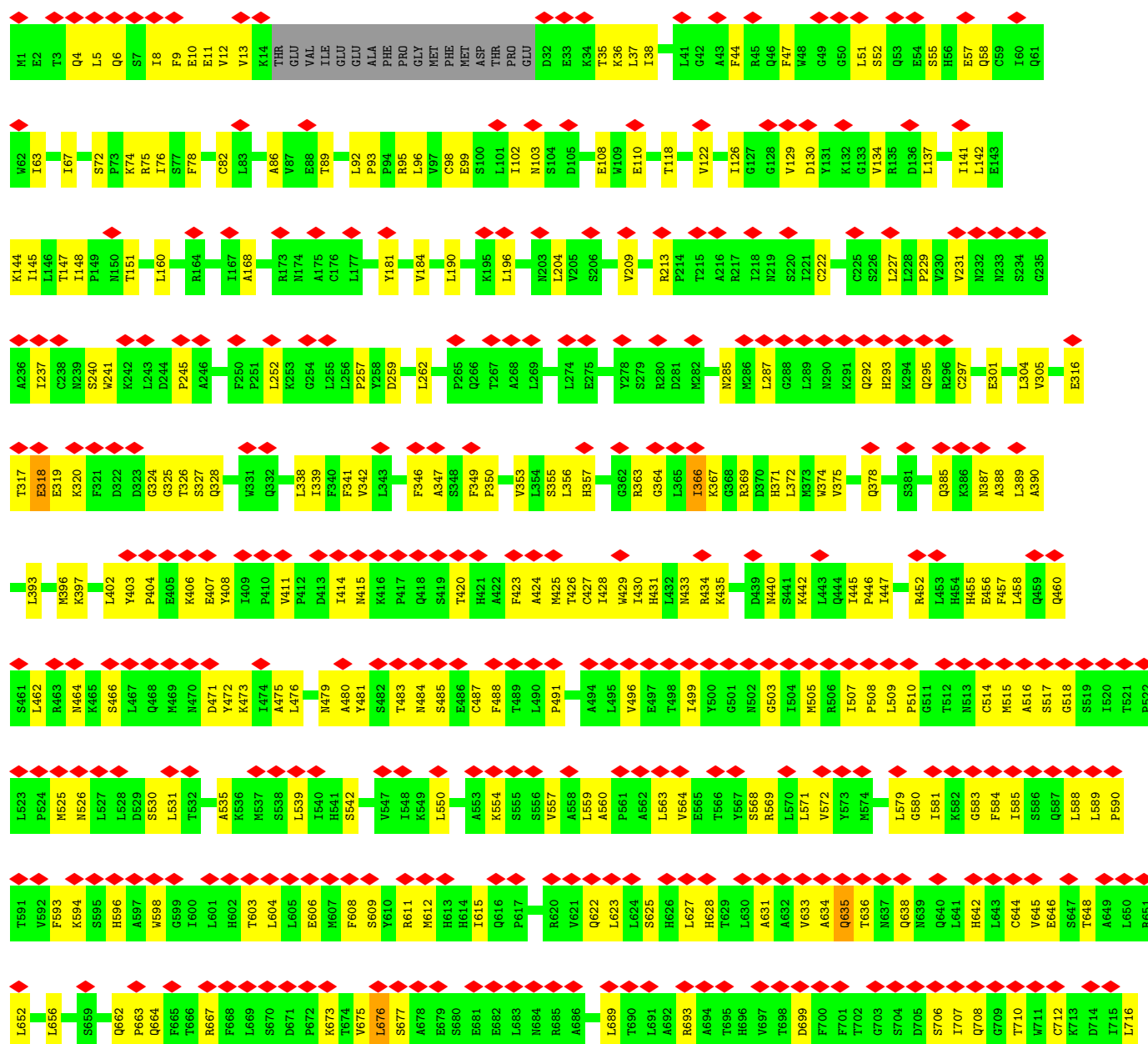
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

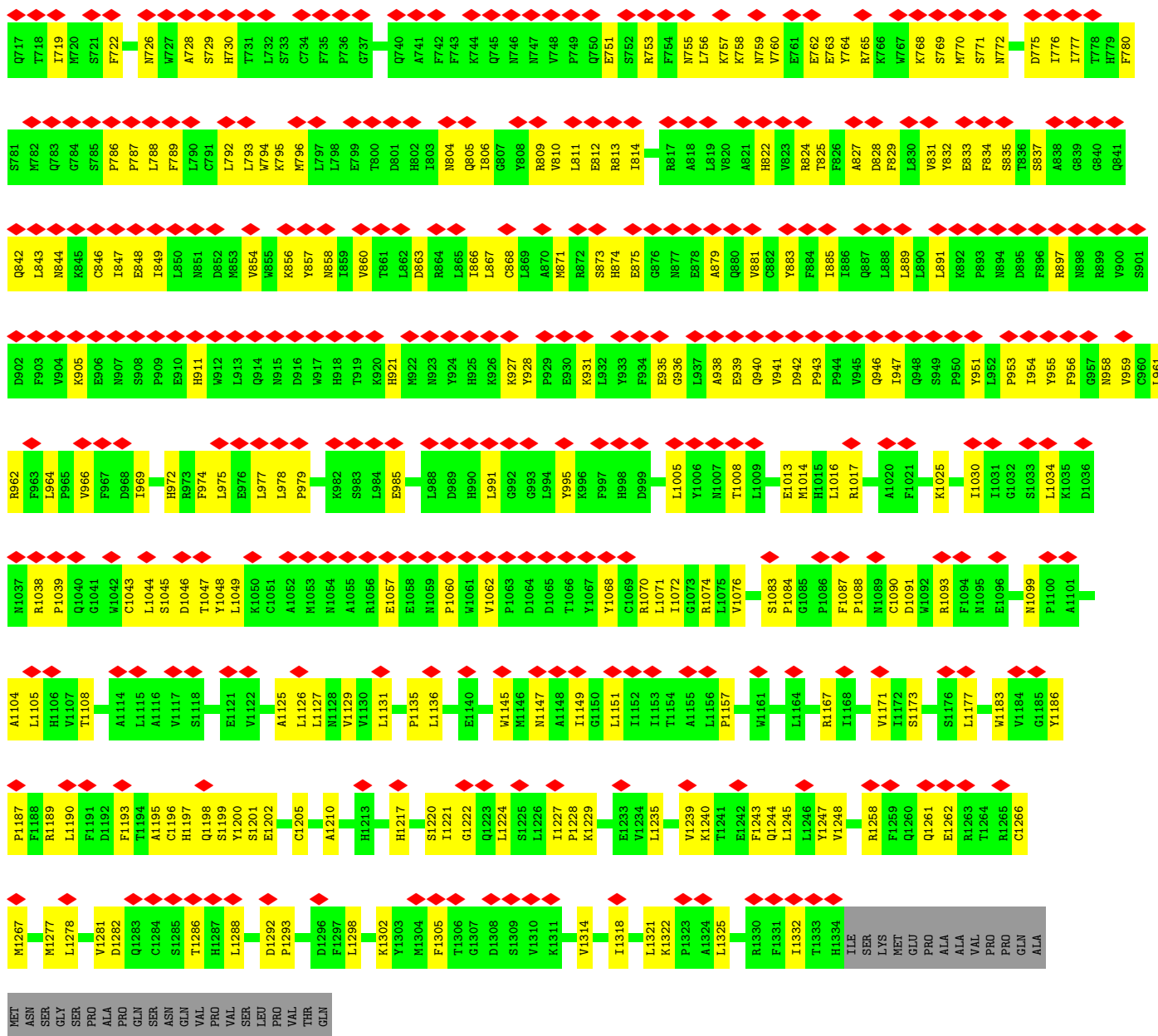
- Molecule 1: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16





• Molecule 2: Mediator of RNA polymerase II transcription subunit 23



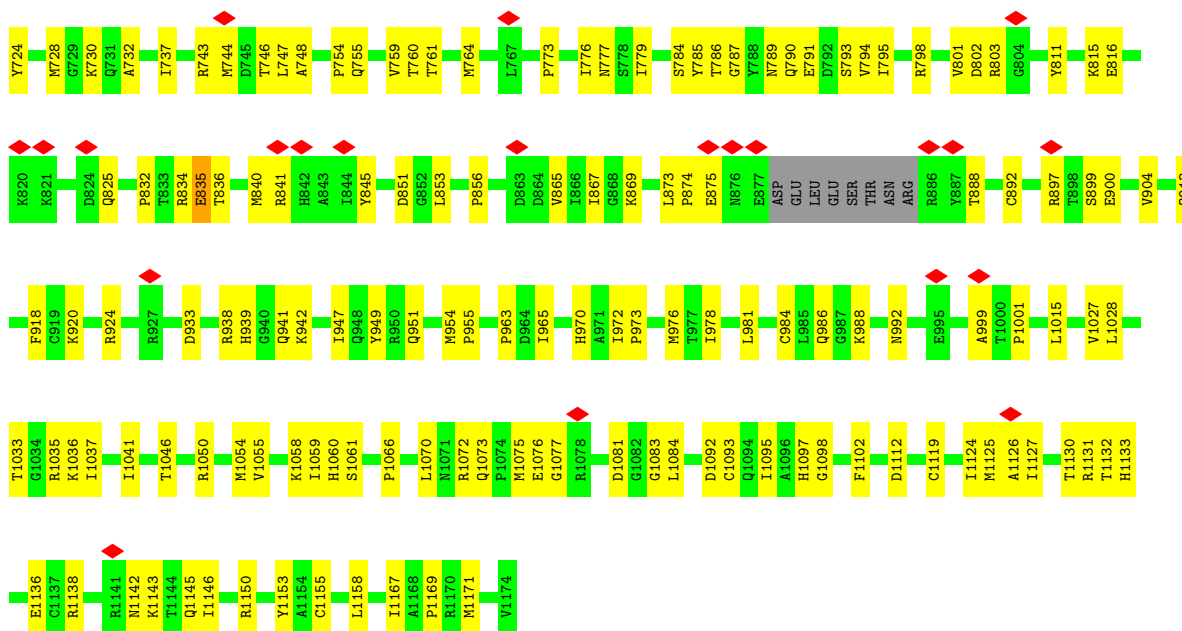




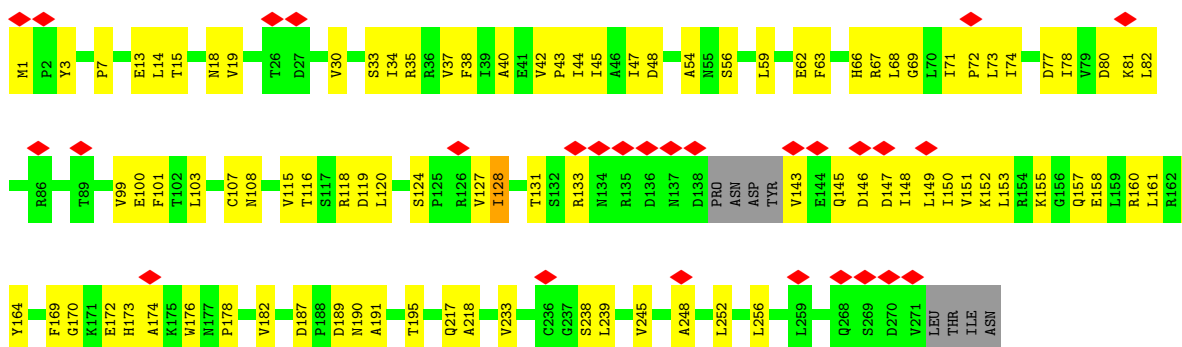
Frequency	Percentage
Often	47%
Sometimes	26%
Rarely	26%



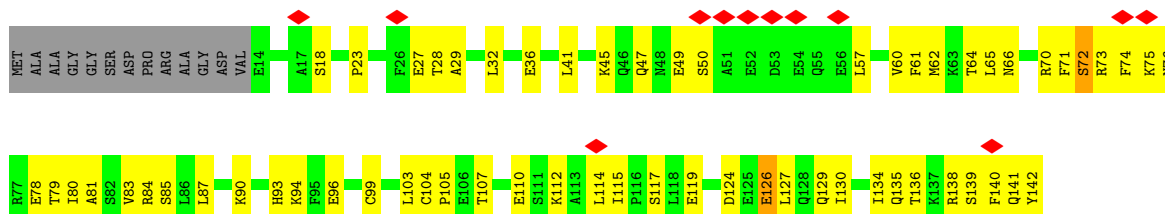
THR	V1436	R1345	N1263	G1120	R890	N780	C641	V538	K445	K344	P262
PRO	V1346	V1346	S1264	V1121	V891	I781	L645	Q539	K446	G345	A263
TRP	L1347	L1347	D1265	R1122	E892	S782	L645	D540	V446	V264	A263
ASN	S1348	S1348	V1195	R1123	E893	A786	L652	D540	R349	V264	V264
GLN	E1349	E1349	Y1196	K1124	Q904	A787	V653	V545	V350	M266	M266
GLY	K1350	K1350	E1198	K1125	N905	Q790	H654	R546	R351	Q267	Q267
ALA	D1351	D1351	M1199	L1128	L906	E794	H655	K547	G352	G268	G268
THR	P1352	P1352	GLN	P1129	A907	R797	E659	F548	N353	S269	S269
PRO	V1353	V1353	GLU	R1129	L907	E660	M660	T549	L354	A270	A270
ALA	L1354	L1354	GLU	I1130	L909	R805	D663	R551	S362	R271	R271
TRP	R1356	R1356	D1202	S1131	E917	F800	I664	R551	A363	N272	N272
ALA	Q1462	Q1462	E1274	K1132	F1041	P808	T665	E556	D775	D775	D775
ALA	Q1461	Q1461	V1275	R1133	N1042	H609	T665	R557	I367	I367	I367
TRP	Q1462	Q1462	V1276	P1134	I1043	F810	I667	R557	I375	I375	I375
SER	D1471	D1471	M1279	P1137	H1044	R805	F668	V560	V380	V380	V380
SER	D1472	D1472	M1280	P1137	H1044	R805	F668	V560	S383	S383	S383
PRO	L1473	L1473	S1208	P1137	H1044	R805	F668	V560	T389	T389	T389
VAL	L1474	L1474	S1208	P1137	H1044	R805	F668	V560	F990	F990	F990
GLY	L1475	L1475	M1279	P1137	H1044	R805	F668	V560	A391	A391	A391
SER	D1476	D1476	M1279	P1137	H1044	R805	F668	V560	V394	V394	V394
GLY	K1479	K1479	D1282	F1142	Y924	P808	F668	V560	F397	F397	F397
GLY	L1480	L1480	V1283	L1143	Y924	P808	F668	V560	L402	L402	L402
THR	K1481	K1481	F1284	L1144	E927	F810	I667	V560	Q311	Q311	Q311
PRO	K1481	K1481	L1285	G1145	R928	R812	I676	F566	H312	H312	H312
GLY	Y1482	Y1482	E1215	Q1146	R931	D813	N677	P575	H313	H313	H313
ALA	G1483	G1483	L1216	S1147	R932	D813	N677	P575	V314	V314	V314
ALA	M1484	M1484	D1217	A1148	T933	D813	N677	P575	A315	A315	A315
GLY	E1485	E1485	R1218	R1149	T933	D813	N677	P575	T316	T316	T316
PHE	I1386	I1386	T1222	D1156	V939	R820	I687	G688	D319	D319	D319
PRO	Y1392	Y1392	R1224	I1157	V942	V823	I689	L585	N320	N320	N320
SER	H1397	H1397	K1225	R1160	Y948	E824	S692	L585	E321	E321	E321
ALA	L1398	L1398	T1227	L1161	L952	L828	T698	Q590	L322	L322	L322
GLY	L1398	L1398	M1228	E1162	L952	E835	T698	Q590	L325	L325	L325
ASP	L1401	L1401	E1229	H1163	F956	E835	I702	F592	P326	P326	P326
ALA	L1411	L1411	I1231	T1164	F956	E835	I702	F592	R327	R327	R327
GLY	M1412	M1412	K1232	L1166	N959	E845	K710	L594	M423	M423	M423
ALA	A1413	A1413	E1233	R1167	D962	E845	H721	L594	G424	G424	G424
PRO	I1414	I1414	K1234	K1168	R963	D849	N722	I595	D425	D425	D425
GLY	H1417	H1417	N1235	V1169	E964	Y859	N723	I595	I427	I427	I427
SER	G1418	G1418	I1236	T1170	V965	Y859	E724	P597	R430	R430	R430
PHE	V1419	V1419	G1240	A1171	L966	E856	P727	C602	F431	F431	F431
ALA	N1420	N1420	D1241	N1172	R967	E856	L733	T605	H432	H432	H432
TRP	R1421	R1421	L1243	V1176	V968	E856	R734	T605	P433	P433	P433
ALA	Q1422	Q1422	C1245	Y1177	Y969	Y859	E724	P597	S338	S338	S338
PRO	D1423	D1423	I1246	D1178	V977	Y859	T752	N601	L339	L339	L339
THR	E1426	E1426	F1247	P1179	V978	Y859	G753	N601	G339	G339	G339
GLY	P1426	P1426	N1248	P1179	L979	Y859	Q757	I621	R334	R334	R334
PRO	L1427	L1427	E1253	Q1182	N982	M668	K767	D625	P335	P335	P335
GLY	M1428	M1428	K1254	T1184	R985	V871	S768	M524	L336	L336	L336
ILE	K1429	K1429	L1255	V1185	R986	N881	H769	P528	K337	K337	K337
SER	C1430	C1430	L1255	V1185	R986	N881	H769	P528	S337	S337	S337
PRO	S1431	S1431	R1258	V1186	R987	S882	V770	P528	P433	P433	P433
ALA	F1432	F1432	L1261	T1189	N988	R883	K778	I639	L438	L438	L438
PRO	E1434	E1434	M1262	L1119	N989	R883	I779	L640	H439	H439	H439
PRO	T1435	T1435	M1262	L1119	N989	R883	I779	L640	L440	L440	L440



• Molecule 7: DNA-directed RNA polymerase II subunit RPB3

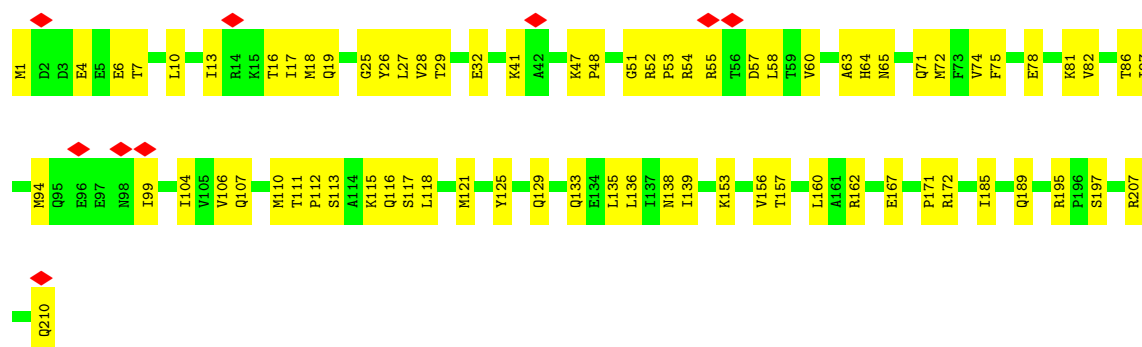


• Molecule 8: DNA-directed RNA polymerase II subunit RPB4

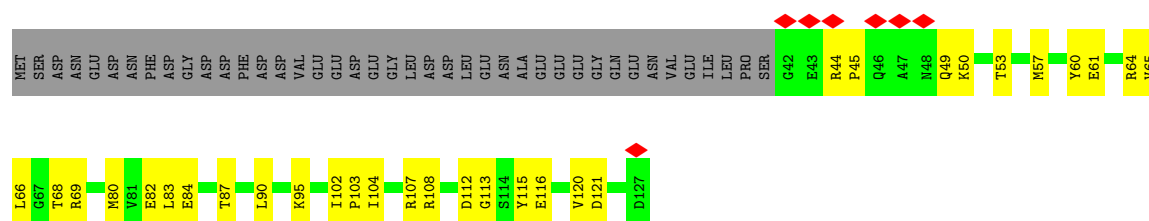


• Molecule 9: DNA-directed RNA polymerase II subunit RPB5

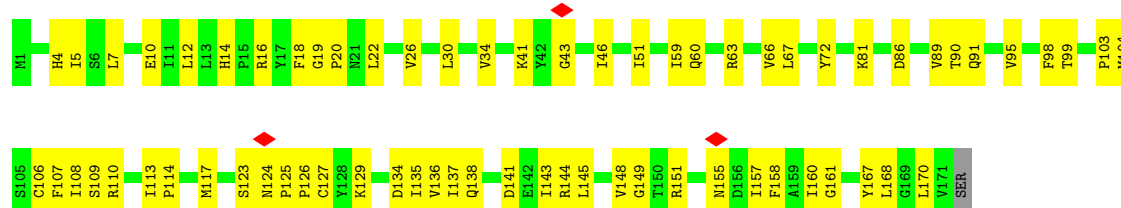




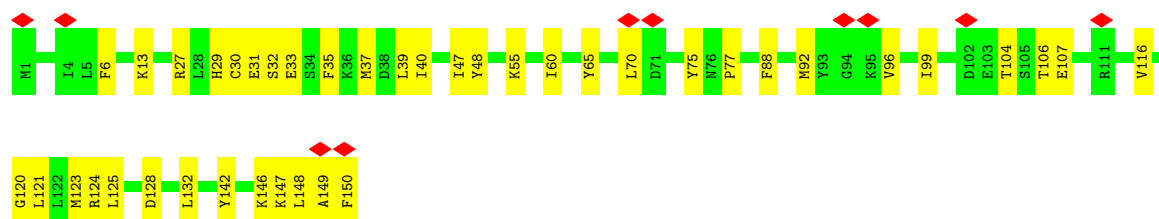
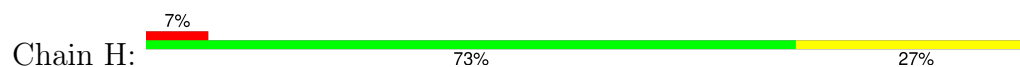
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 11: DNA-directed RNA polymerase II subunit RPB7



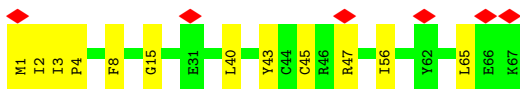
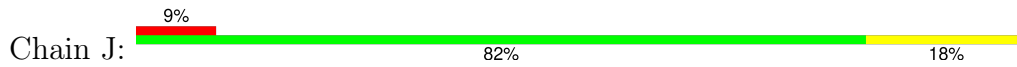
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3



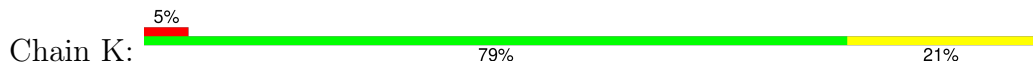
- Molecule 13: DNA-directed RNA polymerase II subunit RPB9



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



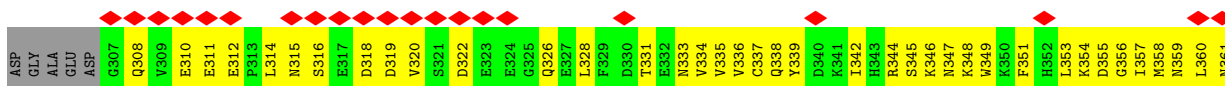
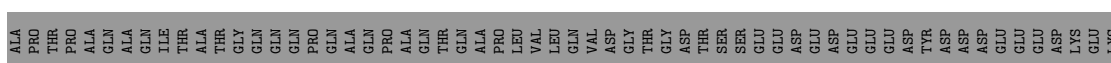
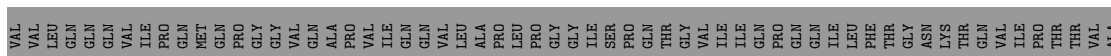
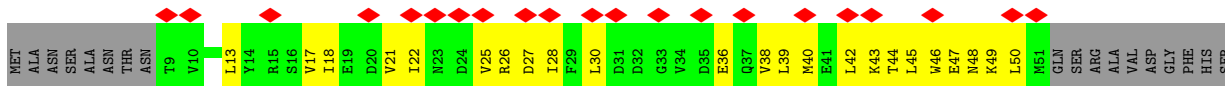
- Molecule 15: DNA-directed RNA polymerase II subunit RPB11-a

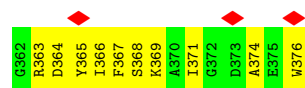


- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4

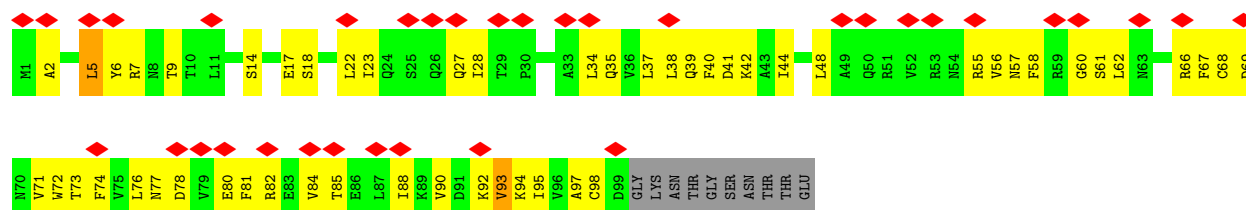
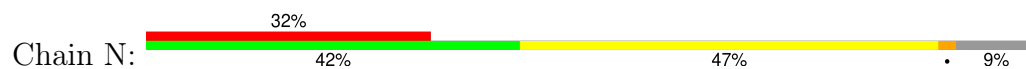


- Molecule 17: Transcription initiation factor IIA subunit 1

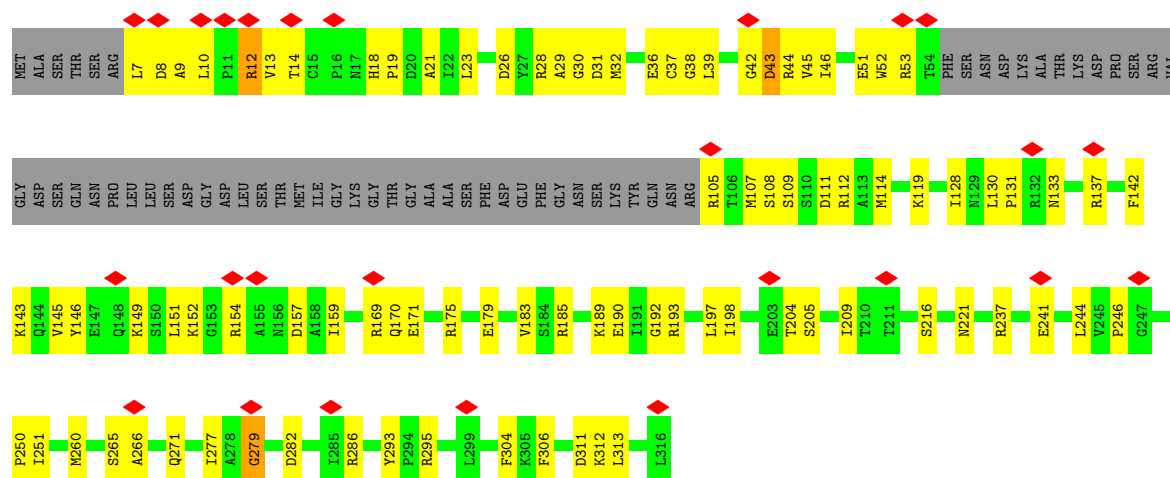




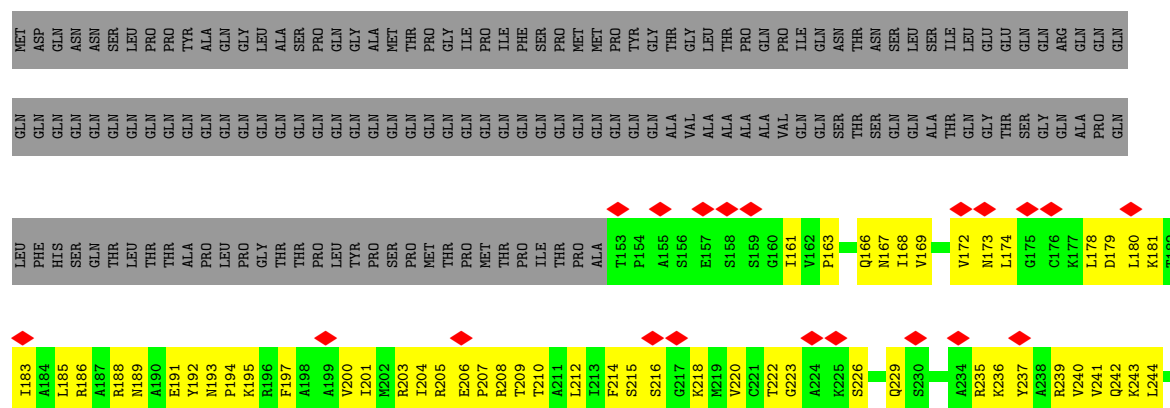
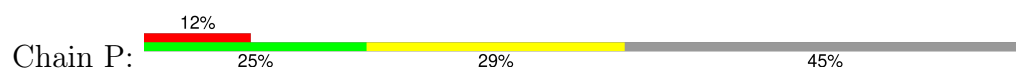
• Molecule 18: Transcription initiation factor IIA subunit 2

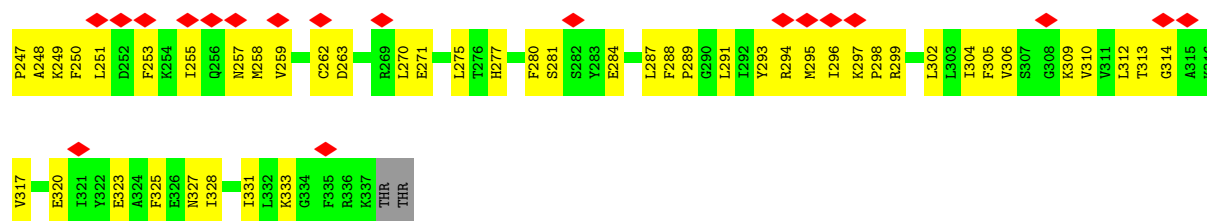


• Molecule 19: Transcription initiation factor IIB

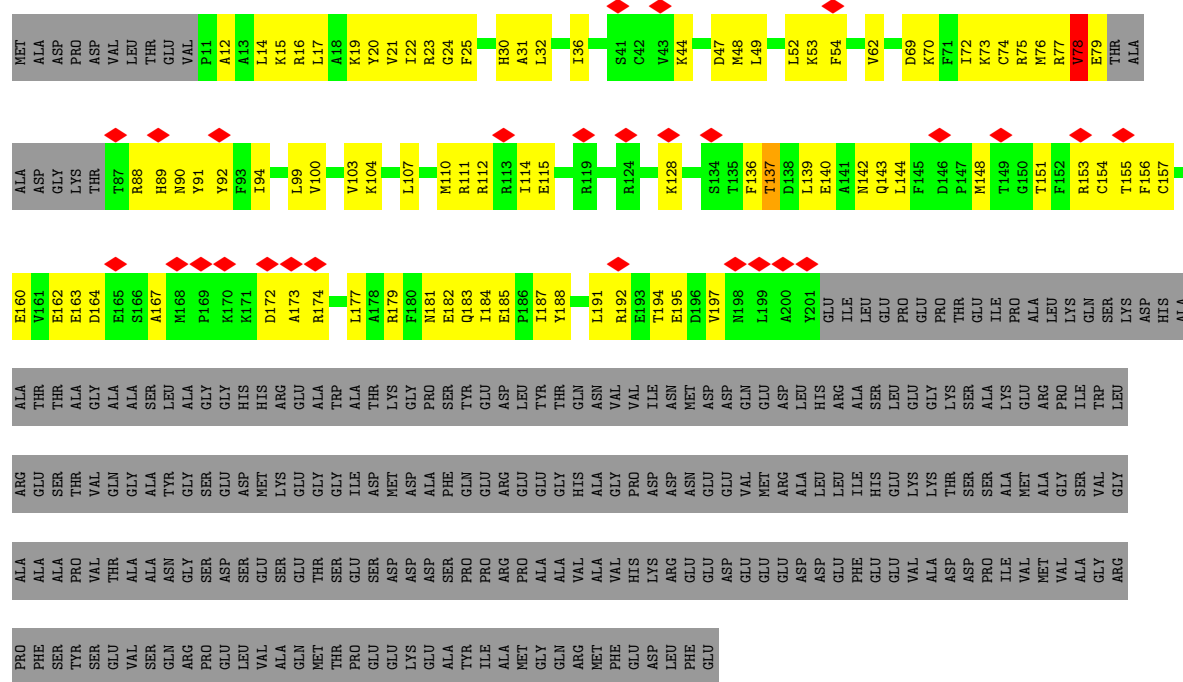


• Molecule 20: TATA-box-binding protein

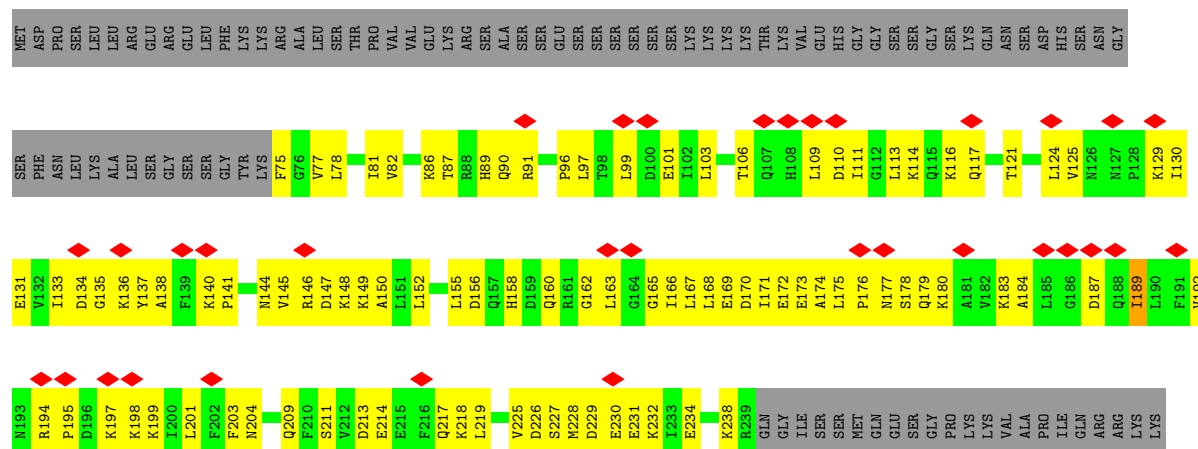
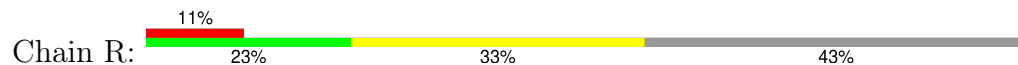




• Molecule 21: General transcription factor IIE subunit 1



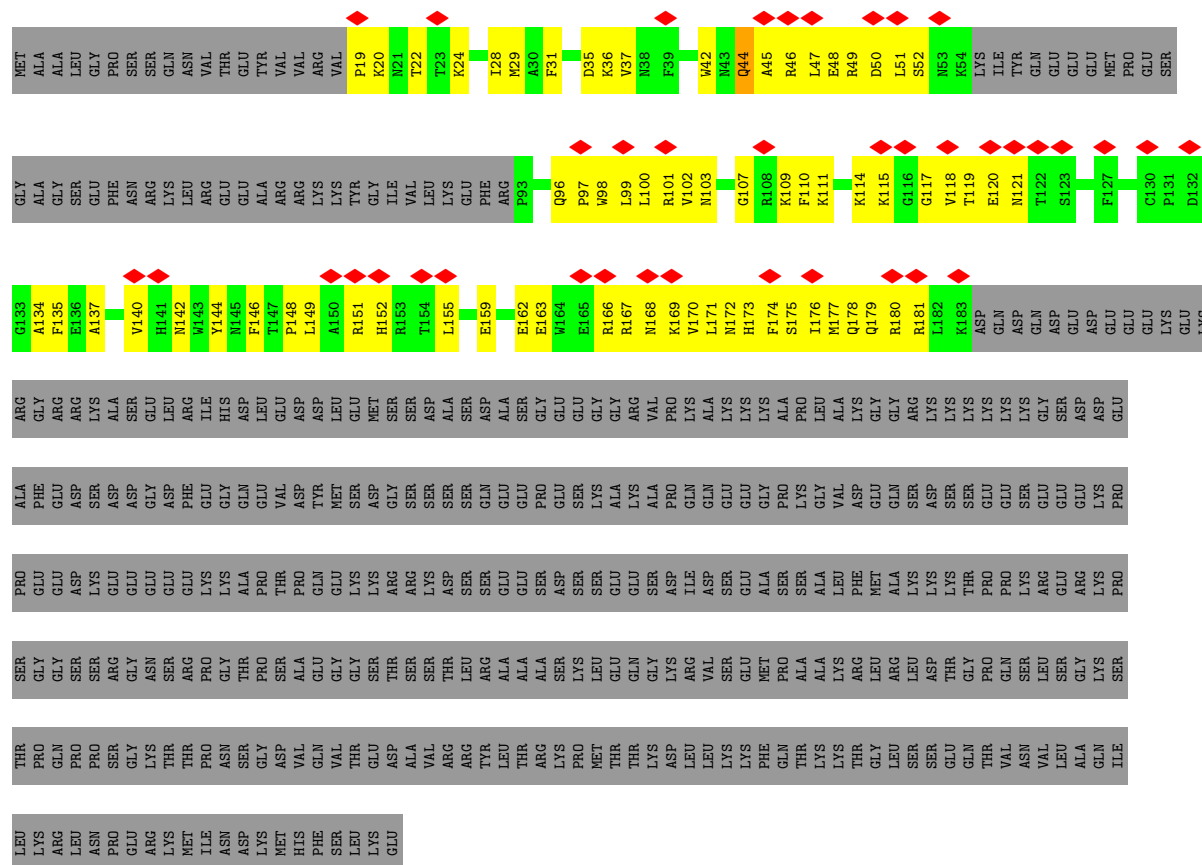
• Molecule 22: Transcription initiation factor IIE subunit beta



PRO
ALA
SER
GLN
LYS
LYS
ARG
ARG
PHE
LYS
THR
HIS
ASN
GLU
HIS
VAL
ALA
VAL
LEU
LYS
ASP
TVR
SER
ASP
TLE
THR
SER
SER
LYS

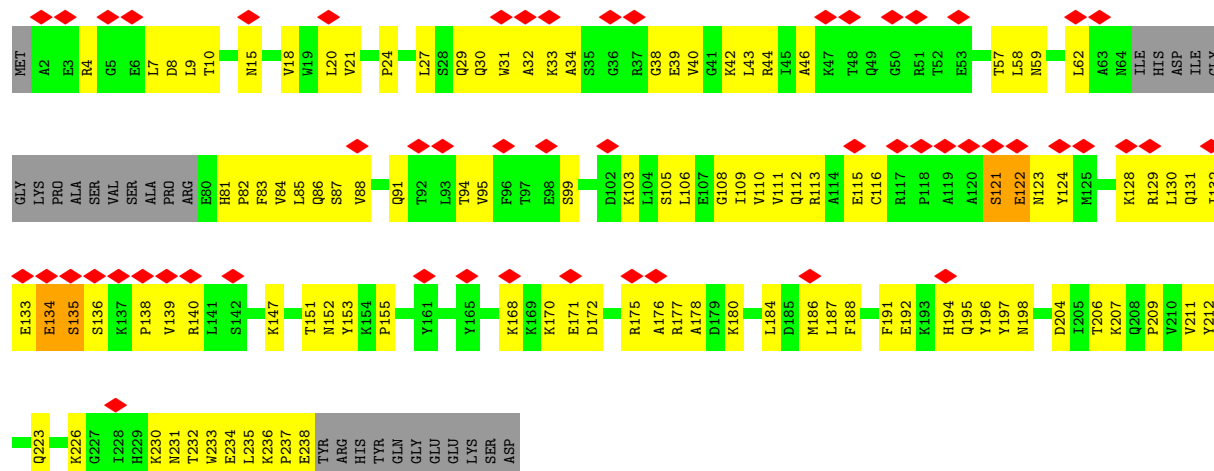
• Molecule 23: General transcription factor IIF subunit 1

Chain S: 

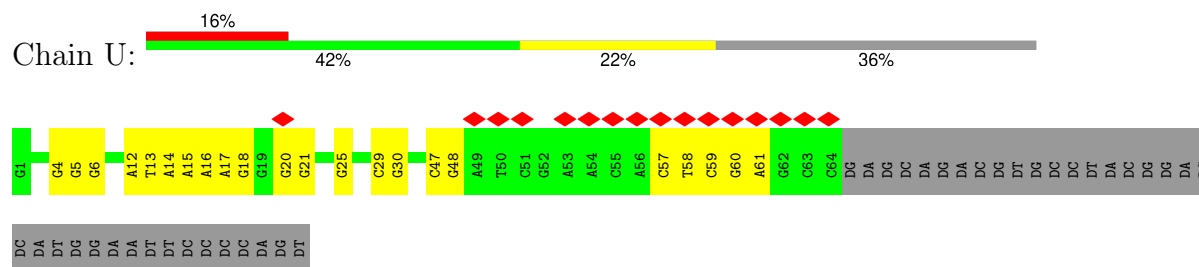


• Molecule 24: General transcription factor IIF subunit 2

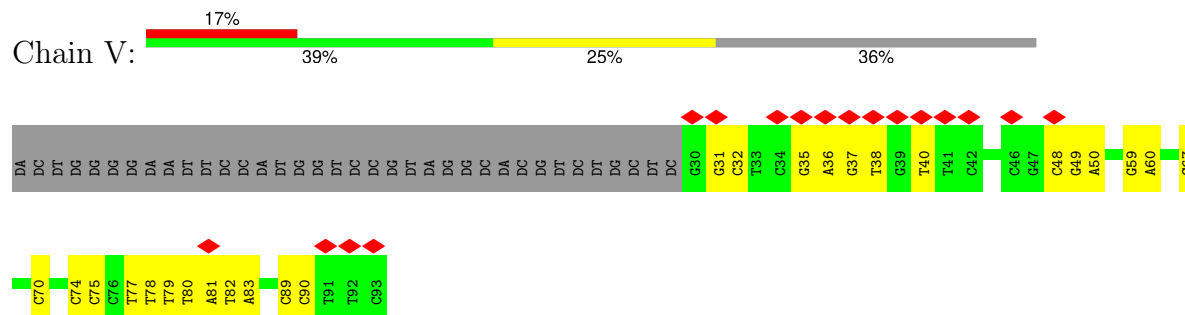
Chain T: 



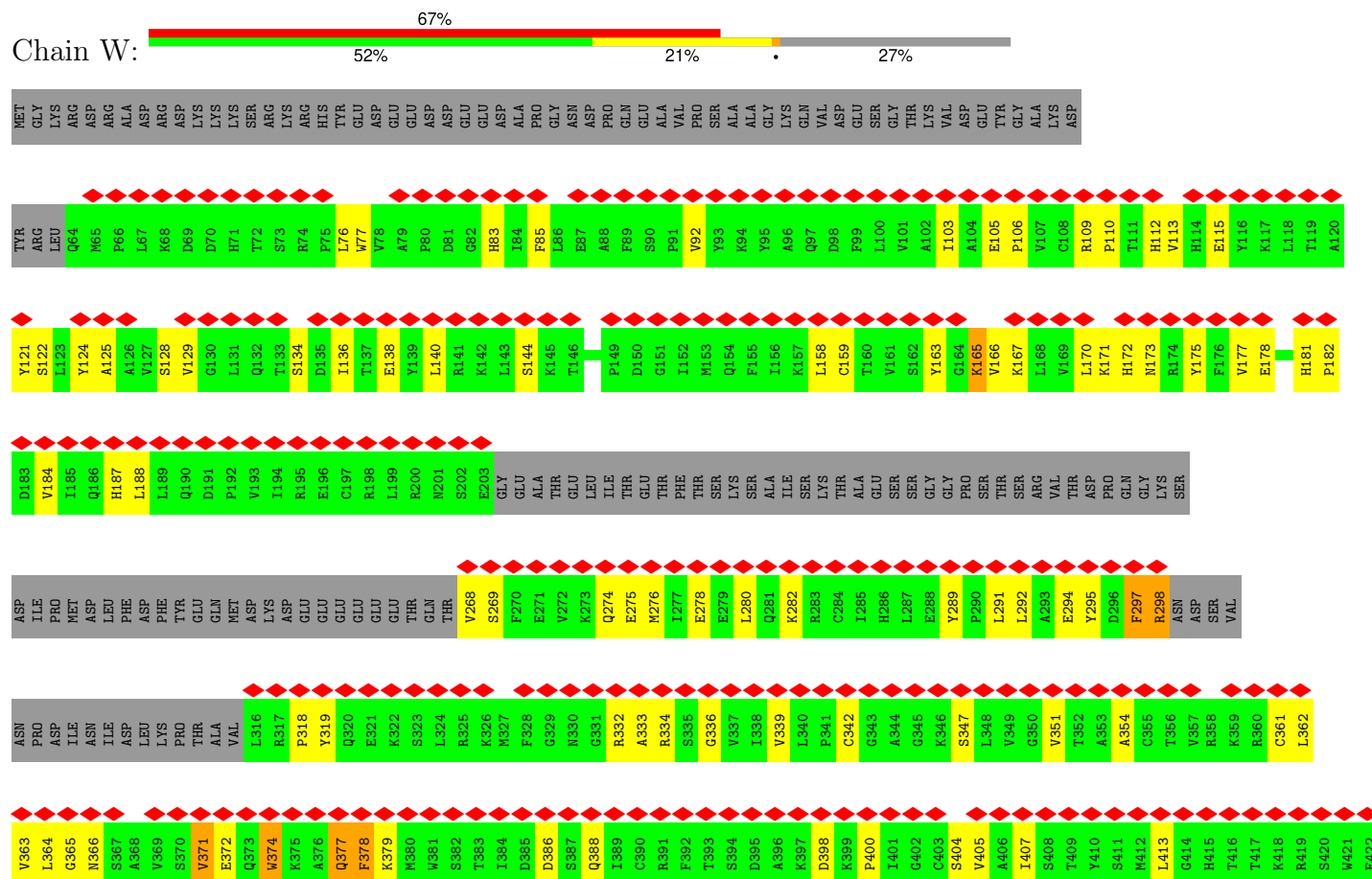
- Chain U:

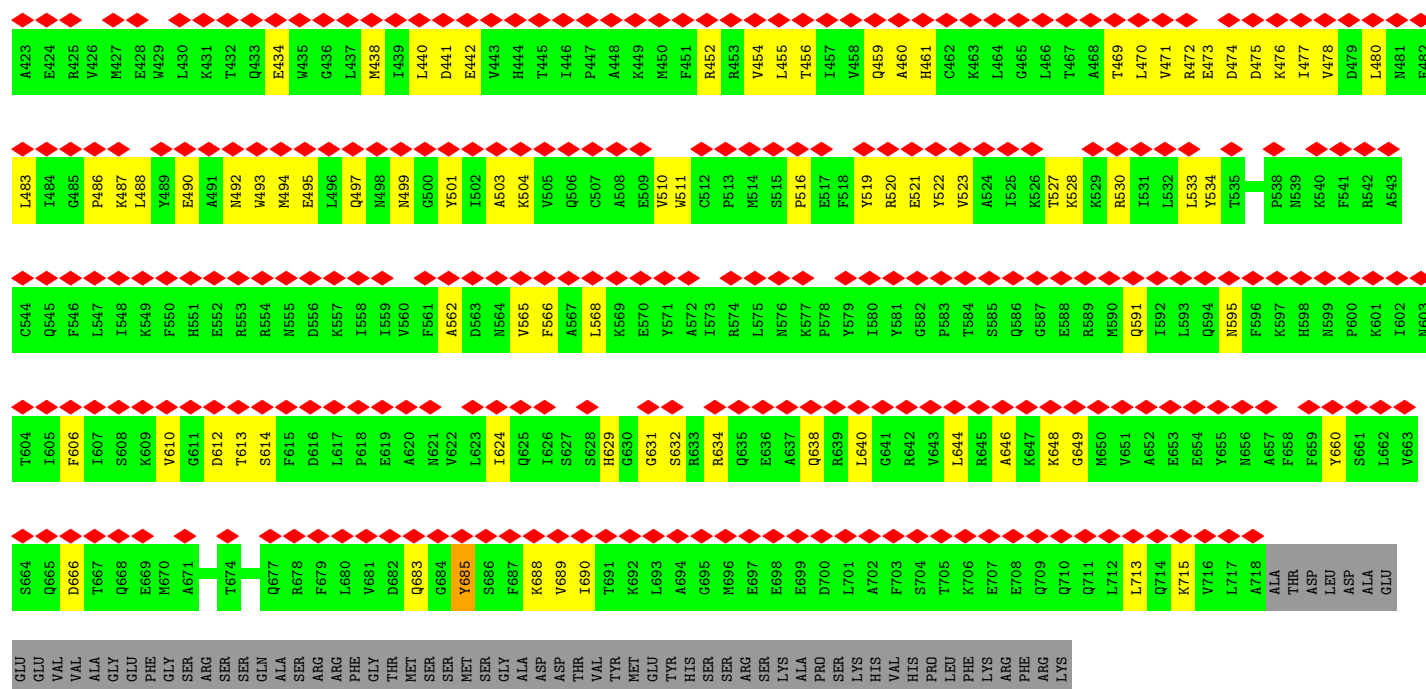


- Chain V:

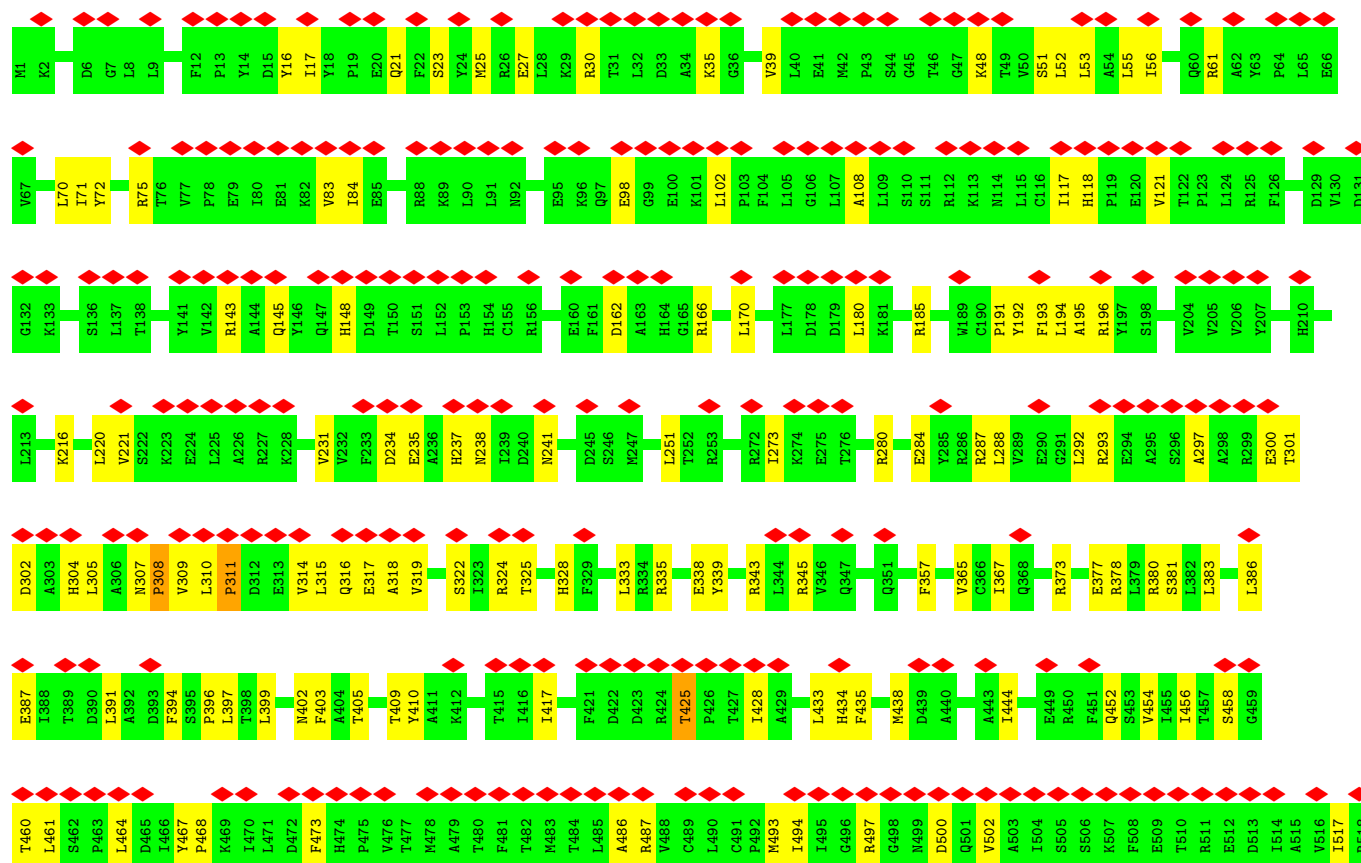
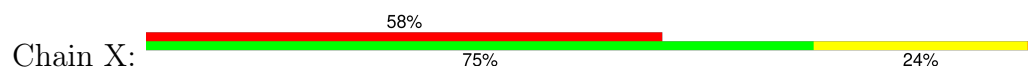


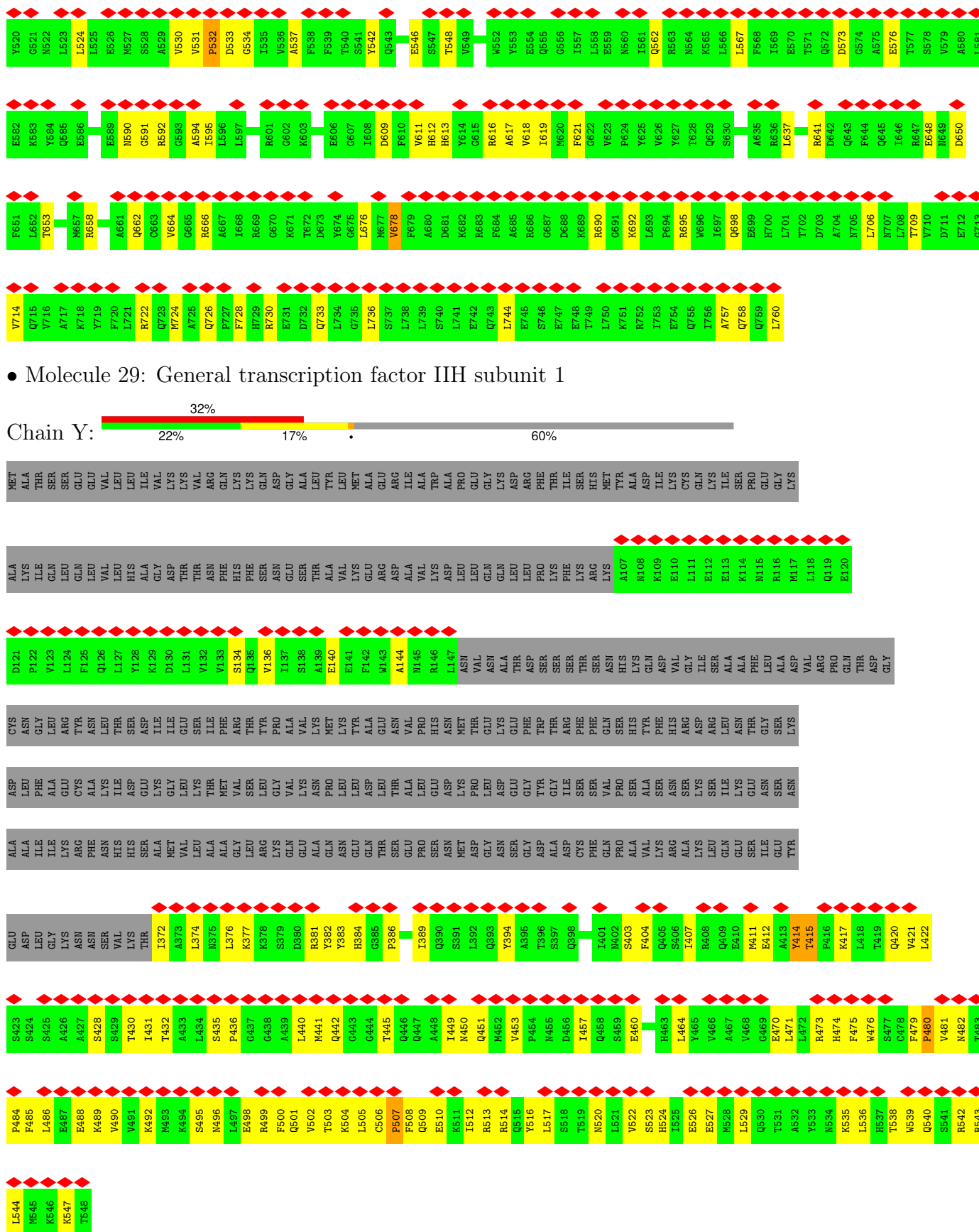
- Chain W:



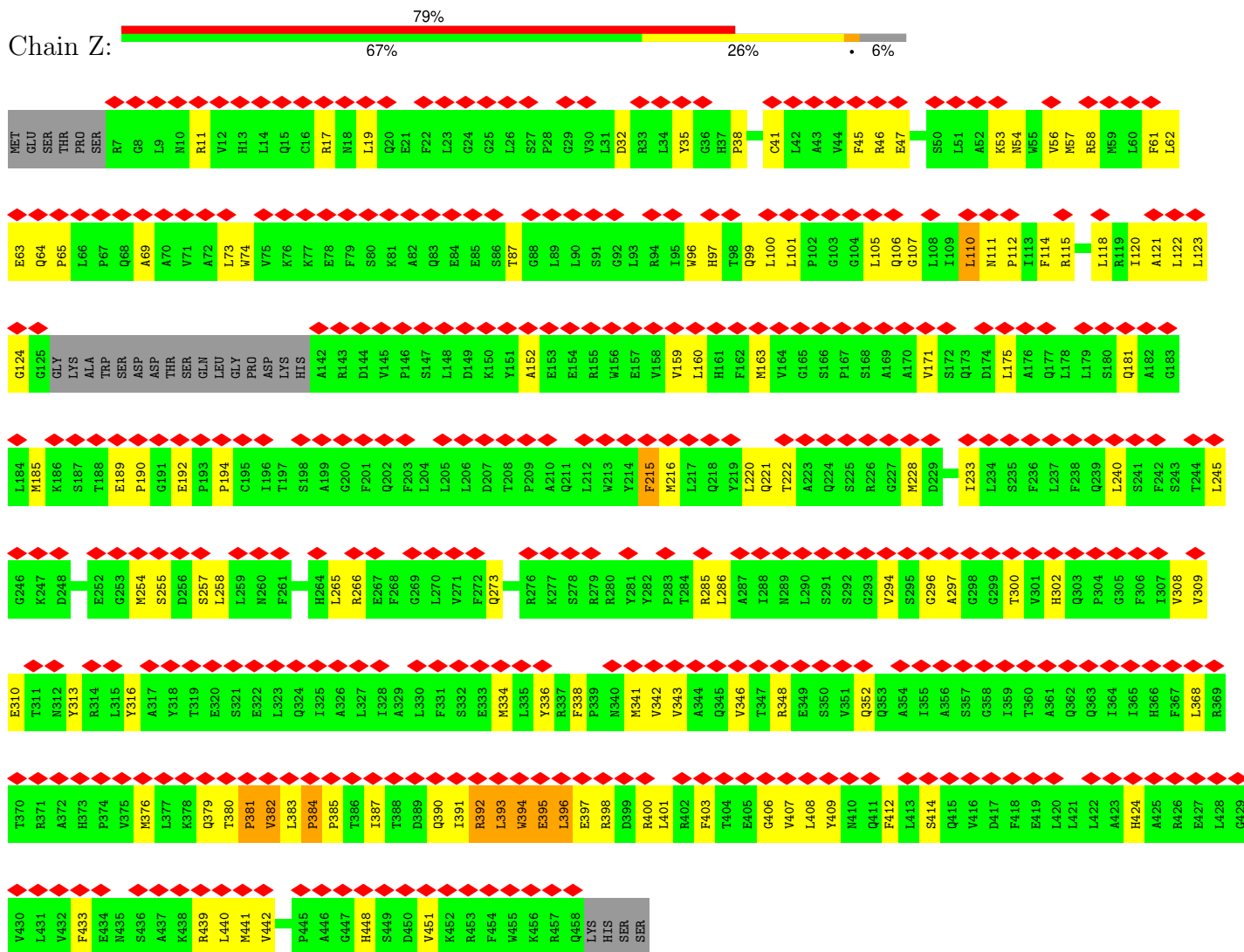


• Molecule 28: TFIID basal transcription factor complex helicase XPD subunit

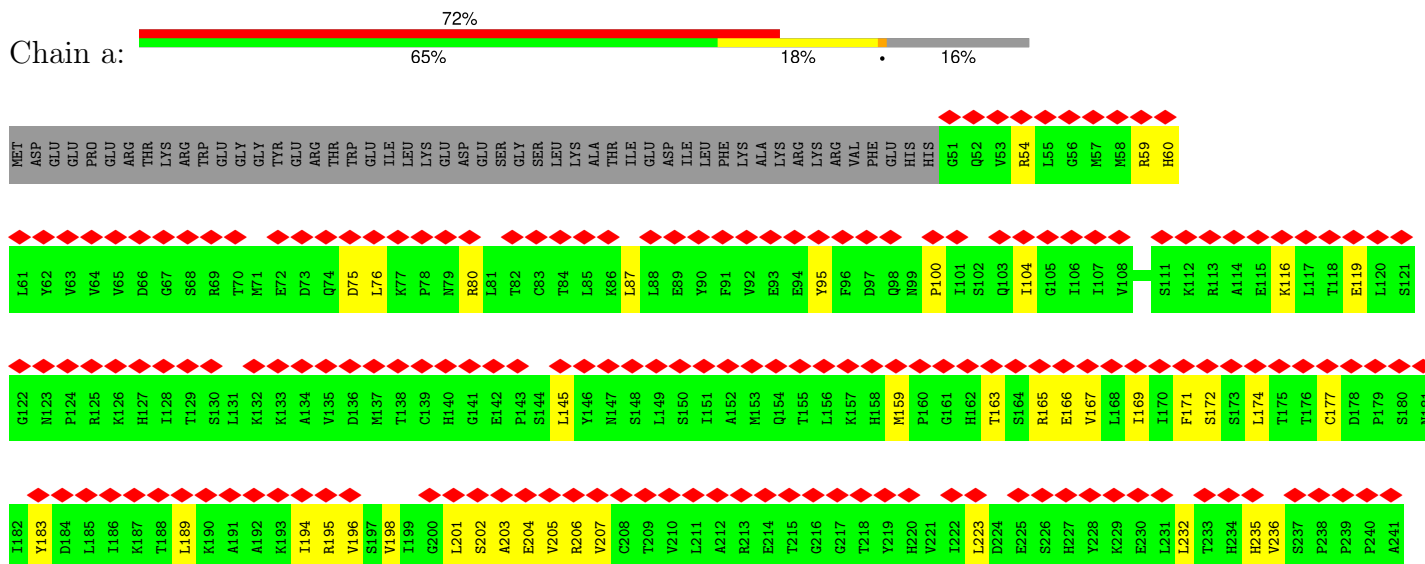


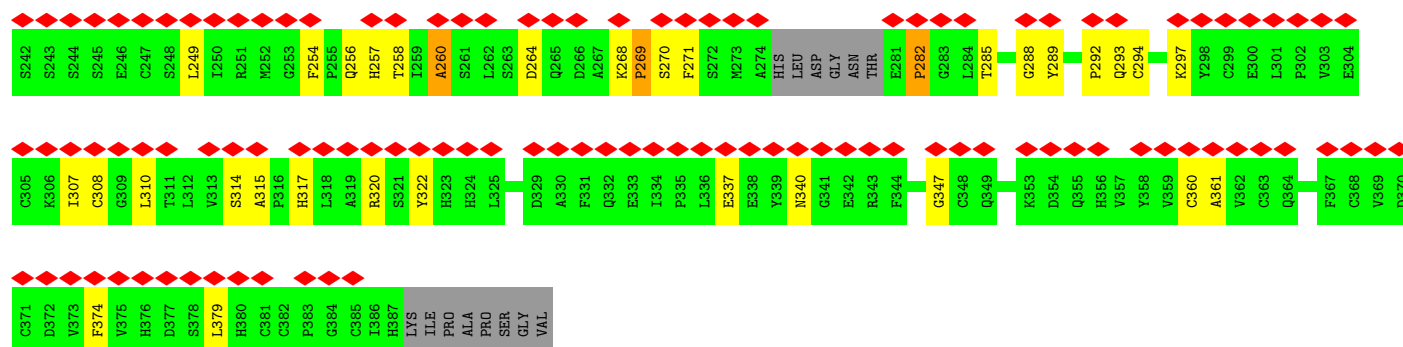


Chain Z:

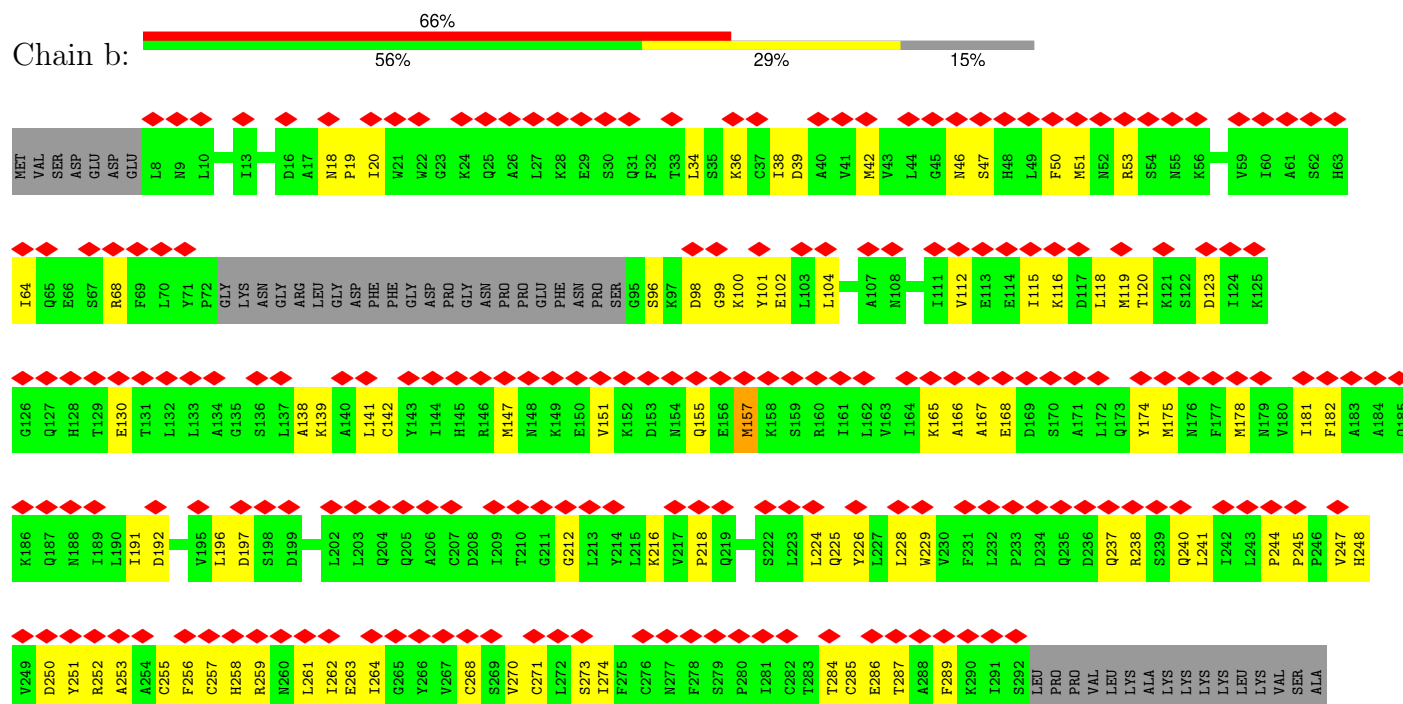


Chain a:

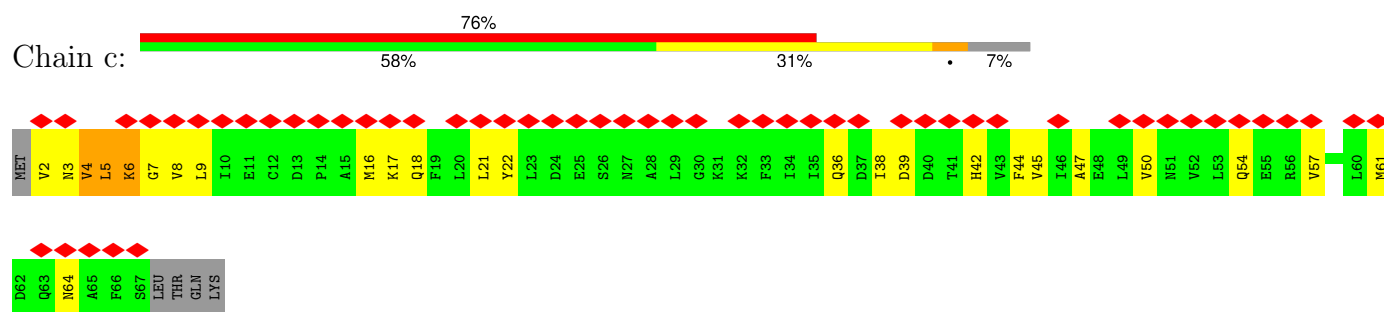




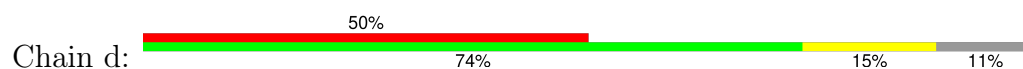
• Molecule 32: General transcription factor IIH subunit 3

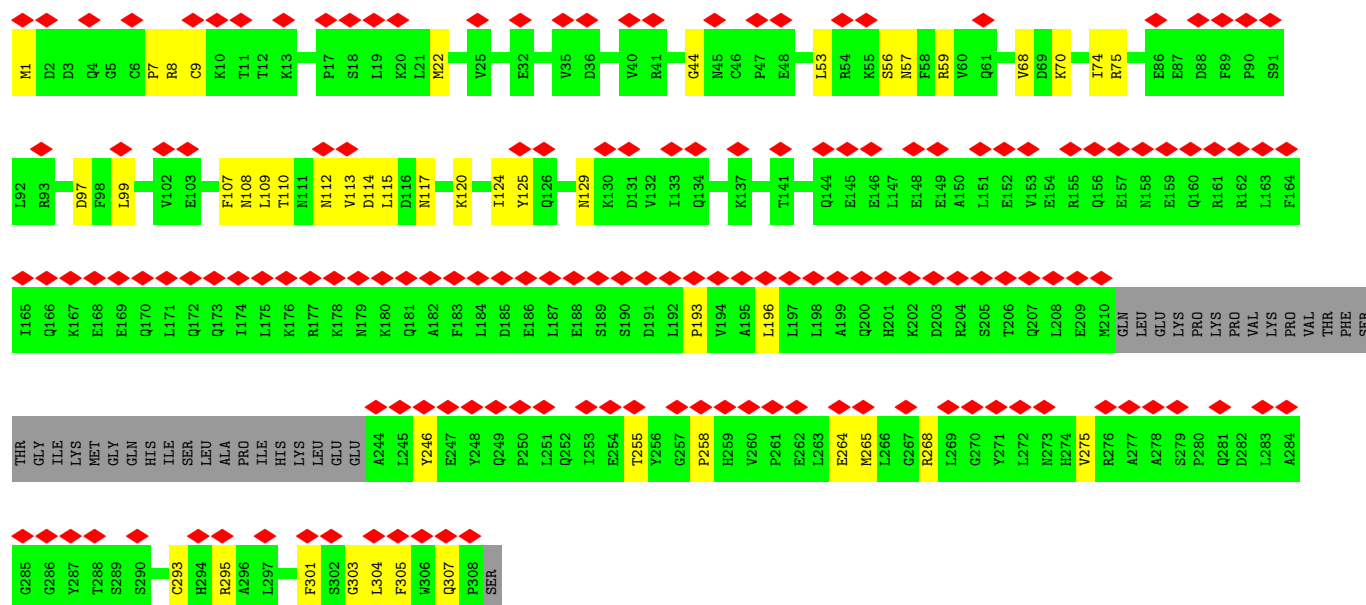


• Molecule 33: General transcription factor IIH subunit 5



• Molecule 34: CDK-activating kinase assembly factor MAT1

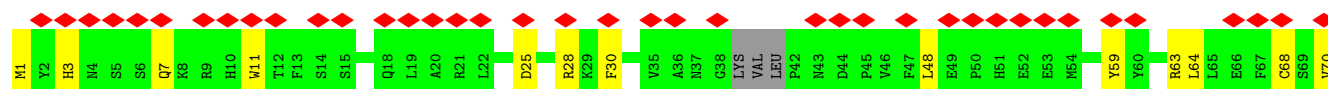




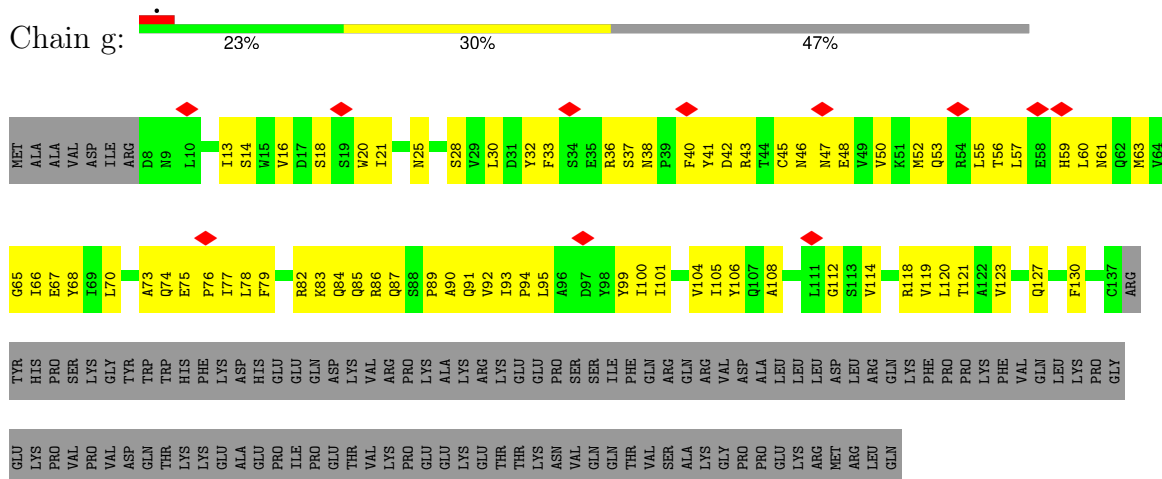
• Molecule 35: Cyclin-dependent kinase 7



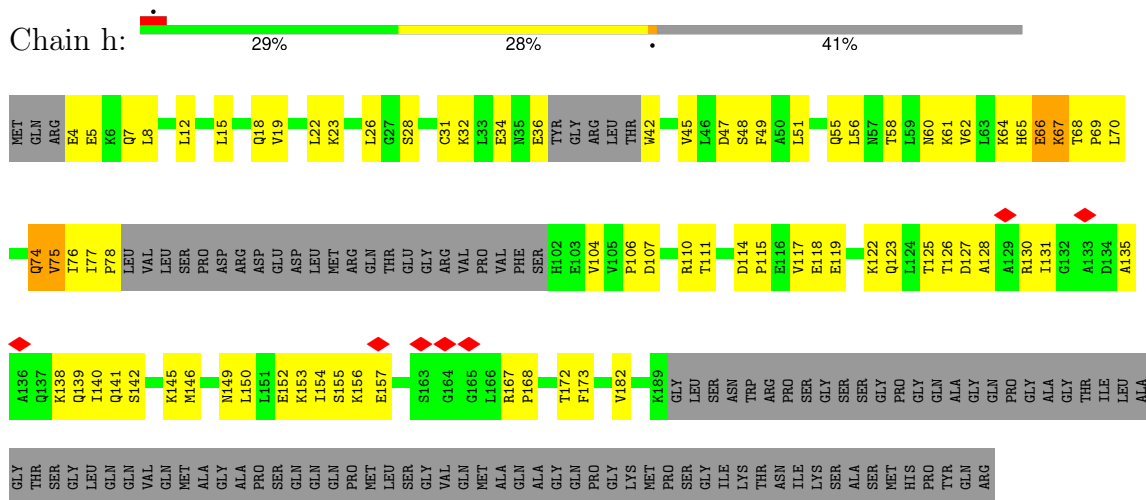
• Molecule 36: Cyclin-H



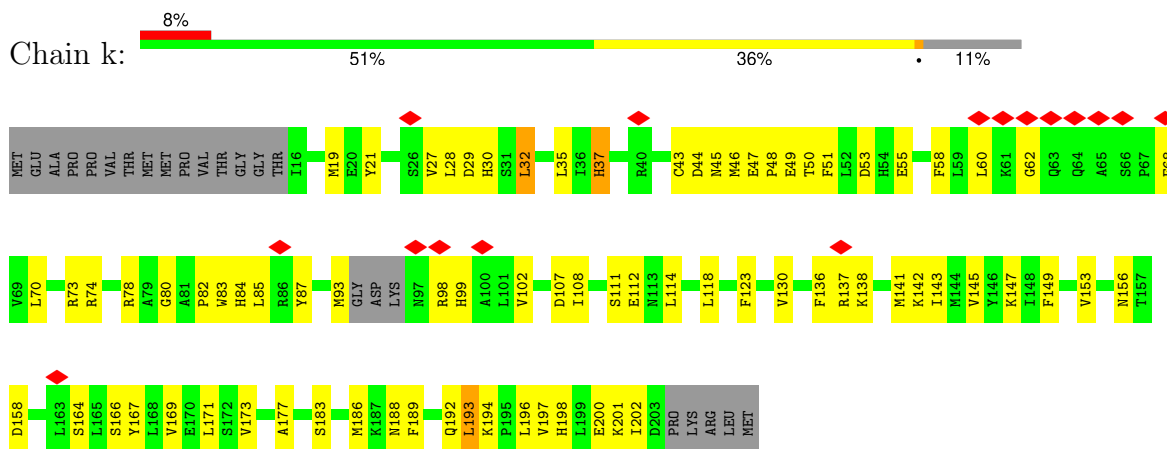
- Molecule 37: Mediator of RNA polymerase II transcription subunit 6



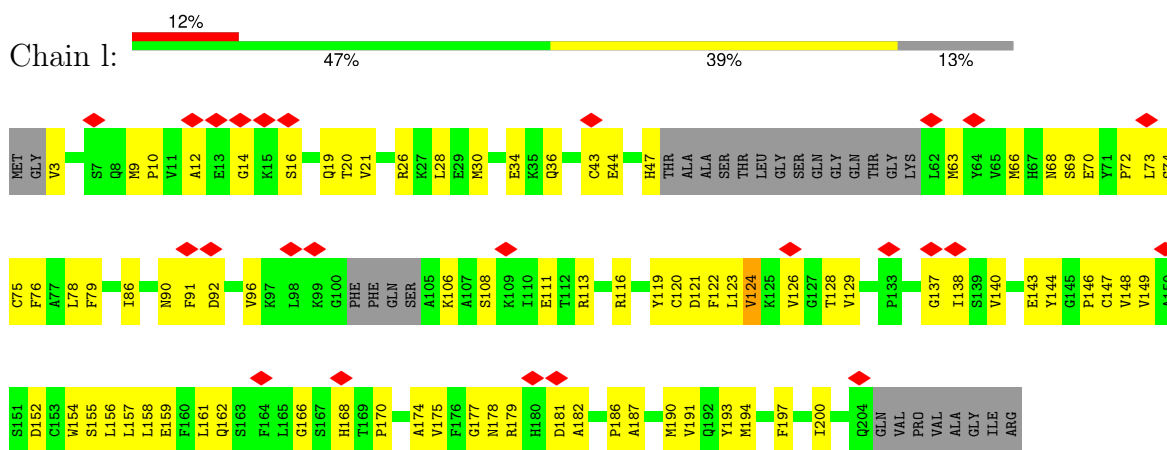
- Molecule 38: Mediator of RNA polymerase II transcription subunit 8



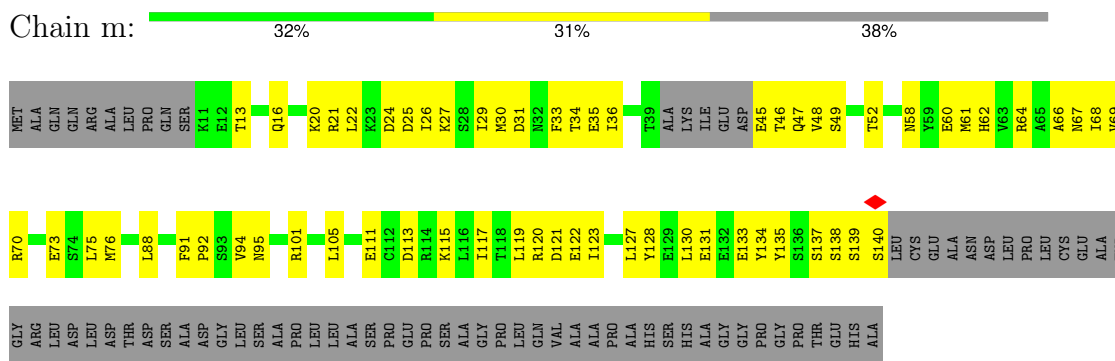
- Molecule 39: Mediator of RNA polymerase II transcription subunit 11



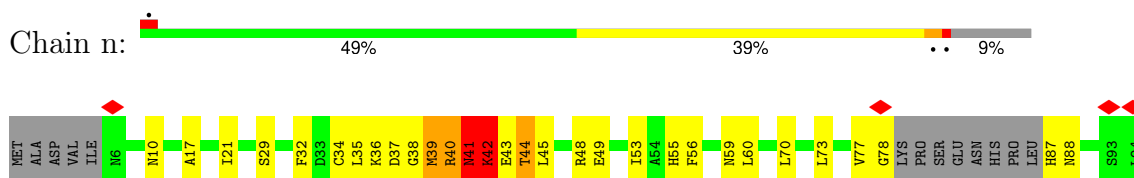
- Molecule 42: Mediator of RNA polymerase II transcription subunit 20

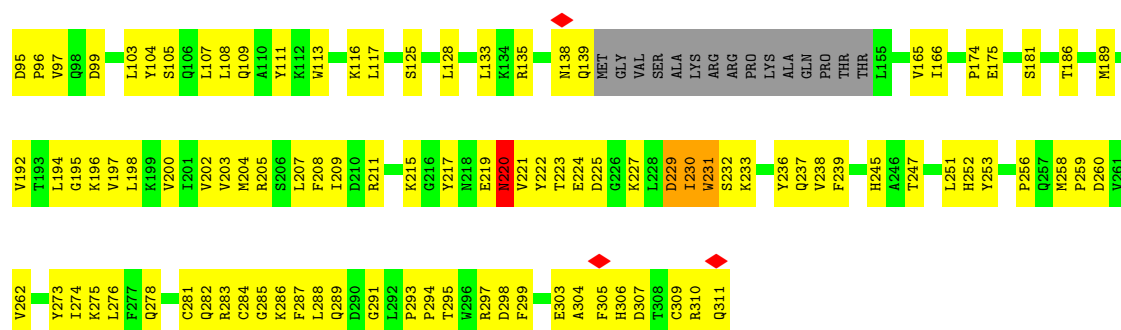


- Molecule 43: Mediator of RNA polymerase II transcription subunit 22

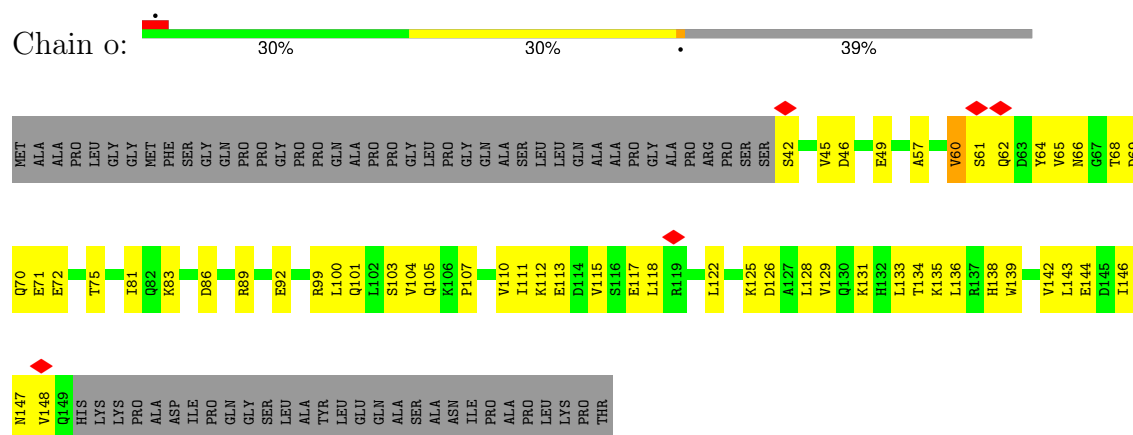


- Molecule 44: Mediator of RNA polymerase II transcription subunit 27

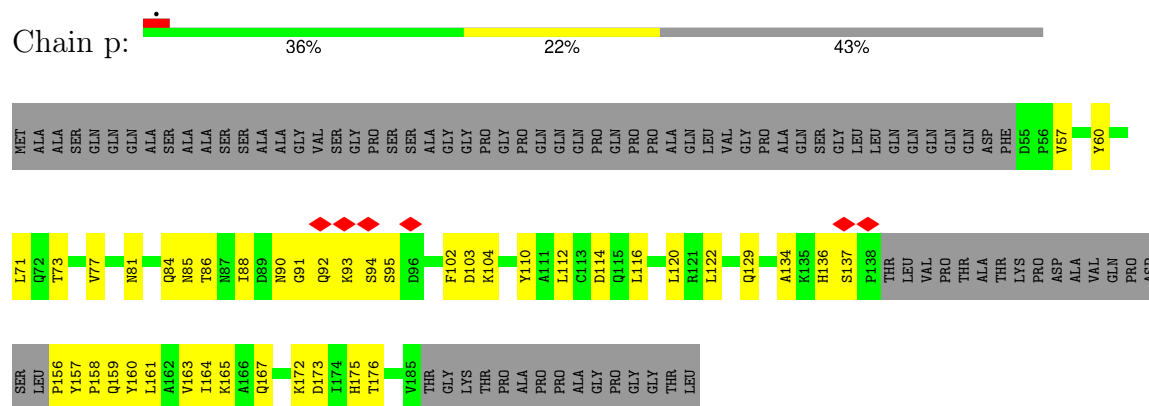




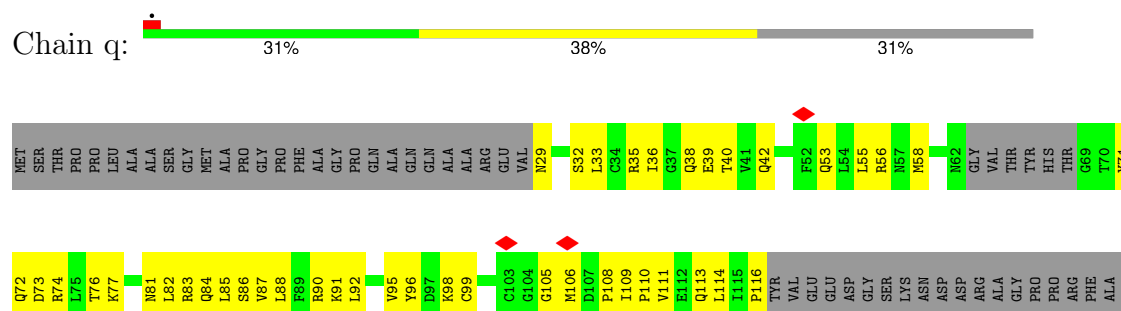
- Molecule 45: Mediator of RNA polymerase II transcription subunit 28



- Molecule 46: Mediator of RNA polymerase II transcription subunit 29

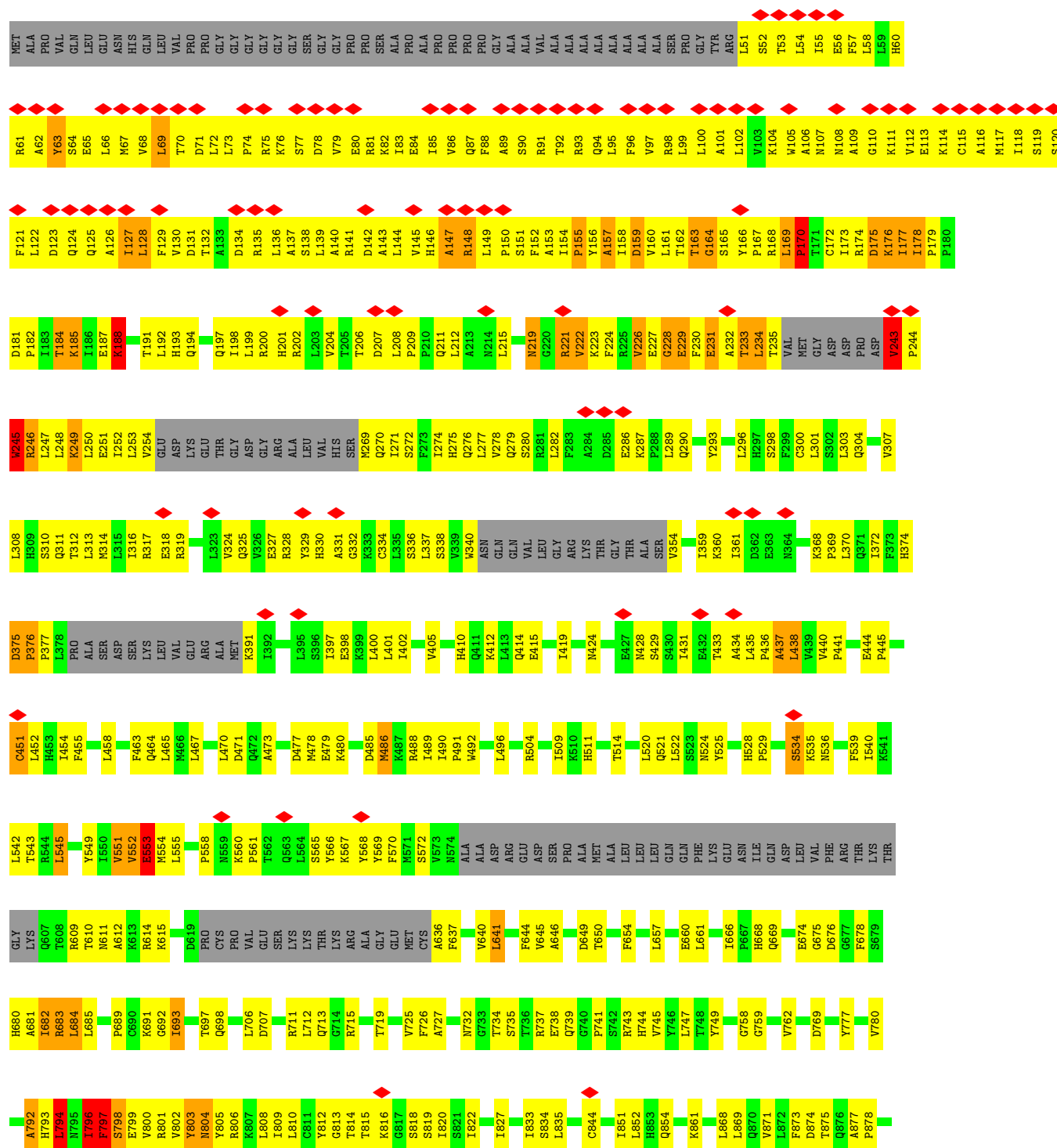


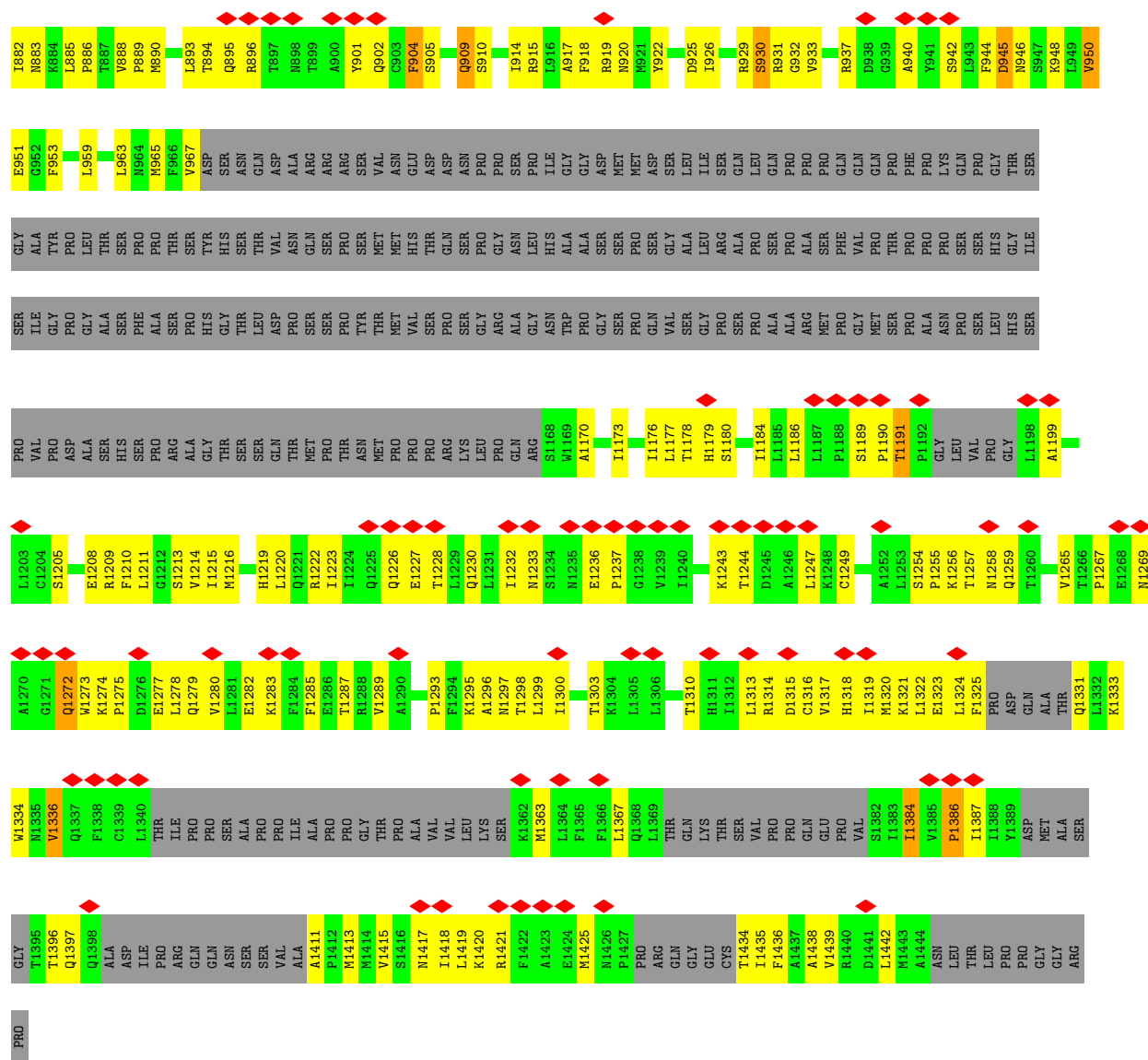
- Molecule 47: Mediator of RNA polymerase II transcription subunit 30



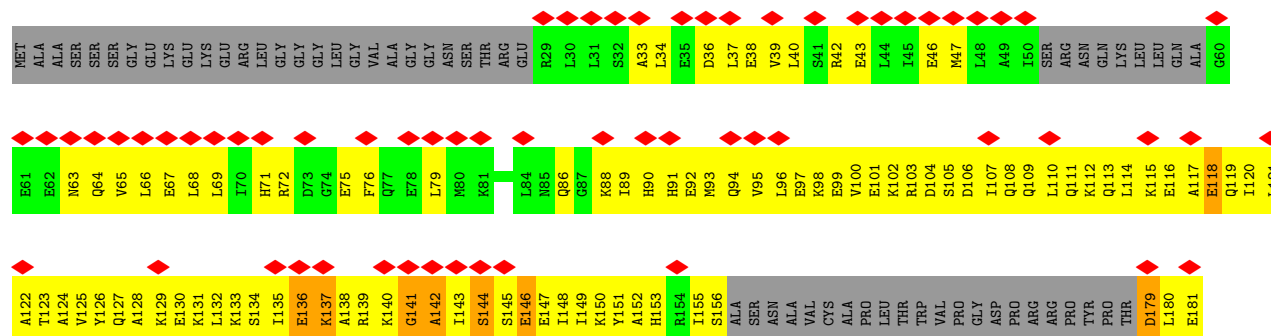


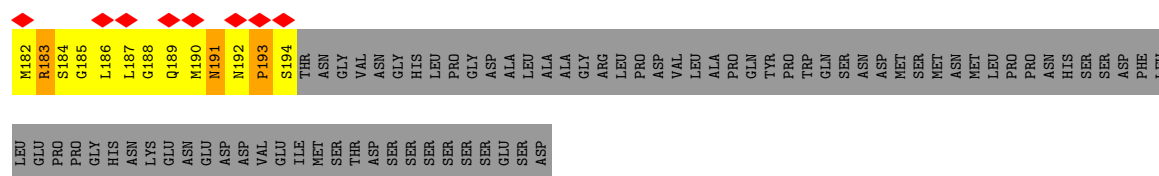
• Molecule 48: Mediator of RNA polymerase II transcription subunit 14



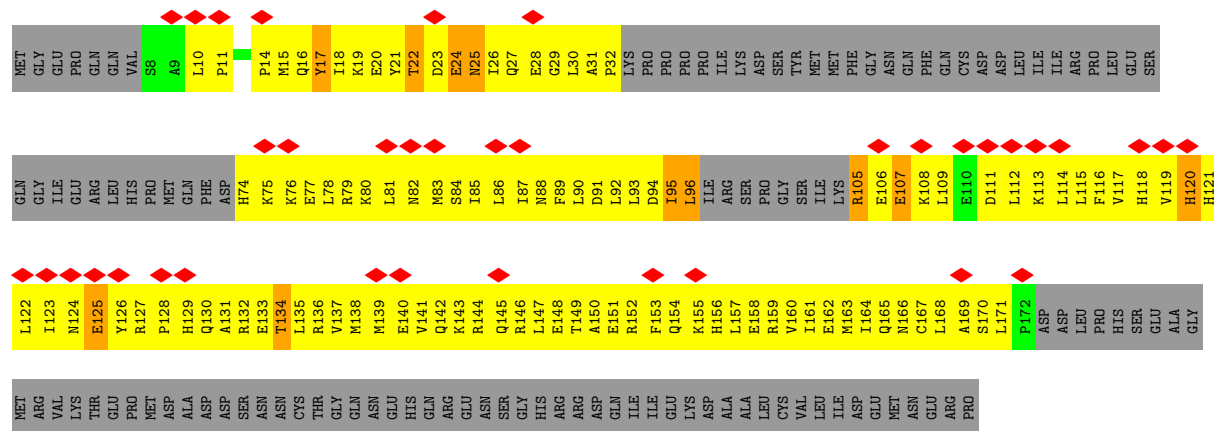


• Molecule 49: Mediator of RNA polymerase II transcription subunit 4

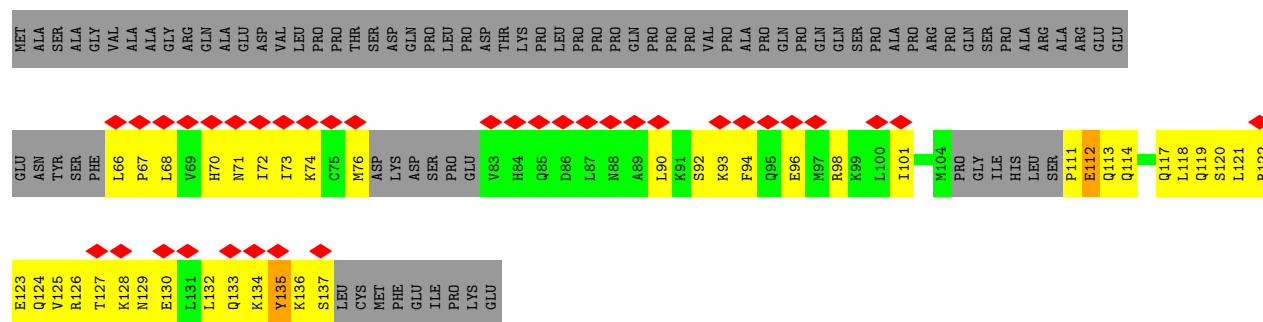




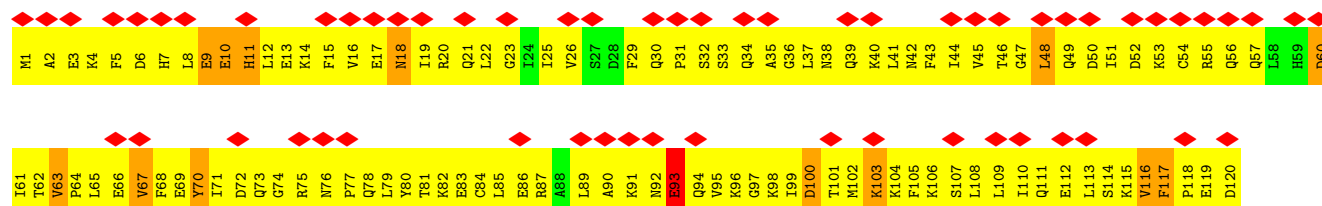
• Molecule 50: Mediator of RNA polymerase II transcription subunit 7

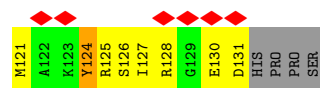


• Molecule 51: Mediator of RNA polymerase II transcription subunit 9

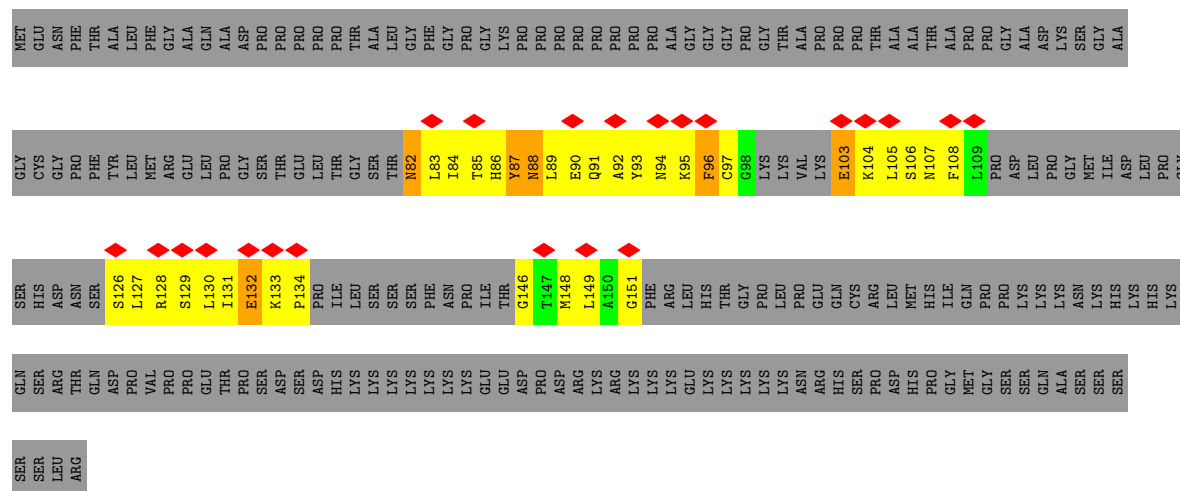


• Molecule 52: Mediator of RNA polymerase II transcription subunit 10

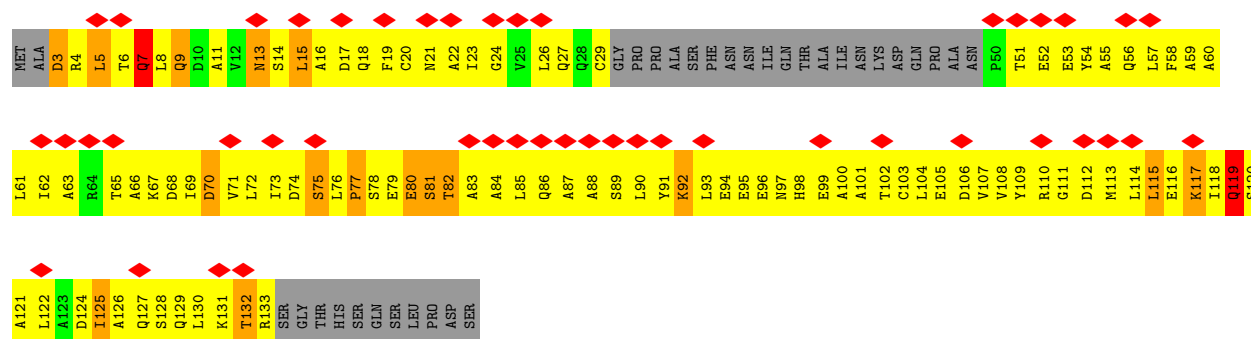




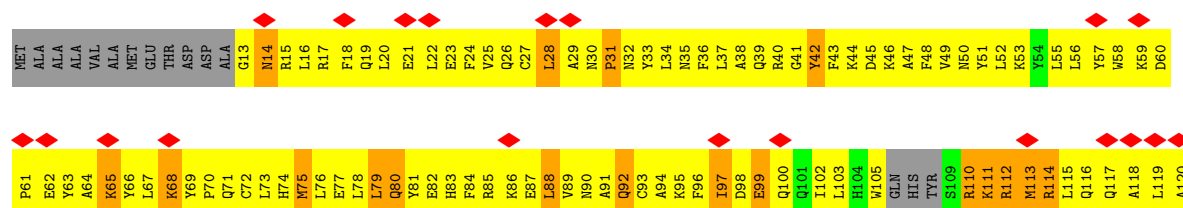
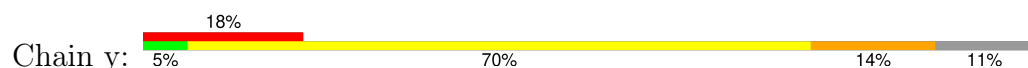
• Molecule 53: Mediator of RNA polymerase II transcription subunit 19

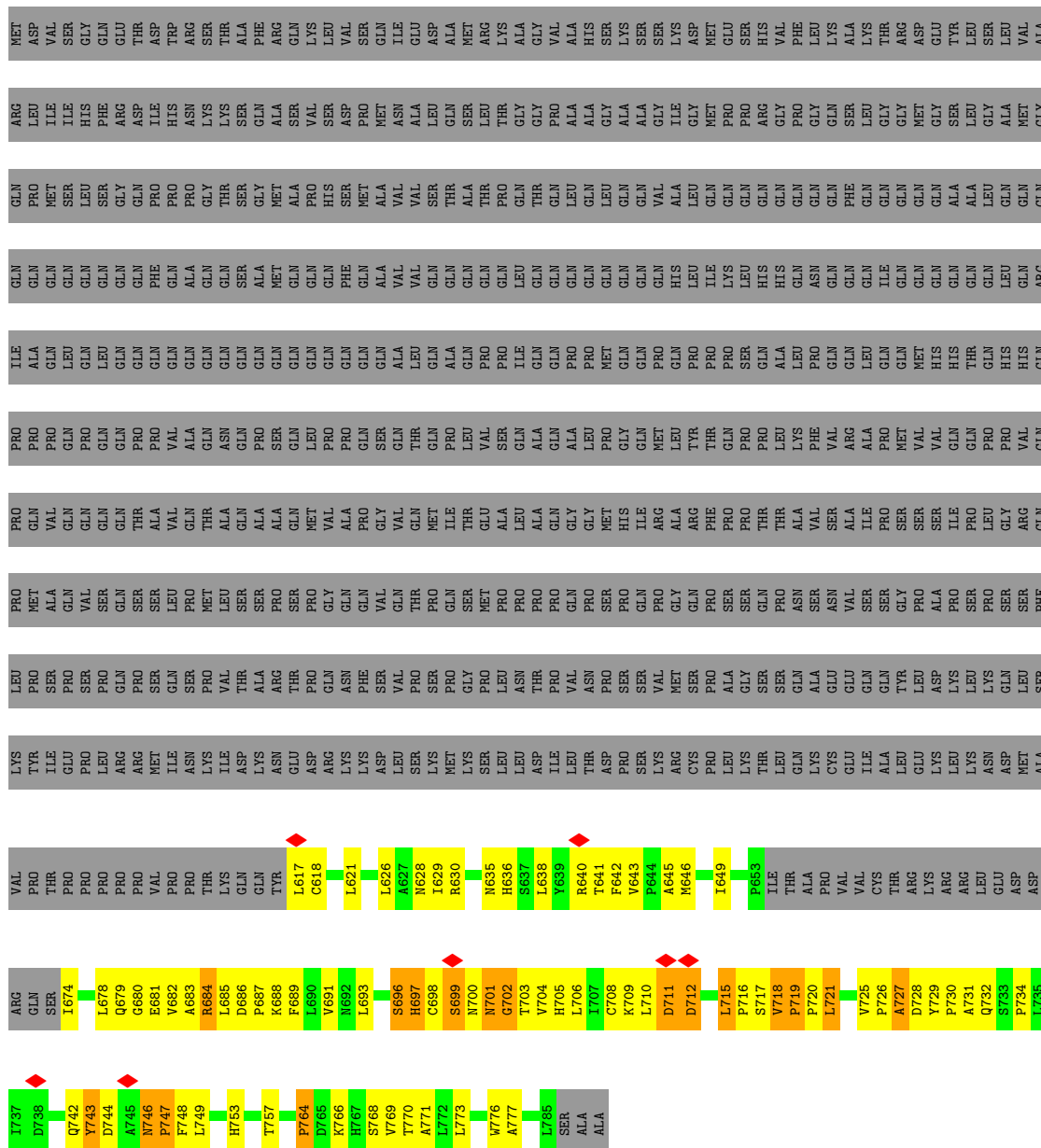


• Molecule 54: Mediator of RNA polymerase II transcription subunit 21



• Molecule 55: Mediator of RNA polymerase II transcription subunit 31





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156383	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 ($e^-/\text{\AA}^2$)	31.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.116	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	444.78, 444.78, 444.78	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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	0.70	18/5990 (0.3%)	0.75	13/8137 (0.2%)
2	1	0.35	0/10913	0.51	0/14828
3	2	0.48	9/7141 (0.1%)	0.59	2/9672 (0.0%)
4	3	0.74	4/1540 (0.3%)	0.73	2/2093 (0.1%)
5	A	0.33	0/11733	0.63	15/15844 (0.1%)
6	B	0.33	0/9310	0.50	2/12567 (0.0%)
7	C	0.34	0/2190	0.52	0/2975
8	D	0.22	0/1077	0.54	1/1446 (0.1%)
9	E	0.28	0/1753	0.50	0/2368
10	F	0.31	0/700	0.48	0/946
11	G	0.27	0/1382	0.53	0/1874
12	H	0.31	0/1227	0.53	0/1654
13	I	0.27	0/964	0.62	2/1305 (0.2%)
14	J	0.36	0/542	0.50	0/730
15	K	0.31	0/947	0.48	0/1282
16	L	0.28	0/394	0.61	0/524
17	M	0.21	0/945	0.60	1/1274 (0.1%)
18	N	0.22	0/816	0.52	0/1105
19	O	0.27	0/2049	0.54	0/2769
20	P	0.22	0/1489	0.47	0/2005
21	Q	0.23	0/1545	0.58	0/2075
22	R	0.22	0/1380	0.57	0/1854
23	S	0.23	0/1086	0.65	1/1461 (0.1%)
24	T	0.23	0/1817	0.61	1/2445 (0.0%)
25	U	0.25	0/1485	0.32	0/2293
26	V	0.26	0/1454	0.35	0/2239
27	W	0.35	0/4744	0.65	1/6402 (0.0%)
28	X	0.40	0/6236	0.73	2/8444 (0.0%)
29	Y	0.35	0/1660	0.79	5/2253 (0.2%)
30	Z	0.38	1/3552 (0.0%)	0.71	5/4814 (0.1%)
31	a	0.38	0/2637	0.67	2/3572 (0.1%)
32	b	0.35	0/2102	0.57	0/2844

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.33	0/528	0.71	0/713
34	d	0.30	0/2137	0.59	0/2890
35	e	0.34	0/2434	0.56	2/3300 (0.1%)
36	f	0.34	0/2342	0.45	0/3159
37	g	0.26	0/1058	0.53	0/1441
38	h	0.32	0/1245	0.60	0/1679
39	i	0.35	0/869	0.53	0/1168
40	j	0.94	32/4079 (0.8%)	0.92	17/5504 (0.3%)
41	k	0.37	0/1512	0.61	0/2034
42	l	0.35	0/1453	0.58	0/1963
43	m	0.41	0/1032	0.57	0/1385
44	n	0.58	2/2324 (0.1%)	0.73	5/3143 (0.2%)
45	o	0.39	0/897	0.59	0/1208
46	p	0.42	0/906	0.48	0/1222
47	q	0.41	0/1015	0.59	0/1360
48	r	0.72	11/8336 (0.1%)	0.89	32/11299 (0.3%)
49	s	0.99	1/1089 (0.1%)	1.05	2/1450 (0.1%)
50	t	1.22	1/991 (0.1%)	1.25	6/1331 (0.5%)
51	u	0.50	0/504	0.71	1/668 (0.1%)
52	v	1.04	3/1082 (0.3%)	1.09	5/1450 (0.3%)
53	w	0.89	0/311	1.02	0/412
54	x	1.22	0/858	1.28	8/1161 (0.7%)
55	y	1.23	3/1027 (0.3%)	1.16	6/1379 (0.4%)
56	z	1.14	8/1202 (0.7%)	1.29	11/1650 (0.7%)
All	All	0.50	93/132031 (0.1%)	0.67	150/179063 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	4
3	2	0	5
4	3	0	2
5	A	0	1
6	B	0	3
7	C	0	1
8	D	0	2
13	I	0	2
17	M	0	1
19	O	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
23	S	0	1
27	W	0	3
28	X	0	3
29	Y	0	1
30	Z	0	2
31	a	0	2
34	d	0	1
37	g	0	1
38	h	0	1
39	i	0	1
40	j	0	9
44	n	0	4
45	o	0	2
48	r	0	13
49	s	0	5
50	t	0	3
52	v	0	1
53	w	0	4
54	x	0	5
55	y	0	1
56	z	0	1
All	All	0	88

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	z	719	PRO	CA-C	-15.14	1.42	1.52
48	r	245	TRP	C-N	14.21	1.53	1.33
40	j	440	LEU	CA-C	-10.54	1.39	1.52
56	z	721	LEU	CA-C	-9.09	1.42	1.52
40	j	497	ILE	CA-C	-8.21	1.43	1.52
40	j	434	GLN	CA-C	-8.14	1.42	1.52
40	j	477	VAL	C-O	-7.80	1.16	1.24
4	3	82	VAL	C-O	-7.75	1.16	1.24
56	z	719	PRO	C-O	-7.60	1.18	1.24
1	0	19	CYS	C-O	-7.46	1.15	1.24
48	r	946	ASN	CA-C	-7.41	1.43	1.52
40	j	499	VAL	CA-C	-7.34	1.44	1.52
3	2	306	THR	C-O	-7.11	1.15	1.24
3	2	306	THR	CA-CB	-6.69	1.42	1.53
1	0	48	THR	CA-C	-6.56	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	833	TRP	CA-CB	-6.53	1.43	1.53
44	n	231	TRP	CB-CG	-6.50	1.30	1.50
40	j	486	GLN	CA-C	-6.38	1.44	1.52
40	j	436	LYS	C-O	-6.35	1.16	1.24
4	3	123	GLN	C-O	-6.34	1.16	1.24
40	j	497	ILE	CA-CB	-6.32	1.46	1.54
40	j	440	LEU	C-O	-6.27	1.16	1.24
40	j	437	HIS	C-O	-6.25	1.16	1.24
1	0	834	TRP	CB-CG	-6.25	1.30	1.50
40	j	501	GLN	C-O	-6.24	1.16	1.24
40	j	433	LYS	CA-C	-6.17	1.45	1.52
56	z	715	LEU	CA-C	-6.13	1.44	1.52
40	j	619	ARG	CA-CB	-6.12	1.43	1.53
44	n	231	TRP	CA-CB	-6.12	1.44	1.53
48	r	798	SER	C-O	-6.11	1.16	1.24
40	j	489	LYS	CA-C	-6.10	1.46	1.53
40	j	491	ILE	C-O	-6.09	1.16	1.24
40	j	615	TRP	CA-C	-6.04	1.44	1.52
3	2	273	MET	C-O	-5.98	1.17	1.24
1	0	833	TRP	CB-CG	-5.94	1.31	1.50
3	2	273	MET	CA-C	-5.88	1.45	1.52
56	z	719	PRO	CA-CB	-5.85	1.49	1.54
40	j	434	GLN	C-O	-5.84	1.17	1.24
40	j	436	LYS	CA-C	-5.84	1.45	1.52
1	0	826	ASN	CA-C	-5.83	1.45	1.52
40	j	615	TRP	CB-CG	-5.82	1.32	1.50
55	y	68	LYS	C-N	-5.79	1.26	1.33
40	j	487	ILE	C-O	-5.78	1.17	1.24
1	0	829	CYS	CA-C	-5.72	1.45	1.52
3	2	269	MET	CA-C	-5.71	1.45	1.52
40	j	615	TRP	C-O	-5.70	1.16	1.24
48	r	798	SER	CA-C	-5.69	1.45	1.52
1	0	62	ILE	C-O	-5.67	1.18	1.24
1	0	833	TRP	C-O	-5.59	1.17	1.23
40	j	439	PHE	CA-C	-5.57	1.45	1.52
48	r	797	PHE	CA-C	-5.57	1.46	1.52
40	j	492	GLN	C-O	-5.55	1.17	1.24
56	z	718	VAL	C-O	-5.55	1.17	1.24
48	r	792	ALA	N-CA	-5.54	1.39	1.46
49	s	191	ASN	CB-CG	-5.53	1.38	1.52
40	j	499	VAL	CA-CB	-5.53	1.47	1.54
40	j	507	ARG	C-O	-5.51	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	j	433	LYS	N-CA	-5.50	1.39	1.46
1	0	833	TRP	CG-CD1	-5.43	1.23	1.36
48	r	684	LEU	CA-C	-5.43	1.45	1.52
3	2	305	TRP	CA-CB	-5.42	1.44	1.53
3	2	304	LYS	CA-C	-5.41	1.45	1.52
52	v	93	GLU	CB-CG	-5.39	1.36	1.52
4	3	122	LEU	C-O	-5.39	1.17	1.24
1	0	833	TRP	CD2-CE2	-5.36	1.32	1.41
48	r	945	ASP	CA-C	-5.36	1.46	1.52
40	j	619	ARG	CA-C	-5.35	1.45	1.52
52	v	124	TYR	CB-CG	-5.30	1.40	1.51
40	j	482	GLN	CA-C	-5.29	1.45	1.52
1	0	831	GLY	CA-C	-5.29	1.47	1.52
55	y	79	LEU	CA-C	-5.28	1.45	1.52
48	r	794	LEU	N-CA	-5.25	1.40	1.46
1	0	827	CYS	CA-CB	-5.25	1.45	1.53
3	2	272	ARG	CA-C	-5.24	1.46	1.52
48	r	188	LYS	N-CA	-5.24	1.39	1.46
1	0	834	TRP	CA-C	-5.24	1.46	1.52
1	0	829	CYS	CA-CB	-5.19	1.45	1.53
55	y	75	MET	CA-C	-5.18	1.45	1.52
40	j	497	ILE	C-O	-5.18	1.18	1.24
1	0	20	GLU	CA-C	-5.17	1.45	1.53
1	0	833	TRP	CA-C	-5.16	1.46	1.52
50	t	17	TYR	CA-C	-5.15	1.45	1.52
40	j	479	ILE	CA-C	-5.14	1.46	1.52
40	j	438	ILE	CA-C	-5.13	1.46	1.52
1	0	19	CYS	CA-CB	-5.10	1.45	1.53
3	2	270	VAL	CA-C	-5.09	1.46	1.52
48	r	797	PHE	C-O	-5.09	1.17	1.24
56	z	715	LEU	CA-CB	-5.08	1.46	1.53
4	3	83	GLN	CA-C	-5.06	1.46	1.53
40	j	501	GLN	N-CA	5.06	1.52	1.46
56	z	717	SER	C-O	-5.01	1.17	1.24
30	Z	110	LEU	C-N	5.01	1.41	1.33
52	v	117	PHE	C-N	-5.00	1.22	1.33

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	z	715	LEU	CA-C-N	23.33	149.00	119.84
56	z	715	LEU	C-N-CA	23.33	149.00	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1623	SER	CA-C-N	19.00	139.04	119.85
5	A	1623	SER	C-N-CA	19.00	139.04	119.85
48	r	245	TRP	CA-C-N	-13.47	102.58	122.65
48	r	245	TRP	C-N-CA	-13.47	102.58	122.65
40	j	194	TRP	N-CA-C	13.01	127.58	109.11
48	r	243	VAL	CA-C-N	12.52	132.43	120.03
48	r	243	VAL	C-N-CA	12.52	132.43	120.03
1	0	640	ARG	CA-C-N	11.58	134.31	119.84
1	0	640	ARG	C-N-CA	11.58	134.31	119.84
44	n	231	TRP	N-CA-C	11.58	126.72	112.59
30	Z	396	LEU	N-CA-C	11.10	127.79	111.81
55	y	68	LYS	CA-C-N	-10.80	107.75	123.30
55	y	68	LYS	C-N-CA	-10.80	107.75	123.30
5	A	1619	SER	CA-C-N	10.78	133.32	119.84
5	A	1619	SER	C-N-CA	10.78	133.32	119.84
4	3	49	GLY	N-CA-C	10.15	124.28	112.50
48	r	827	ILE	N-CA-C	-9.70	104.50	113.71
29	Y	480	PRO	CA-N-CD	-9.68	98.44	112.00
5	A	1655	PRO	CA-C-N	9.37	134.95	122.30
5	A	1655	PRO	C-N-CA	9.37	134.95	122.30
29	Y	484	PRO	CA-N-CD	-9.25	99.05	112.00
29	Y	507	PRO	CA-N-CD	-8.92	99.52	112.00
1	0	19	CYS	N-CA-C	8.90	122.92	108.41
1	0	62	ILE	CB-CA-C	-8.78	100.81	111.08
31	a	282	PRO	CA-N-CD	-8.73	99.78	112.00
28	X	308	PRO	CA-N-CD	-8.72	99.79	112.00
31	a	269	PRO	CA-N-CD	-8.72	99.79	112.00
28	X	311	PRO	CA-N-CD	-8.65	99.89	112.00
5	A	1623	SER	N-CA-C	8.52	120.04	109.57
1	0	829	CYS	CB-CA-C	-8.47	97.51	110.90
55	y	80	GLN	CA-C-N	-8.38	111.21	122.85
55	y	80	GLN	C-N-CA	-8.38	111.21	122.85
56	z	719	PRO	CB-CA-C	-8.08	103.58	111.17
54	x	7	GLN	O-C-N	-8.05	113.66	122.03
40	j	500	GLU	N-CA-C	7.79	122.13	111.54
5	A	1656	SER	N-CA-C	7.68	121.18	108.96
40	j	47	ILE	N-CA-C	7.60	119.55	109.21
40	j	499	VAL	CB-CA-C	-7.58	100.03	111.33
5	A	1656	SER	CA-C-O	-7.35	112.20	120.43
48	r	796	ILE	N-CA-C	-7.13	103.90	110.82
1	0	49	MET	N-CA-C	7.04	120.95	111.24
40	j	479	ILE	CA-C-N	-7.00	111.05	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	j	479	ILE	C-N-CA	-7.00	111.05	122.82
5	A	1628	SER	N-CA-C	6.95	121.92	113.17
48	r	63	TYR	CA-CB-CG	6.91	126.34	113.90
54	x	119	GLN	CA-CB-CG	-6.85	100.40	114.10
3	2	531	THR	CA-C-N	-6.84	114.30	122.44
3	2	531	THR	C-N-CA	-6.84	114.30	122.44
40	j	564	GLY	N-CA-C	-6.71	104.94	112.33
48	r	682	ILE	CB-CA-C	-6.68	102.78	110.73
1	0	58	LEU	N-CA-C	-6.64	97.53	108.49
30	Z	394	TRP	CA-C-N	6.58	129.09	120.28
30	Z	394	TRP	C-N-CA	6.58	129.09	120.28
56	z	715	LEU	C-N-CD	-6.58	98.04	125.00
40	j	497	ILE	CB-CA-C	-6.57	103.40	111.08
30	Z	384	PRO	CA-C-N	6.46	126.23	119.05
30	Z	384	PRO	C-N-CA	6.46	126.23	119.05
1	0	62	ILE	N-CA-C	6.43	118.06	108.54
40	j	438	ILE	CB-CA-C	-6.40	103.50	112.14
4	3	128	PHE	N-CA-C	-6.33	104.38	111.28
48	r	159	ASP	CA-C-N	-6.33	111.43	120.42
48	r	159	ASP	C-N-CA	-6.33	111.43	120.42
48	r	249	LYS	CA-C-N	-6.31	112.70	122.87
48	r	249	LYS	C-N-CA	-6.31	112.70	122.87
48	r	170	PRO	CA-C-N	-6.27	113.17	122.83
48	r	170	PRO	C-N-CA	-6.27	113.17	122.83
35	e	164	SER	CA-C-N	6.18	125.91	119.05
35	e	164	SER	C-N-CA	6.18	125.91	119.05
40	j	479	ILE	CB-CA-C	-6.16	102.54	110.98
27	W	92	VAL	N-CA-C	-6.15	105.37	111.77
5	A	1625	THR	CB-CA-C	-6.09	101.32	110.88
24	T	134	GLU	N-CA-C	-6.08	102.92	110.41
5	A	1619	SER	N-CA-C	6.05	115.27	108.25
48	r	1336	VAL	N-CA-C	6.03	121.88	109.34
48	r	148	ARG	N-CA-C	6.03	119.02	111.24
5	A	1655	PRO	CA-C-O	6.01	128.20	121.34
48	r	797	PHE	CA-C-N	5.99	132.98	121.54
48	r	797	PHE	C-N-CA	5.99	132.98	121.54
54	x	75	SER	CA-CB-OG	-5.99	99.12	111.10
44	n	231	TRP	N-CA-CB	-5.96	101.39	110.92
48	r	1386	PRO	N-CA-CB	5.95	109.50	103.25
52	v	63	VAL	N-CA-C	5.94	113.43	107.55
40	j	479	ILE	CA-C-O	-5.87	114.19	120.59
1	0	16	ALA	N-CA-C	-5.86	104.81	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	z	696	SER	CA-C-N	5.84	132.69	121.54
56	z	696	SER	C-N-CA	5.84	132.69	121.54
48	r	551	VAL	CA-C-N	-5.84	111.46	121.97
48	r	551	VAL	C-N-CA	-5.84	111.46	121.97
50	t	125	GLU	CA-C-N	-5.82	112.48	120.28
50	t	125	GLU	C-N-CA	-5.82	112.48	120.28
5	A	1625	THR	N-CA-C	5.81	117.28	111.07
40	j	34	LEU	CA-C-N	5.80	132.62	121.54
40	j	34	LEU	C-N-CA	5.80	132.62	121.54
13	I	56	ASN	CA-C-N	-5.80	110.46	121.54
13	I	56	ASN	C-N-CA	-5.80	110.46	121.54
50	t	134	THR	CA-C-N	-5.79	113.00	120.65
50	t	134	THR	C-N-CA	-5.79	113.00	120.65
44	n	181	SER	CA-C-N	-5.79	116.32	123.21
44	n	181	SER	C-N-CA	-5.79	116.32	123.21
8	D	126	GLU	N-CA-C	-5.78	106.15	113.43
49	s	183	ARG	CA-C-N	-5.74	110.57	121.54
49	s	183	ARG	C-N-CA	-5.74	110.57	121.54
1	0	832	LEU	N-CA-C	5.73	118.10	110.53
40	j	484	TYR	CA-CB-CG	-5.73	103.59	113.90
29	Y	414	TYR	CA-C-N	5.72	135.75	121.80
29	Y	414	TYR	C-N-CA	5.72	135.75	121.80
54	x	117	LYS	CA-C-N	-5.71	113.26	120.56
54	x	117	LYS	C-N-CA	-5.71	113.26	120.56
52	v	18	ASN	CA-C-N	-5.70	112.66	120.46
52	v	18	ASN	C-N-CA	-5.70	112.66	120.46
48	r	1384	ILE	O-C-N	-5.64	117.09	123.18
1	0	18	VAL	N-CA-C	5.62	116.08	107.77
56	z	697	HIS	N-CA-CB	5.61	119.97	110.49
50	t	96	LEU	N-CA-C	-5.61	95.30	111.00
40	j	488	CYS	N-CA-C	5.61	117.55	108.41
56	z	699	SER	N-CA-C	-5.61	99.39	108.41
56	z	744	ASP	N-CA-C	-5.55	98.97	110.80
54	x	77	PRO	CA-C-N	-5.51	111.02	121.54
54	x	77	PRO	C-N-CA	-5.51	111.02	121.54
6	B	978	ILE	N-CA-C	-5.51	107.01	111.91
50	t	107	GLU	CA-CB-CG	5.47	125.04	114.10
6	B	661	VAL	N-CA-C	-5.46	108.52	113.71
40	j	482	GLN	N-CA-C	5.42	117.19	111.28
23	S	47	LEU	N-CA-C	5.41	116.63	108.46
48	r	436	PRO	CA-C-N	5.39	131.84	121.54
48	r	436	PRO	C-N-CA	5.39	131.84	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	553	GLU	N-CA-C	-5.39	99.32	110.80
1	0	59	THR	N-CA-C	-5.36	99.39	110.80
48	r	157	ALA	CA-C-N	-5.33	114.04	120.70
48	r	157	ALA	C-N-CA	-5.33	114.04	120.70
40	j	620	GLY	N-CA-C	5.31	123.18	112.34
51	u	135	TYR	CA-CB-CG	-5.24	104.47	113.90
56	z	696	SER	N-CA-C	-5.24	102.73	110.48
48	r	641	LEU	CA-CB-CG	-5.23	97.98	116.30
52	v	116	VAL	N-CA-C	-5.21	98.50	109.34
1	0	18	VAL	CB-CA-C	-5.21	103.39	110.42
52	v	70	TYR	CA-CB-CG	5.18	123.23	113.90
17	M	347	ASN	N-CA-C	-5.16	108.00	114.56
5	A	1655	PRO	O-C-N	-5.16	116.78	123.03
54	x	92	LYS	CA-CB-CG	5.10	124.30	114.10
48	r	176	LYS	CA-C-N	-5.10	113.18	120.42
48	r	176	LYS	C-N-CA	-5.10	113.18	120.42
55	y	28	LEU	CA-C-N	-5.09	113.67	120.54
55	y	28	LEU	C-N-CA	-5.09	113.67	120.54
56	z	684	ARG	N-CA-C	5.08	119.06	113.21
48	r	219	ASN	N-CA-C	5.06	116.94	108.23
44	n	41	ASN	N-CA-C	-5.04	100.06	110.80
48	r	534	SER	N-CA-C	5.00	114.84	108.24

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	112	ASP	Peptide
1	0	170	LEU	Peptide
1	0	569	LEU	Peptide
1	0	732	LEU	Peptide
3	2	597	LEU	Peptide
3	2	685	ILE	Peptide
3	2	686	LYS	Peptide
3	2	691	GLY	Peptide
3	2	942	SER	Peptide
4	3	46	TYR	Mainchain
4	3	77	ALA	Peptide
5	A	1202	PHE	Peptide
6	B	563	ASP	Peptide
6	B	594	MET	Peptide
6	B	835	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	C	128	ILE	Peptide
8	D	71	PHE	Peptide
8	D	72	SER	Peptide
13	I	57	LYS	Peptide
13	I	59	THR	Peptide
17	M	316	SER	Peptide
19	O	279	GLY	Peptide
19	O	38	GLY	Peptide
21	Q	78	VAL	Peptide
23	S	44	GLN	Peptide
27	W	400	PRO	Peptide
27	W	475	ASP	Peptide
27	W	476	LYS	Peptide
28	X	102	LEU	Peptide
28	X	425	THR	Peptide
28	X	532	PRO	Peptide
29	Y	415	THR	Peptide
30	Z	189	GLU	Peptide
30	Z	192	GLU	Peptide
31	a	260	ALA	Peptide
31	a	315	ALA	Peptide
34	d	56	SER	Peptide
37	g	108	ALA	Peptide
38	h	66	GLU	Peptide
39	i	74	ALA	Peptide
40	j	194	TRP	Peptide
40	j	317	GLN	Peptide
40	j	399	PRO	Peptide
40	j	414	ASP	Peptide
40	j	457	ASP	Peptide
40	j	485	GLU	Mainchain
40	j	543	VAL	Peptide
40	j	549	LEU	Peptide
40	j	629	LYS	Peptide
44	n	220	ASN	Peptide
44	n	39	MET	Peptide
44	n	41	ASN	Peptide
44	n	42	LYS	Peptide
45	o	60	VAL	Peptide
45	o	62	GLN	Peptide
48	r	1228	THR	Peptide
48	r	147	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
48	r	148	ARG	Peptide
48	r	163	THR	Peptide
48	r	164	GLY	Peptide
48	r	178	ILE	Peptide
48	r	228	GLY	Peptide
48	r	375	ASP	Peptide
48	r	376	PRO	Peptide
48	r	486	MET	Peptide
48	r	803	TYR	Peptide
48	r	909	GLN	Peptide
48	r	930	SER	Peptide
49	s	137	LYS	Peptide
49	s	141	GLY	Peptide
49	s	142	ALA	Peptide
49	s	179	ASP	Peptide
49	s	193	PRO	Peptide
50	t	105	ARG	Peptide
50	t	22	THR	Peptide
50	t	95	ILE	Peptide
52	v	60	ASP	Peptide
53	w	103	GLU	Peptide
53	w	82	ASN	Peptide
53	w	87	TYR	Peptide
53	w	96	PHE	Peptide
54	x	3	ASP	Peptide
54	x	7	GLN	Mainchain
54	x	80	GLU	Peptide
54	x	81	SER	Peptide
54	x	82	THR	Peptide
55	y	42	TYR	Peptide
56	z	764	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	5864	0	5967	384	0
2	1	10636	0	10706	350	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	7007	0	7171	331	0
4	3	1504	0	1492	119	0
5	A	11519	0	11611	513	0
6	B	9129	0	9143	291	0
7	C	2147	0	2091	78	0
8	D	1062	0	1042	125	0
9	E	1723	0	1744	58	0
10	F	689	0	715	29	0
11	G	1351	0	1358	63	0
12	H	1205	0	1168	35	0
13	I	942	0	871	43	0
14	J	533	0	554	12	0
15	K	928	0	953	23	0
16	L	388	0	394	10	0
17	M	930	0	888	76	0
18	N	806	0	818	60	0
19	O	2018	0	2061	80	0
20	P	1462	0	1549	118	0
21	Q	1520	0	1520	110	0
22	R	1357	0	1381	86	0
23	S	1059	0	1036	65	0
24	T	1788	0	1819	119	0
25	U	1321	0	716	44	0
26	V	1300	0	718	49	0
27	W	4645	0	4692	485	0
28	X	6109	0	6137	223	0
29	Y	1631	0	1532	267	0
30	Z	3473	0	3511	450	0
31	a	2580	0	2550	147	0
32	b	2065	0	2096	302	0
33	c	522	0	526	173	0
34	d	2104	0	1946	37	0
35	e	2376	0	2402	109	0
36	f	2293	0	2315	65	0
37	g	1035	0	1023	84	0
38	h	1230	0	1236	106	0
39	i	863	0	869	116	0
40	j	4005	0	4053	659	0
41	k	1484	0	1488	142	0
42	l	1425	0	1409	159	0
43	m	1024	0	1000	260	0
44	n	2279	0	2285	206	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	o	887	0	880	103	0
46	p	893	0	900	99	0
47	q	1007	0	1044	172	0
48	r	8174	0	8275	803	0
49	s	1084	0	1118	231	0
50	t	975	0	1005	284	0
51	u	501	0	530	56	0
52	v	1067	0	1080	307	0
53	w	309	0	309	82	0
54	x	852	0	842	255	0
55	y	1003	0	991	311	0
56	z	1168	0	1162	233	0
57	A	2	0	0	0	0
58	A	2	0	0	0	0
58	B	1	0	0	0	0
58	C	1	0	0	0	0
58	I	2	0	0	0	0
58	J	1	0	0	0	0
58	L	1	0	0	0	0
58	O	1	0	0	0	0
58	Q	1	0	0	0	0
58	a	3	0	0	0	0
58	b	1	0	0	0	0
58	d	2	0	0	0	0
59	X	8	0	0	0	0
All	All	129277	0	128692	8213	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 32.

All (8213) 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)
30:Z:57:MET:HG2	32:b:51:MET:SD	1.28	1.71
27:W:85:PHE:HZ	30:Z:336:TYR:CD2	1.07	1.67
27:W:520:ARG:HA	33:c:22:TYR:CE1	1.19	1.64
27:W:85:PHE:CZ	30:Z:336:TYR:CD2	1.77	1.63
43:m:130:LEU:CB	47:q:160:MET:HE2	1.23	1.63
39:i:114:MET:CE	47:q:159:ILE:CD1	1.75	1.61
27:W:170:LEU:HD21	27:W:175:TYR:CD2	1.15	1.61
27:W:159:CYS:HA	27:W:163:TYR:CE2	1.34	1.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:85:PHE:HZ	30:Z:336:TYR:CE2	1.19	1.60
44:n:56:PHE:HZ	56:z:621:LEU:CD2	1.11	1.59
30:Z:38:PRO:HB3	30:Z:121:ALA:CB	1.14	1.58
43:m:123:ILE:HD11	47:q:163:LEU:CD1	1.17	1.57
27:W:85:PHE:CZ	30:Z:336:TYR:CE2	1.91	1.57
56:z:719:PRO:CB	56:z:742:GLN:HE21	1.08	1.57
43:m:140:SER:HB2	47:q:146:ASN:CB	1.34	1.56
30:Z:440:LEU:CD1	33:c:36:GLN:NE2	1.67	1.56
39:i:114:MET:HE1	47:q:159:ILE:CG1	1.33	1.56
40:j:392:MET:HG2	41:k:49:GLU:CD	1.22	1.55
43:m:123:ILE:CD1	47:q:163:LEU:HD11	1.10	1.55
27:W:129:VAL:CA	27:W:334:ARG:HH12	1.14	1.54
30:Z:408:LEU:CD1	33:c:44:PHE:CE2	1.84	1.54
27:W:112:HIS:HD2	30:Z:310:GLU:CG	1.21	1.54
40:j:479:ILE:HD13	40:j:529:MET:CE	1.28	1.54
30:Z:61:PHE:CG	32:b:228:LEU:HD13	1.04	1.53
48:r:230:PHE:CZ	48:r:296:LEU:CD1	1.91	1.52
21:Q:148:MET:CE	41:k:200:GLU:CG	1.85	1.52
30:Z:38:PRO:CB	30:Z:121:ALA:CB	1.84	1.52
30:Z:57:MET:HE3	32:b:51:MET:CG	1.38	1.52
30:Z:57:MET:CE	32:b:51:MET:HG2	1.28	1.51
27:W:473:GLU:CD	27:W:632:SER:HB3	1.30	1.51
30:Z:61:PHE:CG	32:b:228:LEU:CD1	1.85	1.50
43:m:130:LEU:CB	47:q:160:MET:CE	1.75	1.50
30:Z:440:LEU:CD2	33:c:36:GLN:NE2	1.74	1.50
1:0:812:ARG:CZ	46:p:90:ASN:HB3	1.39	1.50
30:Z:46:ARG:NH2	32:b:53:ARG:CB	1.70	1.50
30:Z:408:LEU:HD13	33:c:44:PHE:CE2	1.00	1.50
30:Z:122:LEU:HD21	32:b:50:PHE:CD1	1.42	1.49
56:z:697:HIS:HD2	56:z:705:HIS:CD2	1.27	1.49
8:D:141:GLN:CG	43:m:70:ARG:NH1	1.71	1.49
39:i:78:PRO:HG2	40:j:197:ARG:CD	1.38	1.49
5:A:1650:TYR:CZ	35:e:216:ASP:HA	1.46	1.48
28:X:591:GLY:CA	31:a:207:VAL:HG21	1.42	1.48
43:m:130:LEU:C	47:q:160:MET:CE	1.74	1.48
27:W:497:GLN:NE2	27:W:685:TYR:CE1	1.80	1.48
43:m:130:LEU:HB3	47:q:160:MET:CE	1.07	1.48
44:n:56:PHE:CZ	56:z:621:LEU:CD2	1.96	1.47
27:W:473:GLU:CG	27:W:632:SER:HB3	1.44	1.47
40:j:395:PRO:HD2	40:j:406:ARG:NH1	1.26	1.47
48:r:247:LEU:HD13	48:r:275:HIS:NE2	1.25	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:721:LEU:CD1	56:z:736:TRP:CZ2	1.98	1.46
27:W:109:ARG:NH1	27:W:492:ASN:HA	1.16	1.46
43:m:140:SER:HB2	47:q:146:ASN:CA	1.45	1.46
40:j:491:ILE:CD1	40:j:532:HIS:CA	1.94	1.45
27:W:112:HIS:CD2	30:Z:310:GLU:HG3	1.50	1.45
43:m:122:GLU:HB3	45:o:135:LYS:NZ	1.17	1.45
27:W:170:LEU:CD2	27:W:175:TYR:CD2	1.94	1.45
40:j:491:ILE:HD12	40:j:532:HIS:CB	1.44	1.45
30:Z:61:PHE:CD2	32:b:228:LEU:HD13	1.49	1.45
40:j:412:ALA:HB2	42:l:76:PHE:CZ	1.49	1.45
40:j:479:ILE:CD1	40:j:529:MET:HE1	1.43	1.45
27:W:175:TYR:HE1	27:W:459:GLN:CB	1.29	1.44
56:z:715:LEU:HB3	56:z:716:PRO:CD	1.44	1.44
27:W:175:TYR:HE1	27:W:459:GLN:CG	1.31	1.44
30:Z:408:LEU:CD1	33:c:44:PHE:HE2	1.20	1.44
30:Z:57:MET:CG	32:b:51:MET:SD	2.06	1.44
48:r:669:GLN:HE21	56:z:770:THR:CB	1.30	1.44
30:Z:433:PHE:CE1	33:c:42:HIS:CD2	2.05	1.43
29:Y:464:LEU:CD1	29:Y:513:ARG:NH1	1.78	1.43
30:Z:313:TYR:CZ	30:Z:390:GLN:HG2	1.53	1.43
48:r:230:PHE:CE2	48:r:296:LEU:HD22	1.51	1.43
48:r:1323:GLU:CG	48:r:1331:GLN:O	1.65	1.43
40:j:491:ILE:CD1	40:j:532:HIS:HA	1.48	1.42
8:D:141:GLN:HG3	43:m:70:ARG:CZ	1.46	1.42
21:Q:107:LEU:CD1	21:Q:111:ARG:HH12	1.29	1.41
40:j:491:ILE:CD1	40:j:532:HIS:HB2	1.46	1.41
56:z:721:LEU:HD13	56:z:736:TRP:CH2	1.53	1.41
27:W:159:CYS:HA	27:W:163:TYR:CZ	1.54	1.41
40:j:393:PRO:HB3	40:j:406:ARG:NH2	1.33	1.41
27:W:109:ARG:NH1	27:W:492:ASN:CA	1.82	1.40
40:j:198:LYS:HB2	43:m:88:LEU:CD2	1.47	1.40
21:Q:107:LEU:HD13	21:Q:111:ARG:NH1	1.32	1.40
39:i:114:MET:CE	47:q:159:ILE:CG1	1.92	1.40
48:r:669:GLN:HG2	56:z:770:THR:CG2	1.50	1.40
27:W:159:CYS:CA	27:W:163:TYR:CE2	2.05	1.40
27:W:342:CYS:SG	27:W:638:GLN:HA	1.60	1.40
43:m:130:LEU:C	47:q:160:MET:HE1	0.98	1.39
43:m:133:GLU:OE2	45:o:125:LYS:CE	1.71	1.39
21:Q:148:MET:CE	41:k:200:GLU:HG2	0.92	1.38
56:z:697:HIS:CD2	56:z:705:HIS:CD2	2.11	1.38
27:W:129:VAL:HA	27:W:334:ARG:NH1	1.32	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:715:LEU:CB	56:z:716:PRO:CD	2.00	1.38
27:W:129:VAL:CA	27:W:334:ARG:NH1	1.81	1.38
1:0:13:MET:CE	1:0:405:PHE:HB2	1.53	1.38
44:n:49:GLU:OE1	56:z:629:ILE:CG2	1.71	1.38
27:W:520:ARG:CA	33:c:22:TYR:HE1	1.36	1.38
29:Y:514:ARG:HE	29:Y:522:VAL:CG2	1.05	1.38
39:i:114:MET:HE3	47:q:159:ILE:CD1	1.39	1.38
27:W:175:TYR:CE1	27:W:459:GLN:HG2	1.57	1.37
39:i:114:MET:CE	47:q:159:ILE:HG13	1.49	1.37
1:0:671:SER:OG	46:p:88:ILE:CD1	1.72	1.37
28:X:193:PHE:CZ	28:X:302:ASP:OD1	1.75	1.37
29:Y:372:ILE:HG21	31:a:54:ARG:CZ	1.53	1.37
40:j:491:ILE:HD11	40:j:532:HIS:CA	1.49	1.37
27:W:274:GLN:HA	27:W:459:GLN:NE2	1.39	1.36
30:Z:313:TYR:OH	30:Z:390:GLN:CG	1.73	1.36
39:i:78:PRO:CG	40:j:197:ARG:HD2	1.55	1.36
28:X:591:GLY:N	31:a:207:VAL:HG21	1.09	1.36
42:l:30:MET:CE	48:r:521:GLN:HE22	1.39	1.36
27:W:85:PHE:CZ	30:Z:336:TYR:CG	2.11	1.35
1:0:640:ARG:CG	1:0:641:PRO:HD2	1.57	1.35
43:m:130:LEU:CA	47:q:160:MET:CE	2.05	1.35
29:Y:464:LEU:CG	29:Y:513:ARG:HH12	1.40	1.35
30:Z:46:ARG:CZ	32:b:53:ARG:HB2	1.55	1.34
30:Z:57:MET:SD	32:b:51:MET:HG2	1.65	1.34
1:0:812:ARG:NH2	46:p:90:ASN:HB3	1.43	1.33
8:D:70:ARG:HG3	43:m:20:LYS:CE	1.56	1.33
29:Y:513:ARG:O	29:Y:516:TYR:CD2	1.80	1.33
40:j:396:ALA:CB	41:k:73:ARG:HH21	1.42	1.33
8:D:78:GLU:OE1	38:h:51:LEU:CB	1.75	1.33
8:D:142:TYR:HD2	43:m:24:ASP:C	1.12	1.33
39:i:114:MET:SD	47:q:155:GLN:HB3	1.69	1.33
27:W:175:TYR:CE1	27:W:459:GLN:CB	2.13	1.32
56:z:715:LEU:CB	56:z:716:PRO:HD2	1.52	1.32
48:r:669:GLN:CG	56:z:770:THR:HG21	1.58	1.32
39:i:114:MET:CG	47:q:155:GLN:HB3	1.58	1.31
29:Y:524:HIS:CG	31:a:270:SER:HB3	1.65	1.31
39:i:114:MET:O	47:q:152:LYS:NZ	1.64	1.31
43:m:140:SER:CB	47:q:146:ASN:CG	2.03	1.31
27:W:112:HIS:CD2	30:Z:310:GLU:CG	2.06	1.31
40:j:412:ALA:CB	42:l:76:PHE:HZ	1.40	1.31
30:Z:61:PHE:CD1	32:b:228:LEU:CD1	2.12	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:491:ILE:CD1	40:j:532:HIS:CB	1.99	1.31
40:j:609:VAL:CG1	56:z:682:VAL:HG11	1.61	1.31
30:Z:57:MET:CE	32:b:51:MET:CG	2.00	1.30
43:m:140:SER:HB3	47:q:146:ASN:OD1	1.13	1.30
43:m:140:SER:CB	47:q:146:ASN:OD1	1.79	1.30
27:W:295:TYR:O	27:W:332:ARG:HD2	1.31	1.30
48:r:674:GLU:OE2	48:r:681:ALA:CB	1.77	1.30
31:a:260:ALA:HB1	31:a:264:ASP:OD1	1.31	1.30
40:j:197:ARG:NE	40:j:204:LEU:HD21	1.43	1.30
8:D:142:TYR:OH	43:m:21:ARG:HA	1.12	1.29
27:W:172:HIS:HA	27:W:434:GLU:CD	1.55	1.29
27:W:520:ARG:CA	33:c:22:TYR:CE1	2.09	1.29
53:w:92:ALA:O	53:w:96:PHE:HB2	1.28	1.29
27:W:292:LEU:CD2	27:W:294:GLU:OE2	1.80	1.29
30:Z:46:ARG:NH2	32:b:53:ARG:HB2	0.97	1.29
40:j:197:ARG:HE	40:j:204:LEU:CD2	1.43	1.29
28:X:309:VAL:CG2	28:X:402:ASN:HD21	1.45	1.29
27:W:278:GLU:OE2	27:W:452:ARG:HA	1.31	1.29
48:r:230:PHE:CE2	48:r:296:LEU:HD13	1.66	1.29
28:X:591:GLY:N	31:a:207:VAL:CG2	1.94	1.28
48:r:247:LEU:CD1	48:r:275:HIS:NE2	1.94	1.28
27:W:106:PRO:HD2	27:W:490:GLU:OE1	1.28	1.28
56:z:721:LEU:HD11	56:z:736:TRP:CE2	1.67	1.28
8:D:142:TYR:CD2	43:m:24:ASP:C	1.91	1.28
30:Z:57:MET:HG2	32:b:51:MET:CE	1.62	1.28
27:W:175:TYR:CZ	27:W:459:GLN:HA	1.68	1.28
30:Z:57:MET:SD	32:b:51:MET:CG	2.21	1.28
48:r:230:PHE:CZ	48:r:296:LEU:HD13	1.60	1.28
27:W:175:TYR:CE1	27:W:459:GLN:CG	2.13	1.27
30:Z:313:TYR:OH	30:Z:390:GLN:HG2	1.13	1.27
21:Q:148:MET:HE3	41:k:200:GLU:CG	1.52	1.27
28:X:591:GLY:H	31:a:207:VAL:CG2	1.44	1.27
40:j:392:MET:CG	41:k:49:GLU:OE1	1.83	1.27
27:W:85:PHE:CE2	30:Z:336:TYR:CG	2.22	1.27
27:W:292:LEU:HD21	27:W:294:GLU:OE2	1.34	1.27
30:Z:403:PHE:CE2	33:c:54:GLN:OE1	1.85	1.27
48:r:202:ARG:HD3	48:r:243:VAL:N	1.45	1.26
52:v:126:SER:O	52:v:130:GLU:HB2	1.30	1.26
40:j:392:MET:SD	41:k:49:GLU:OE2	1.94	1.26
27:W:124:TYR:OH	27:W:292:LEU:CA	1.83	1.26
40:j:479:ILE:CD1	40:j:529:MET:CE	2.01	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1625:THR:O	55:y:39:GLN:HG2	1.30	1.25
30:Z:57:MET:HG2	32:b:51:MET:CG	1.66	1.25
30:Z:122:LEU:CD2	32:b:104:LEU:CD1	2.13	1.25
48:r:1320:MET:HE1	48:r:1333:LYS:CB	1.65	1.25
30:Z:122:LEU:HD21	32:b:50:PHE:CE1	1.71	1.25
40:j:197:ARG:NE	40:j:204:LEU:CD2	1.98	1.25
40:j:396:ALA:CB	41:k:73:ARG:NH2	1.98	1.25
1:0:795:CYS:O	1:0:836:VAL:HG23	1.31	1.24
29:Y:513:ARG:O	29:Y:516:TYR:HD2	1.09	1.24
48:r:230:PHE:CE2	48:r:296:LEU:CD2	2.20	1.24
43:m:130:LEU:O	47:q:160:MET:HE1	1.35	1.24
43:m:140:SER:CB	47:q:146:ASN:CB	2.16	1.24
48:r:1323:GLU:HG2	48:r:1331:GLN:O	1.08	1.24
8:D:78:GLU:OE1	38:h:51:LEU:HB2	1.10	1.24
27:W:351:VAL:HG22	27:W:378:PHE:CD1	1.72	1.24
27:W:471:VAL:HB	27:W:634:ARG:NE	1.53	1.24
46:p:110:TYR:HD2	56:z:649:ILE:CD1	1.51	1.24
5:A:1622:TYR:OH	37:g:118:ARG:NH1	1.67	1.23
30:Z:57:MET:HE3	32:b:51:MET:CB	1.67	1.23
43:m:115:LYS:HD3	45:o:143:LEU:CD1	1.68	1.23
1:0:74:HIS:CB	1:0:116:ASN:OD1	1.86	1.23
39:i:78:PRO:HB3	40:j:197:ARG:CB	1.69	1.23
5:A:1629:TYR:O	37:g:13:ILE:CD1	1.86	1.23
30:Z:440:LEU:CG	33:c:36:GLN:NE2	2.01	1.23
48:r:230:PHE:CZ	48:r:296:LEU:HD11	1.65	1.23
46:p:103:ASP:OD1	48:r:944:PHE:CD2	1.75	1.23
40:j:415:LYS:HD2	42:l:116:ARG:NH1	1.53	1.22
27:W:125:ALA:CB	27:W:486:PRO:HB2	1.67	1.22
27:W:473:GLU:CD	27:W:632:SER:CB	2.13	1.22
28:X:311:PRO:HG3	28:X:410:TYR:OH	1.35	1.22
28:X:297:ALA:HA	28:X:300:GLU:CD	1.61	1.22
30:Z:38:PRO:CB	30:Z:121:ALA:HB2	1.55	1.22
40:j:607:SER:OG	56:z:691:VAL:O	1.54	1.22
27:W:274:GLN:CA	27:W:459:GLN:NE2	2.00	1.22
40:j:392:MET:HG2	41:k:49:GLU:OE1	1.05	1.22
42:l:121:ASP:OD2	44:n:237:GLN:N	1.72	1.22
30:Z:122:LEU:CG	32:b:50:PHE:CE1	2.23	1.21
30:Z:403:PHE:CD2	33:c:54:GLN:OE1	1.91	1.21
56:z:719:PRO:CB	56:z:742:GLN:NE2	1.76	1.21
29:Y:504:LYS:O	29:Y:507:PRO:CD	1.88	1.21
56:z:721:LEU:HD13	56:z:736:TRP:CZ2	1.63	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:142:TYR:CD2	43:m:25:ASP:N	2.07	1.21
27:W:469:THR:CG2	27:W:634:ARG:NH1	1.72	1.21
29:Y:372:ILE:CG2	31:a:54:ARG:CZ	2.16	1.21
48:r:222:VAL:HG21	48:r:234:LEU:O	1.37	1.21
48:r:669:GLN:NE2	56:z:770:THR:HB	1.53	1.21
56:z:719:PRO:HB2	56:z:742:GLN:NE2	0.88	1.21
27:W:469:THR:CG2	27:W:634:ARG:HH11	1.21	1.21
40:j:191:ARG:HH12	40:j:203:ILE:CG2	1.52	1.21
55:y:116:GLN:OE1	55:y:119:LEU:HB2	1.38	1.21
27:W:129:VAL:N	27:W:334:ARG:NH1	1.90	1.20
30:Z:408:LEU:HD13	33:c:44:PHE:CZ	1.74	1.20
31:a:257:HIS:ND1	32:b:248:HIS:HE1	1.36	1.20
40:j:392:MET:CG	41:k:49:GLU:CD	2.12	1.20
27:W:473:GLU:OE2	27:W:632:SER:CB	1.89	1.20
28:X:193:PHE:HZ	28:X:302:ASP:OD1	1.04	1.20
56:z:697:HIS:HD2	56:z:705:HIS:NE2	1.38	1.20
30:Z:401:LEU:HD11	33:c:57:VAL:CG1	1.69	1.20
8:D:141:GLN:HG3	43:m:70:ARG:NH1	0.88	1.20
52:v:101:THR:O	52:v:105:PHE:HB2	1.41	1.20
27:W:473:GLU:OE2	27:W:632:SER:CA	1.90	1.20
43:m:134:TYR:OH	47:q:157:LYS:HD2	1.39	1.20
30:Z:41:CYS:SG	30:Z:114:PHE:CE1	2.35	1.19
44:n:56:PHE:HZ	56:z:621:LEU:HD22	1.05	1.19
48:r:233:THR:O	48:r:248:LEU:CB	1.88	1.19
39:i:114:MET:SD	47:q:155:GLN:C	2.24	1.19
42:l:30:MET:HE3	48:r:521:GLN:NE2	1.58	1.19
43:m:133:GLU:OE2	45:o:125:LYS:HE3	1.09	1.19
56:z:702:GLY:O	56:z:727:ALA:HB2	1.42	1.19
27:W:124:TYR:OH	27:W:292:LEU:HA	1.04	1.19
27:W:125:ALA:HB2	27:W:486:PRO:CB	1.71	1.19
27:W:175:TYR:OH	27:W:459:GLN:HA	1.04	1.18
28:X:532:PRO:HG3	31:a:203:ALA:HB1	1.20	1.18
42:l:121:ASP:CG	44:n:237:GLN:H	1.49	1.18
48:r:233:THR:O	48:r:248:LEU:HB2	1.02	1.18
56:z:718:VAL:HB	56:z:719:PRO:CD	1.73	1.18
27:W:274:GLN:NE2	27:W:459:GLN:HG3	1.52	1.18
40:j:464:TRP:HA	40:j:475:VAL:HG23	1.26	1.18
1:O:812:ARG:NH2	46:p:90:ASN:CB	2.06	1.18
27:W:689:VAL:HB	30:Z:393:LEU:CD1	1.73	1.18
40:j:393:PRO:CB	40:j:406:ARG:HH22	1.56	1.18
5:A:1623:SER:OG	55:y:92:GLN:CG	1.91	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1650:TYR:OH	35:e:216:ASP:HA	1.44	1.17
30:Z:74:TRP:CZ2	32:b:229:TRP:CH2	2.31	1.17
27:W:85:PHE:CZ	30:Z:336:TYR:CZ	2.30	1.17
40:j:463:HIS:CD2	43:m:128:TYR:CE1	2.32	1.17
43:m:140:SER:HB2	47:q:146:ASN:CG	1.65	1.17
29:Y:414:TYR:CZ	32:b:115:ILE:HD11	1.80	1.17
29:Y:498:GLU:O	29:Y:502:VAL:HG23	1.42	1.17
28:X:310:LEU:HD22	28:X:409:THR:HG21	1.17	1.17
40:j:456:GLU:OE1	43:m:138:SER:C	1.88	1.17
30:Z:122:LEU:O	32:b:100:LYS:HG2	1.43	1.17
28:X:726:GLN:HE22	31:a:223:LEU:HD11	1.04	1.16
30:Z:57:MET:CG	32:b:51:MET:CG	2.22	1.16
30:Z:122:LEU:CD2	32:b:50:PHE:CE1	2.27	1.16
48:r:202:ARG:CD	48:r:243:VAL:N	2.07	1.16
27:W:165:LYS:HG3	27:W:181:HIS:NE2	1.60	1.16
29:Y:507:PRO:HD2	29:Y:508:PHE:H	1.10	1.16
27:W:112:HIS:HB2	30:Z:310:GLU:OE2	1.44	1.16
30:Z:46:ARG:HH22	32:b:53:ARG:CG	1.57	1.16
30:Z:58:ARG:CD	32:b:241:LEU:HD21	1.75	1.16
39:i:87:ARG:NH2	40:j:299:GLN:OE1	1.79	1.16
43:m:122:GLU:CB	45:o:135:LYS:NZ	2.08	1.16
1:0:74:HIS:HB2	1:0:116:ASN:OD1	1.01	1.15
3:2:915:ARG:NH2	56:z:701:ASN:HA	1.59	1.15
29:Y:414:TYR:CE2	32:b:115:ILE:HD11	1.79	1.15
30:Z:433:PHE:CE2	33:c:38:ILE:CD1	2.29	1.15
1:0:13:MET:HE1	1:0:405:PHE:HB2	1.19	1.15
30:Z:122:LEU:CD2	32:b:50:PHE:CD1	2.30	1.15
39:i:99:TYR:OH	40:j:366:ASP:OD2	1.64	1.15
40:j:392:MET:CG	41:k:49:GLU:OE2	1.94	1.15
40:j:396:ALA:HB3	41:k:73:ARG:HH21	0.99	1.15
48:r:233:THR:HG23	48:r:248:LEU:CB	1.77	1.15
30:Z:74:TRP:CH2	32:b:229:TRP:HH2	1.65	1.15
29:Y:464:LEU:HD11	29:Y:513:ARG:NH1	1.49	1.15
30:Z:401:LEU:HD11	33:c:57:VAL:HG11	1.19	1.15
8:D:142:TYR:HD2	43:m:25:ASP:N	1.38	1.15
27:W:109:ARG:HD3	27:W:492:ASN:OD1	1.45	1.15
27:W:351:VAL:HA	27:W:378:PHE:CE1	1.81	1.15
56:z:721:LEU:CD1	56:z:736:TRP:CH2	2.23	1.15
28:X:307:ASN:HB3	28:X:308:PRO:HD3	1.17	1.14
30:Z:58:ARG:NH1	32:b:241:LEU:CD2	2.10	1.14
40:j:198:LYS:CB	43:m:88:LEU:CD2	2.25	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:247:LEU:HD13	48:r:275:HIS:CD2	1.82	1.14
1:0:13:MET:HB3	1:0:456:ARG:O	1.47	1.14
1:0:640:ARG:HG3	1:0:641:PRO:CD	1.76	1.14
40:j:392:MET:HG2	41:k:49:GLU:OE2	1.46	1.14
43:m:134:TYR:CZ	47:q:157:LYS:HD2	1.81	1.14
46:p:110:TYR:CD2	56:z:649:ILE:CD1	2.29	1.14
1:0:640:ARG:CG	1:0:641:PRO:CD	2.25	1.14
1:0:812:ARG:HH12	46:p:92:GLN:HB2	1.06	1.14
27:W:85:PHE:CE1	30:Z:336:TYR:CE2	2.36	1.14
30:Z:46:ARG:NH2	32:b:53:ARG:CG	2.10	1.14
30:Z:440:LEU:HD22	33:c:36:GLN:NE2	1.55	1.14
40:j:414:ASP:O	42:l:70:GLU:O	1.64	1.14
20:P:218:LYS:CE	25:U:18:DG:OP1	1.95	1.14
30:Z:368:LEU:CB	30:Z:383:LEU:HD11	1.76	1.14
30:Z:440:LEU:HD13	33:c:38:ILE:HG22	1.22	1.14
40:j:412:ALA:HB3	42:l:186:PRO:HG2	1.23	1.14
43:m:138:SER:OG	47:q:150:LYS:CD	1.86	1.14
27:W:172:HIS:CA	27:W:434:GLU:OE2	1.96	1.13
46:p:71:LEU:CD2	56:z:617:LEU:HD11	1.77	1.13
29:Y:414:TYR:HB3	32:b:116:LYS:HE2	1.19	1.13
29:Y:475:PHE:CE2	29:Y:499:ARG:HG2	1.82	1.13
27:W:170:LEU:HD21	27:W:175:TYR:CE2	1.81	1.13
30:Z:74:TRP:CH2	32:b:229:TRP:CH2	2.37	1.13
8:D:70:ARG:CG	43:m:20:LYS:HE2	1.78	1.13
40:j:198:LYS:HG3	40:j:203:ILE:HD13	1.27	1.13
43:m:140:SER:HB2	47:q:146:ASN:HA	1.20	1.13
48:r:1367:LEU:O	48:r:1384:ILE:CB	1.95	1.13
27:W:105:GLU:HG2	27:W:487:LYS:NZ	1.62	1.13
29:Y:464:LEU:HG	29:Y:513:ARG:HH12	0.98	1.13
43:m:123:ILE:CG1	47:q:163:LEU:HD11	1.78	1.12
30:Z:61:PHE:CD1	32:b:228:LEU:HD13	1.79	1.12
40:j:487:ILE:HB	44:n:135:ARG:HA	1.14	1.12
44:n:49:GLU:OE1	56:z:629:ILE:HG21	0.95	1.12
46:p:110:TYR:HD2	56:z:649:ILE:HD11	1.06	1.12
27:W:274:GLN:CB	27:W:459:GLN:NE2	2.08	1.12
30:Z:57:MET:HE3	32:b:51:MET:CA	1.80	1.12
31:a:257:HIS:ND1	32:b:248:HIS:CE1	2.17	1.12
31:a:374:PHE:CZ	32:b:141:LEU:HB3	1.85	1.12
40:j:463:HIS:CD2	43:m:128:TYR:HE1	1.65	1.12
48:r:202:ARG:CG	48:r:243:VAL:N	2.12	1.12
48:r:799:GLU:HG3	48:r:816:LYS:HE3	1.17	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:718:VAL:HB	56:z:719:PRO:HD2	1.28	1.12
27:W:473:GLU:HG3	27:W:632:SER:HB3	1.24	1.11
29:Y:524:HIS:CD2	31:a:270:SER:CB	2.33	1.11
40:j:415:LYS:NZ	42:l:123:LEU:HD12	1.62	1.11
27:W:121:TYR:CZ	27:W:486:PRO:HA	1.85	1.11
27:W:175:TYR:OH	27:W:459:GLN:CA	1.98	1.11
28:X:591:GLY:HA2	31:a:207:VAL:HG21	1.32	1.11
30:Z:45:PHE:HE2	32:b:51:MET:O	1.32	1.11
40:j:191:ARG:HG2	40:j:196:LEU:HD13	1.15	1.11
40:j:396:ALA:HB2	41:k:51:PHE:HE1	1.12	1.11
48:r:1323:GLU:CD	48:r:1331:GLN:O	1.93	1.11
27:W:171:LYS:HA	27:W:461:HIS:CE1	1.83	1.11
28:X:309:VAL:HG23	28:X:402:ASN:ND2	1.65	1.11
27:W:351:VAL:HA	27:W:378:PHE:HE1	0.96	1.11
39:i:114:MET:CE	47:q:159:ILE:HD12	1.76	1.11
40:j:410:PRO:O	42:l:86:ILE:HB	1.50	1.11
27:W:503:ALA:CB	27:W:646:ALA:HB2	1.80	1.11
40:j:394:HIS:CG	41:k:78:ARG:HG3	1.85	1.11
40:j:191:ARG:NH2	40:j:196:LEU:HB2	1.65	1.10
40:j:395:PRO:CD	40:j:406:ARG:NH1	2.13	1.10
46:p:110:TYR:CD2	56:z:649:ILE:HD11	1.86	1.10
48:r:230:PHE:HE2	48:r:296:LEU:CD2	1.61	1.10
27:W:85:PHE:HZ	30:Z:336:TYR:CG	1.58	1.10
27:W:274:GLN:HE22	27:W:459:GLN:HG3	1.03	1.10
35:e:164:SER:OG	35:e:167:ARG:HD3	1.51	1.10
40:j:449:ASP:HB2	47:q:157:LYS:NZ	1.66	1.10
1:0:13:MET:HE2	1:0:405:PHE:HB2	1.31	1.10
40:j:190:LEU:HG	40:j:194:TRP:CZ3	1.85	1.10
40:j:396:ALA:HB1	41:k:73:ARG:NH2	1.64	1.10
40:j:492:GLN:HE21	40:j:507:ARG:HD3	1.07	1.10
44:n:56:PHE:CZ	56:z:621:LEU:HD21	1.70	1.10
39:i:114:MET:SD	47:q:155:GLN:CB	2.40	1.10
39:i:114:MET:HG2	47:q:155:GLN:HB3	1.20	1.10
20:P:167:ASN:HD21	26:V:79:DT:H1'	1.04	1.09
27:W:351:VAL:CA	27:W:378:PHE:HE1	1.65	1.09
27:W:503:ALA:HB2	27:W:646:ALA:HB2	1.26	1.09
29:Y:504:LYS:O	29:Y:507:PRO:HD2	1.48	1.09
43:m:115:LYS:HD3	45:o:143:LEU:HD12	1.12	1.09
27:W:172:HIS:HA	27:W:434:GLU:OE2	1.46	1.09
27:W:689:VAL:HG12	30:Z:393:LEU:HD11	1.34	1.09
30:Z:57:MET:CB	32:b:51:MET:HE3	1.82	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:135:ARG:HD2	50:t:109:LEU:HD22	1.33	1.09
48:r:201:HIS:NE2	49:s:111:GLN:HG3	1.66	1.09
30:Z:57:MET:CG	32:b:51:MET:HG2	1.79	1.09
48:r:669:GLN:CG	56:z:770:THR:CG2	2.24	1.09
30:Z:38:PRO:CB	30:Z:121:ALA:HB1	1.59	1.09
40:j:608:ASP:HB3	56:z:693:LEU:HD21	1.30	1.09
27:W:520:ARG:HA	33:c:22:TYR:CD1	1.86	1.09
30:Z:440:LEU:HD11	33:c:36:GLN:NE2	1.66	1.09
30:Z:442:VAL:HG21	33:c:9:LEU:HD13	1.34	1.09
40:j:394:HIS:ND1	41:k:78:ARG:CG	2.15	1.09
8:D:142:TYR:OH	43:m:21:ARG:CA	2.00	1.08
27:W:471:VAL:CB	27:W:634:ARG:HE	1.65	1.08
29:Y:374:LEU:HD13	32:b:270:VAL:CG1	1.81	1.08
29:Y:504:LYS:O	29:Y:508:PHE:CD2	2.06	1.08
44:n:53:ILE:HD11	56:z:629:ILE:HD13	1.28	1.08
48:r:202:ARG:HB3	48:r:243:VAL:N	1.66	1.08
5:A:1619:SER:CB	5:A:1620:PRO:HD2	1.77	1.08
27:W:128:SER:C	27:W:334:ARG:CZ	2.26	1.08
27:W:175:TYR:CE1	27:W:459:GLN:HB3	1.86	1.08
54:x:15:LEU:HD11	54:x:72:LEU:HD11	1.34	1.08
21:Q:107:LEU:CD1	21:Q:111:ARG:NH1	1.99	1.08
27:W:109:ARG:HD3	27:W:492:ASN:CG	1.76	1.08
27:W:167:LYS:HG2	27:W:294:GLU:HG3	1.35	1.08
27:W:689:VAL:CB	30:Z:393:LEU:HD12	1.83	1.08
40:j:410:PRO:O	42:l:86:ILE:CB	2.01	1.08
43:m:140:SER:CB	47:q:146:ASN:HA	1.82	1.08
48:r:669:GLN:OE1	48:r:683:ARG:HD3	1.50	1.08
5:A:1625:THR:O	55:y:39:GLN:CG	2.02	1.08
30:Z:440:LEU:CD1	33:c:38:ILE:HG22	1.83	1.08
1:O:640:ARG:HG3	1:O:641:PRO:HD3	1.35	1.08
27:W:342:CYS:SG	27:W:638:GLN:CA	2.41	1.08
27:W:351:VAL:HG13	27:W:378:PHE:CE1	1.88	1.08
28:X:591:GLY:CA	31:a:207:VAL:CG2	2.30	1.08
30:Z:58:ARG:HD3	32:b:241:LEU:HD21	1.32	1.08
40:j:608:ASP:CB	56:z:693:LEU:HD21	1.82	1.08
27:W:473:GLU:OE2	27:W:632:SER:HA	1.49	1.07
28:X:309:VAL:CG2	28:X:402:ASN:ND2	2.17	1.07
30:Z:440:LEU:HD13	33:c:36:GLN:NE2	1.48	1.07
31:a:294:CYS:HB3	31:a:308:CYS:SG	1.93	1.07
40:j:393:PRO:HG2	41:k:137:ARG:NH2	1.69	1.07
40:j:398:ALA:H	41:k:84:HIS:CE1	1.72	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:55:GLU:HG2	41:k:73:ARG:HG2	1.32	1.07
43:m:131:GLU:N	47:q:160:MET:HE1	1.69	1.07
27:W:105:GLU:HA	27:W:487:LYS:HZ1	1.15	1.07
27:W:274:GLN:CB	27:W:459:GLN:HE22	1.65	1.07
27:W:278:GLU:OE2	27:W:452:ARG:CA	2.03	1.07
30:Z:63:GLU:OE2	30:Z:115:ARG:NH2	1.87	1.07
30:Z:401:LEU:CA	33:c:16:MET:HE1	1.82	1.07
31:a:292:PRO:HB2	32:b:264:ILE:HG13	1.26	1.07
39:i:78:PRO:HB3	40:j:197:ARG:HB3	1.34	1.07
40:j:191:ARG:NH1	40:j:203:ILE:HG23	1.70	1.07
48:r:674:GLU:OE2	48:r:681:ALA:HB2	1.50	1.07
5:A:1650:TYR:OH	35:e:216:ASP:CA	2.02	1.07
29:Y:372:ILE:O	31:a:54:ARG:HG3	1.52	1.07
40:j:608:ASP:HB2	56:z:693:LEU:CD2	1.84	1.06
48:r:669:GLN:NE2	56:z:770:THR:CB	2.12	1.06
5:A:1657:TYR:OH	35:e:157:GLY:O	1.73	1.06
28:X:297:ALA:HA	28:X:300:GLU:OE2	1.52	1.06
30:Z:122:LEU:HG	32:b:50:PHE:CE1	1.86	1.06
20:P:167:ASN:ND2	26:V:79:DT:H1'	1.69	1.06
28:X:591:GLY:HA2	31:a:207:VAL:CG2	1.86	1.06
30:Z:61:PHE:CD1	32:b:228:LEU:HD11	1.87	1.06
56:z:697:HIS:CD2	56:z:705:HIS:NE2	2.20	1.06
1:0:790:CYS:HB3	44:n:41:ASN:HB2	1.31	1.06
27:W:292:LEU:CG	27:W:294:GLU:OE2	2.03	1.06
27:W:473:GLU:HG3	27:W:632:SER:CB	1.85	1.06
44:n:53:ILE:HD11	56:z:629:ILE:CD1	1.84	1.06
39:i:114:MET:HE1	47:q:159:ILE:CD1	1.60	1.06
50:t:81:LEU:O	50:t:84:SER:OG	1.71	1.06
54:x:14:SER:OG	54:x:68:ASP:OD2	1.73	1.06
1:0:640:ARG:HG2	1:0:641:PRO:HD2	1.31	1.05
28:X:309:VAL:HG23	28:X:402:ASN:HD21	0.90	1.05
4:3:85:HIS:CD2	4:3:97:TRP:CE3	2.44	1.05
5:A:1619:SER:HB3	5:A:1620:PRO:HD2	1.07	1.05
40:j:198:LYS:HB2	43:m:88:LEU:HD23	1.16	1.05
42:l:30:MET:CE	48:r:521:GLN:NE2	2.14	1.05
1:0:792:THR:HG22	44:n:41:ASN:HA	1.29	1.05
5:A:1629:TYR:C	37:g:13:ILE:HD12	1.82	1.05
28:X:293:ARG:HH12	28:X:378:ARG:N	1.54	1.05
29:Y:514:ARG:NE	29:Y:522:VAL:HG23	0.98	1.05
40:j:609:VAL:HG11	56:z:682:VAL:HG11	1.37	1.05
1:0:13:MET:N	1:0:13:MET:SD	2.30	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1622:TYR:CE2	38:h:107:ASP:OD1	2.09	1.05
5:A:1650:TYR:CE1	35:e:216:ASP:HA	1.91	1.05
40:j:393:PRO:CB	40:j:406:ARG:NH2	2.14	1.05
43:m:130:LEU:HB2	47:q:160:MET:HE2	1.36	1.05
21:Q:148:MET:HE1	41:k:200:GLU:CG	1.64	1.05
27:W:158:LEU:O	27:W:163:TYR:OH	1.73	1.05
27:W:173:ASN:ND2	27:W:434:GLU:HA	1.72	1.05
27:W:318:PRO:HD2	27:W:501:TYR:OH	1.57	1.05
27:W:112:HIS:CB	30:Z:310:GLU:OE2	2.05	1.04
27:W:129:VAL:N	27:W:334:ARG:CZ	2.20	1.04
27:W:159:CYS:O	27:W:163:TYR:CD2	2.10	1.04
27:W:278:GLU:CD	27:W:452:ARG:HG2	1.82	1.04
28:X:216:LYS:HD3	28:X:309:VAL:HG22	1.06	1.04
30:Z:440:LEU:CD1	33:c:36:GLN:CD	2.29	1.04
43:m:115:LYS:CD	45:o:146:ILE:HD12	1.87	1.04
43:m:122:GLU:CB	45:o:135:LYS:HZ1	1.65	1.04
5:A:1622:TYR:CD2	38:h:107:ASP:OD1	2.10	1.04
27:W:473:GLU:CG	27:W:632:SER:CB	2.34	1.04
30:Z:122:LEU:HD23	32:b:104:LEU:HD12	1.38	1.04
43:m:123:ILE:HD11	47:q:163:LEU:HD13	1.39	1.04
48:r:230:PHE:CE2	48:r:296:LEU:CD1	2.31	1.04
11:G:125:PRO:HG3	38:h:168:PRO:HD2	1.35	1.04
30:Z:58:ARG:CZ	32:b:241:LEU:CD2	2.33	1.04
1:O:792:THR:HG22	44:n:41:ASN:CA	1.81	1.04
27:W:511:TRP:CZ3	30:Z:397:GLU:OE2	2.09	1.04
30:Z:122:LEU:HD23	32:b:104:LEU:CD1	1.88	1.04
53:w:103:GLU:N	53:w:106:SER:HG	1.55	1.04
54:x:60:ALA:O	54:x:63:ALA:N	1.91	1.04
1:O:671:SER:OG	46:p:88:ILE:HD11	0.86	1.04
27:W:85:PHE:HZ	30:Z:336:TYR:CZ	1.72	1.04
39:i:78:PRO:CB	40:j:197:ARG:CB	2.36	1.04
40:j:415:LYS:NZ	42:l:123:LEU:CD1	2.20	1.04
27:W:274:GLN:CA	27:W:459:GLN:HE22	1.63	1.03
30:Z:433:PHE:HE2	33:c:38:ILE:CD1	1.64	1.03
43:m:115:LYS:CD	45:o:143:LEU:HD12	1.88	1.03
48:r:199:LEU:HD11	48:r:222:VAL:HG13	1.06	1.03
27:W:109:ARG:O	27:W:494:MET:SD	2.15	1.03
28:X:305:LEU:HD21	28:X:391:LEU:HD12	1.37	1.03
30:Z:440:LEU:HD11	33:c:36:GLN:CD	1.84	1.03
42:l:120:CYS:SG	44:n:291:GLY:HA3	1.97	1.03
27:W:85:PHE:CZ	30:Z:336:TYR:CD1	2.46	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:471:VAL:O	27:W:634:ARG:HD2	1.59	1.03
27:W:511:TRP:HZ3	30:Z:397:GLU:OE2	1.39	1.03
28:X:305:LEU:HD21	28:X:391:LEU:CD1	1.89	1.03
39:i:114:MET:CE	47:q:159:ILE:HD11	1.60	1.03
30:Z:58:ARG:NH1	32:b:241:LEU:HD23	1.71	1.02
30:Z:122:LEU:HD22	32:b:104:LEU:HD13	1.39	1.02
30:Z:401:LEU:HA	33:c:16:MET:HE1	1.03	1.02
30:Z:433:PHE:CD1	33:c:42:HIS:CD2	2.46	1.02
43:m:130:LEU:HB3	47:q:160:MET:HE3	1.07	1.02
44:n:306:HIS:HE2	44:n:309:CYS:HG	1.05	1.02
20:P:218:LYS:NZ	25:U:18:DG:OP1	1.93	1.02
30:Z:38:PRO:HB3	30:Z:121:ALA:HB3	1.37	1.02
30:Z:38:PRO:CG	30:Z:121:ALA:CB	2.37	1.02
30:Z:41:CYS:SG	30:Z:114:PHE:CD1	2.51	1.02
48:r:669:GLN:HE21	56:z:770:THR:CG2	1.72	1.02
4:3:125:PHE:CE2	4:3:178:ILE:HD12	1.93	1.02
27:W:112:HIS:CD2	30:Z:310:GLU:HG2	1.95	1.02
28:X:311:PRO:CG	28:X:410:TYR:OH	2.07	1.02
30:Z:74:TRP:CZ2	32:b:229:TRP:HH2	1.72	1.02
5:A:1629:TYR:O	37:g:13:ILE:HD12	1.56	1.02
5:A:1650:TYR:CE2	35:e:215:GLY:O	2.12	1.02
27:W:342:CYS:SG	27:W:638:GLN:HG3	1.99	1.02
29:Y:374:LEU:CD1	32:b:270:VAL:CG1	2.36	1.02
56:z:715:LEU:CD1	56:z:716:PRO:HD3	1.89	1.02
27:W:77:TRP:HB3	30:Z:338:PHE:CE2	1.95	1.02
30:Z:58:ARG:CZ	32:b:241:LEU:HD21	1.89	1.02
40:j:608:ASP:CB	56:z:693:LEU:CD2	2.37	1.02
48:r:233:THR:HG23	48:r:248:LEU:HB3	1.36	1.02
30:Z:368:LEU:HB2	30:Z:383:LEU:HD11	1.02	1.01
40:j:191:ARG:NH1	40:j:203:ILE:CG2	2.23	1.01
48:r:202:ARG:CB	48:r:243:VAL:N	2.23	1.01
55:y:91:ALA:O	55:y:94:ALA:N	1.93	1.01
28:X:305:LEU:HD11	28:X:391:LEU:HD13	1.41	1.01
29:Y:372:ILE:HG22	31:a:54:ARG:NE	1.75	1.01
40:j:197:ARG:HE	40:j:204:LEU:HD21	0.93	1.01
40:j:396:ALA:HB3	41:k:73:ARG:NH2	1.63	1.01
40:j:598:ARG:HH12	56:z:683:ALA:HA	1.23	1.01
1:0:812:ARG:CZ	46:p:90:ASN:CB	2.36	1.01
27:W:170:LEU:CD2	27:W:175:TYR:CE2	2.38	1.01
27:W:170:LEU:HD13	27:W:460:ALA:O	1.60	1.01
27:W:689:VAL:CB	30:Z:393:LEU:CD1	2.38	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:99:GLU:O	2:1:103:ASN:HB2	1.60	1.01
5:A:1650:TYR:CZ	35:e:216:ASP:CA	2.41	1.01
27:W:85:PHE:CD2	30:Z:338:PHE:CZ	2.48	1.01
40:j:415:LYS:HD2	42:l:116:ARG:HH12	1.25	1.01
29:Y:514:ARG:HE	29:Y:522:VAL:HG21	1.21	1.01
30:Z:297:ALA:O	30:Z:382:VAL:HG11	1.61	1.01
30:Z:433:PHE:HE2	33:c:38:ILE:HD12	1.25	1.01
46:p:85:ASN:HD22	56:z:641:THR:HG22	1.26	1.01
52:v:126:SER:O	52:v:130:GLU:CB	2.08	1.01
8:D:142:TYR:CZ	43:m:21:ARG:HA	1.95	1.00
27:W:129:VAL:N	27:W:334:ARG:HH12	1.53	1.00
30:Z:46:ARG:HH22	32:b:53:ARG:CD	1.74	1.00
40:j:191:ARG:HH12	40:j:203:ILE:HG23	0.85	1.00
48:r:1387:ILE:O	48:r:1396:THR:O	1.79	1.00
55:y:36:PHE:O	55:y:40:ARG:HB2	1.61	1.00
55:y:38:ALA:O	55:y:41:GLY:N	1.94	1.00
28:X:216:LYS:HD3	28:X:309:VAL:CG2	1.90	1.00
39:i:114:MET:SD	47:q:155:GLN:O	2.20	1.00
40:j:392:MET:SD	41:k:137:ARG:HD2	2.00	1.00
46:p:85:ASN:HD22	56:z:641:THR:CG2	1.74	1.00
48:r:230:PHE:CZ	48:r:296:LEU:CD2	2.44	1.00
27:W:124:TYR:CZ	27:W:292:LEU:HA	1.97	1.00
27:W:167:LYS:CG	27:W:294:GLU:HG3	1.92	1.00
29:Y:414:TYR:HB3	32:b:116:LYS:CE	1.89	1.00
29:Y:464:LEU:HG	29:Y:513:ARG:NH1	1.70	1.00
29:Y:524:HIS:CD2	31:a:270:SER:HB3	1.93	1.00
40:j:395:PRO:CD	40:j:406:ARG:HH12	1.70	1.00
43:m:115:LYS:CG	45:o:146:ILE:HD12	1.89	1.00
46:p:71:LEU:HD23	56:z:617:LEU:CD1	1.92	1.00
48:r:669:GLN:HE21	56:z:770:THR:HB	0.84	1.00
40:j:398:ALA:N	41:k:84:HIS:CE1	2.29	1.00
30:Z:74:TRP:O	32:b:240:GLN:O	1.78	1.00
30:Z:403:PHE:HE2	33:c:54:GLN:OE1	1.43	1.00
40:j:211:SER:OG	41:k:45:ASN:CB	1.94	1.00
46:p:85:ASN:OD1	56:z:640:ARG:CZ	2.08	1.00
30:Z:58:ARG:HB3	32:b:229:TRP:HZ3	1.25	1.00
39:i:78:PRO:HB3	40:j:197:ARG:HB2	1.38	1.00
48:r:1397:GLN:CB	48:r:1419:LEU:HD21	1.91	0.99
29:Y:457:ILE:HD13	29:Y:520:ASN:HD22	1.25	0.99
48:r:657:LEU:CD2	48:r:682:ILE:HD12	1.92	0.99
30:Z:408:LEU:HD11	33:c:44:PHE:HE2	1.23	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:293:ARG:HH12	28:X:378:ARG:CA	1.74	0.99
29:Y:374:LEU:HD11	32:b:270:VAL:HG12	1.44	0.99
30:Z:440:LEU:HD21	33:c:36:GLN:NE2	1.73	0.99
1:O:812:ARG:NH1	46:p:92:GLN:HB2	1.75	0.99
3:2:301:GLU:OE1	3:2:304:LYS:HE3	1.61	0.99
8:D:141:GLN:NE2	43:m:70:ARG:HH11	1.59	0.99
31:a:271:PHE:O	31:a:285:THR:HG23	1.63	0.99
31:a:374:PHE:HZ	32:b:141:LEU:HB3	1.17	0.99
43:m:115:LYS:CE	45:o:142:VAL:HG12	1.92	0.99
1:O:832:LEU:H	1:O:832:LEU:HD22	1.24	0.99
28:X:316:GLN:HG3	28:X:373:ARG:NH2	1.77	0.99
29:Y:513:ARG:HA	29:Y:516:TYR:HE2	1.22	0.99
40:j:608:ASP:HB2	56:z:693:LEU:HD23	1.43	0.99
31:a:292:PRO:HB2	32:b:264:ILE:CG1	1.92	0.99
40:j:198:LYS:CB	43:m:88:LEU:HD23	1.90	0.99
42:l:156:LEU:HD11	44:n:288:LEU:CG	1.93	0.99
27:W:109:ARG:NH1	27:W:492:ASN:CB	2.26	0.99
49:s:145:SER:O	49:s:148:ILE:N	1.96	0.99
30:Z:368:LEU:HB2	30:Z:383:LEU:CD1	1.92	0.98
39:i:114:MET:HE3	47:q:159:ILE:HD11	1.00	0.98
40:j:415:LYS:HZ2	42:l:123:LEU:CD1	1.74	0.98
28:X:307:ASN:HB3	28:X:308:PRO:CD	1.92	0.98
29:Y:524:HIS:CG	31:a:270:SER:CB	2.45	0.98
29:Y:524:HIS:CD2	31:a:270:SER:HB2	1.95	0.98
40:j:412:ALA:HB3	42:l:186:PRO:CG	1.93	0.98
28:X:534:GLY:HA2	28:X:594:ALA:O	1.61	0.98
27:W:129:VAL:CB	27:W:334:ARG:HH12	1.75	0.98
43:m:115:LYS:HD2	45:o:146:ILE:HD12	1.43	0.98
1:O:15:LEU:HD13	1:O:455:LEU:CD2	1.92	0.98
48:r:233:THR:C	48:r:248:LEU:HB2	1.88	0.98
55:y:46:LYS:O	55:y:49:VAL:N	1.96	0.98
56:z:721:LEU:HD11	56:z:736:TRP:CZ2	1.77	0.98
21:Q:148:MET:HE3	41:k:200:GLU:HG2	1.01	0.98
40:j:396:ALA:HB2	41:k:51:PHE:CE1	1.98	0.98
52:v:117:PHE:HB2	52:v:119:GLU:HG2	1.43	0.98
27:W:442:GLU:OE2	27:W:638:GLN:NE2	1.97	0.98
30:Z:122:LEU:O	32:b:100:LYS:CG	2.11	0.98
30:Z:122:LEU:HD22	32:b:104:LEU:CD1	1.87	0.98
27:W:274:GLN:HA	27:W:459:GLN:HE21	1.26	0.98
30:Z:57:MET:CG	32:b:51:MET:HE3	1.94	0.98
46:p:71:LEU:CD2	56:z:617:LEU:CD1	2.41	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:719:PRO:HB2	56:z:742:GLN:HE22	1.25	0.98
27:W:105:GLU:HG2	27:W:487:LYS:CE	1.94	0.97
46:p:85:ASN:OD1	56:z:640:ARG:NH2	1.96	0.97
39:i:114:MET:HG2	47:q:155:GLN:CB	1.93	0.97
30:Z:46:ARG:HH12	32:b:53:ARG:HD2	1.29	0.97
39:i:78:PRO:CG	40:j:197:ARG:CD	2.26	0.97
40:j:410:PRO:HA	42:l:86:ILE:HG22	1.45	0.97
40:j:479:ILE:CD1	40:j:529:MET:HE2	1.94	0.97
27:W:442:GLU:CD	27:W:638:GLN:NE2	2.22	0.97
49:s:179:ASP:O	49:s:183:ARG:N	1.98	0.97
29:Y:504:LYS:C	29:Y:507:PRO:HD3	1.88	0.97
39:i:114:MET:HE1	47:q:159:ILE:HG13	0.99	0.97
29:Y:539:TRP:CH2	29:Y:543:ARG:HD3	1.99	0.97
54:x:72:LEU:O	54:x:75:SER:OG	1.81	0.97
27:W:172:HIS:CB	27:W:434:GLU:OE2	2.12	0.97
29:Y:504:LYS:O	29:Y:508:PHE:HD2	1.42	0.97
27:W:85:PHE:HD2	30:Z:338:PHE:CE2	1.83	0.97
30:Z:38:PRO:CG	30:Z:121:ALA:HB2	1.94	0.97
30:Z:122:LEU:C	32:b:100:LYS:HG2	1.88	0.97
46:p:85:ASN:OD1	56:z:640:ARG:NH1	1.98	0.97
48:r:232:ALA:HB2	48:r:250:LEU:HD11	1.42	0.97
8:D:70:ARG:CB	43:m:20:LYS:HZ1	1.78	0.97
52:v:112:GLU:O	52:v:116:VAL:N	1.96	0.97
21:Q:177:LEU:HD21	34:d:9:CYS:HA	1.44	0.97
27:W:128:SER:HB3	27:W:334:ARG:NH2	1.79	0.97
27:W:493:TRP:CD1	27:W:683:GLN:O	2.17	0.97
30:Z:57:MET:CE	32:b:51:MET:HA	1.95	0.96
48:r:201:HIS:HE2	49:s:111:GLN:HG3	1.30	0.96
29:Y:510:GLU:OE1	29:Y:526:GLU:OE2	1.83	0.96
4:3:45:GLU:O	4:3:48:ASN:O	1.83	0.96
5:A:1623:SER:OG	55:y:92:GLN:NE2	1.98	0.96
40:j:615:TRP:CH2	56:z:680:GLY:HA2	2.00	0.96
40:j:415:LYS:HZ2	42:l:123:LEU:HD12	1.29	0.96
27:W:442:GLU:CD	27:W:638:GLN:HE22	1.74	0.96
30:Z:61:PHE:O	32:b:225:GLN:NE2	1.99	0.96
39:i:114:MET:HE2	47:q:159:ILE:HG13	1.46	0.96
50:t:132:ARG:NH2	54:x:83:ALA:O	1.98	0.96
52:v:98:LYS:O	52:v:101:THR:OG1	1.84	0.96
55:y:92:GLN:OE1	55:y:92:GLN:N	1.99	0.96
27:W:159:CYS:CB	27:W:163:TYR:CE2	2.47	0.96
28:X:726:GLN:HE22	31:a:223:LEU:CD1	1.77	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:191:ARG:NH1	40:j:203:ILE:HD12	1.81	0.96
8:D:141:GLN:CD	43:m:70:ARG:NH1	2.24	0.96
27:W:371:VAL:HG13	27:W:407:ILE:CG2	1.96	0.96
39:i:78:PRO:CB	40:j:197:ARG:HB3	1.96	0.96
39:i:114:MET:HE3	47:q:159:ILE:HD12	1.36	0.96
55:y:25:VAL:O	55:y:28:LEU:N	1.98	0.96
20:P:197:PHE:CD1	26:V:77:DT:H5''	2.01	0.96
29:Y:471:LEU:HD13	29:Y:502:VAL:HG11	1.47	0.96
39:i:104:LEU:HD22	45:o:136:LEU:HD22	1.46	0.96
40:j:492:GLN:HE21	40:j:507:ARG:CD	1.78	0.96
52:v:70:TYR:HH	52:v:80:TYR:H	1.10	0.96
5:A:1623:SER:OG	55:y:92:GLN:HG2	1.66	0.96
46:p:110:TYR:CD2	56:z:649:ILE:HD13	2.00	0.96
25:U:61:DA:OP1	27:W:527:THR:HA	1.65	0.95
49:s:180:LEU:O	49:s:184:SER:N	1.97	0.95
27:W:128:SER:HB3	27:W:334:ARG:HH21	1.25	0.95
28:X:300:GLU:HB3	28:X:304:HIS:NE2	1.81	0.95
52:v:70:TYR:OH	52:v:80:TYR:N	1.99	0.95
29:Y:504:LYS:C	29:Y:507:PRO:CD	2.39	0.95
43:m:140:SER:CA	47:q:146:ASN:HB3	1.95	0.95
30:Z:61:PHE:CB	32:b:228:LEU:CD1	2.44	0.95
48:r:121:PHE:O	48:r:125:GLN:NE2	1.99	0.95
48:r:230:PHE:CE1	48:r:296:LEU:CD1	2.48	0.95
50:t:84:SER:O	50:t:87:ILE:N	1.99	0.95
52:v:105:PHE:O	52:v:109:LEU:HB2	1.65	0.95
1:0:13:MET:CB	1:0:456:ARG:O	2.13	0.95
27:W:371:VAL:HG13	27:W:407:ILE:HG21	1.48	0.95
28:X:592:ARG:NH1	31:a:177:CYS:HA	1.82	0.95
52:v:104:LYS:O	52:v:107:SER:N	2.00	0.95
27:W:109:ARG:HH12	27:W:492:ASN:CA	1.62	0.95
27:W:469:THR:HG23	27:W:634:ARG:NH1	0.89	0.95
27:W:493:TRP:NE1	27:W:683:GLN:HB3	1.82	0.95
40:j:198:LYS:HD2	43:m:88:LEU:HD22	1.47	0.95
48:r:245:TRP:O	48:r:282:LEU:HD11	1.66	0.95
53:w:92:ALA:O	53:w:96:PHE:CB	2.14	0.95
30:Z:313:TYR:OH	30:Z:390:GLN:CD	2.10	0.95
44:n:49:GLU:CD	56:z:629:ILE:CG2	2.39	0.95
29:Y:464:LEU:CG	29:Y:513:ARG:NH1	2.09	0.95
27:W:497:GLN:NE2	27:W:685:TYR:HE1	1.57	0.94
30:Z:122:LEU:CD2	32:b:104:LEU:HD11	1.96	0.94
55:y:31:PRO:O	55:y:34:LEU:N	1.99	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:13:MET:CE	1:0:405:PHE:CB	2.44	0.94
29:Y:372:ILE:HG21	31:a:54:ARG:NH1	1.80	0.94
27:W:105:GLU:HG2	27:W:487:LYS:HZ3	1.23	0.94
40:j:412:ALA:HB2	42:l:76:PHE:HZ	0.79	0.94
55:y:55:LEU:O	55:y:58:TRP:N	1.98	0.94
29:Y:464:LEU:CD1	29:Y:513:ARG:HH12	1.56	0.94
54:x:129:GLN:O	54:x:133:ARG:N	2.01	0.94
28:X:293:ARG:NH1	28:X:377:GLU:C	2.26	0.94
30:Z:61:PHE:CB	32:b:228:LEU:HD13	1.97	0.94
40:j:336:PHE:CE1	40:j:500:GLU:HG3	2.03	0.94
42:l:146:PRO:HB3	44:n:236:TYR:CD2	2.03	0.94
53:w:93:TYR:O	53:w:97:CYS:N	1.99	0.94
44:n:36:LYS:CG	56:z:643:VAL:HG22	1.98	0.94
42:l:30:MET:HE3	48:r:521:GLN:HE22	0.79	0.94
5:A:1629:TYR:O	37:g:13:ILE:HD11	1.64	0.93
27:W:109:ARG:CD	27:W:492:ASN:OD1	2.15	0.93
27:W:167:LYS:HG2	27:W:294:GLU:CG	1.97	0.93
28:X:591:GLY:HA2	31:a:207:VAL:CB	1.98	0.93
30:Z:433:PHE:CE2	33:c:38:ILE:HD12	1.96	0.93
27:W:125:ALA:O	27:W:334:ARG:NH2	2.00	0.93
31:a:320:ARG:CZ	32:b:182:PHE:CE1	2.51	0.93
48:r:96:PHE:HA	48:r:99:LEU:HD12	1.49	0.93
27:W:113:VAL:HB	30:Z:316:TYR:CE2	2.03	0.93
28:X:293:ARG:NH1	28:X:378:ARG:N	2.17	0.93
30:Z:442:VAL:CB	33:c:9:LEU:HD22	1.98	0.93
44:n:56:PHE:CZ	56:z:621:LEU:HD23	1.99	0.93
48:r:657:LEU:HD22	48:r:682:ILE:HD12	1.51	0.93
30:Z:442:VAL:HG21	33:c:9:LEU:CD1	1.97	0.93
27:W:167:LYS:CD	27:W:294:GLU:HG3	1.99	0.93
29:Y:464:LEU:CD1	29:Y:513:ARG:HH11	1.67	0.93
33:c:8:VAL:HG21	33:c:47:ALA:HA	1.51	0.93
27:W:85:PHE:CZ	30:Z:336:TYR:CE1	2.56	0.93
30:Z:58:ARG:NE	32:b:241:LEU:HD21	1.81	0.93
44:n:49:GLU:CD	56:z:629:ILE:HG21	1.93	0.93
1:0:812:ARG:HH12	46:p:92:GLN:CB	1.82	0.93
27:W:158:LEU:O	27:W:163:TYR:CZ	2.21	0.93
30:Z:45:PHE:CE2	32:b:51:MET:O	2.22	0.93
40:j:595:GLN:OE1	40:j:619:ARG:HG2	1.68	0.93
56:z:719:PRO:HG3	56:z:743:TYR:CE1	2.03	0.93
8:D:129:GLN:HG3	38:h:65:HIS:CE1	2.04	0.93
27:W:689:VAL:CG1	30:Z:393:LEU:CD1	2.47	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:191:ILE:O	32:b:212:GLY:HA3	1.67	0.93
40:j:409:GLY:HA2	42:l:74:SER:OG	1.67	0.93
55:y:58:TRP:HA	55:y:63:TYR:CD2	2.03	0.93
27:W:516:PRO:HG3	33:c:18:GLN:HB3	1.49	0.92
27:W:689:VAL:CG1	30:Z:393:LEU:HD11	1.97	0.92
30:Z:433:PHE:CE1	33:c:42:HIS:HD2	1.67	0.92
44:n:35:LEU:HD23	56:z:642:PHE:CE2	2.05	0.92
20:P:309:LYS:HD2	26:V:83:DA:OP1	1.69	0.92
27:W:523:VAL:HG21	33:c:22:TYR:CE2	2.04	0.92
30:Z:313:TYR:CD2	30:Z:394:TRP:CH2	2.56	0.92
40:j:198:LYS:CB	43:m:88:LEU:HD22	1.99	0.92
40:j:598:ARG:NH1	56:z:683:ALA:HA	1.83	0.92
54:x:117:LYS:O	54:x:120:SER:OG	1.86	0.92
27:W:106:PRO:CD	27:W:490:GLU:OE1	2.16	0.92
28:X:310:LEU:HD22	28:X:409:THR:CG2	1.98	0.92
28:X:310:LEU:HD21	28:X:409:THR:CB	1.99	0.92
30:Z:313:TYR:CE2	30:Z:394:TRP:CZ2	2.57	0.92
48:r:669:GLN:OE1	48:r:683:ARG:CD	2.16	0.92
20:P:167:ASN:HB2	26:V:80:DT:O4'	1.69	0.92
29:Y:464:LEU:HD12	29:Y:513:ARG:NH1	1.83	0.92
43:m:130:LEU:CB	47:q:160:MET:HE3	1.64	0.92
50:t:24:GLU:OE1	50:t:24:GLU:N	2.01	0.92
27:W:175:TYR:CE1	27:W:459:GLN:CA	2.52	0.92
40:j:197:ARG:NE	40:j:204:LEU:HD23	1.83	0.92
43:m:133:GLU:OE2	45:o:125:LYS:HE2	1.69	0.92
48:r:674:GLU:CD	48:r:681:ALA:HB2	1.95	0.92
8:D:76:ASN:HD22	8:D:79:THR:HB	1.33	0.92
29:Y:514:ARG:NE	29:Y:522:VAL:CG2	1.74	0.92
49:s:183:ARG:NH1	50:t:10:LEU:O	2.01	0.92
27:W:129:VAL:N	27:W:334:ARG:NH2	2.17	0.92
40:j:393:PRO:HB3	40:j:406:ARG:HH21	1.32	0.92
46:p:71:LEU:HD23	56:z:617:LEU:HD12	1.52	0.92
52:v:52:ASP:HA	52:v:55:ARG:HB3	1.52	0.92
49:s:120:ILE:O	49:s:123:THR:OG1	1.85	0.92
5:A:1657:TYR:OH	35:e:61:ARG:NH1	2.02	0.91
20:P:218:LYS:CD	25:U:18:DG:OP1	2.17	0.91
27:W:121:TYR:CE2	27:W:487:LYS:N	2.38	0.91
27:W:689:VAL:HB	30:Z:393:LEU:HD12	0.94	0.91
30:Z:57:MET:HE3	32:b:51:MET:HA	1.47	0.91
30:Z:58:ARG:CZ	32:b:241:LEU:HG	2.00	0.91
30:Z:433:PHE:HZ	33:c:39:ASP:HB2	1.35	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:99:LEU:O	48:r:102:LEU:N	2.03	0.91
48:r:797:PHE:HE2	48:r:873:PHE:HD1	1.14	0.91
50:t:25:ASN:O	50:t:28:GLU:N	2.02	0.91
27:W:85:PHE:HE2	30:Z:336:TYR:CG	1.82	0.91
5:A:1619:SER:HB3	5:A:1620:PRO:CD	1.99	0.91
27:W:112:HIS:HD2	30:Z:310:GLU:HG2	1.31	0.91
28:X:293:ARG:NH1	28:X:378:ARG:HA	1.85	0.91
27:W:121:TYR:CZ	27:W:486:PRO:CA	2.54	0.91
40:j:394:HIS:CD2	41:k:78:ARG:HG3	2.06	0.91
54:x:94:GLU:O	54:x:98:HIS:ND1	2.01	0.91
29:Y:374:LEU:HD13	32:b:270:VAL:HG13	1.53	0.91
30:Z:57:MET:HG2	32:b:51:MET:HE3	1.51	0.91
43:m:134:TYR:HE1	47:q:153:ASN:OD1	1.52	0.91
29:Y:374:LEU:CD1	32:b:270:VAL:HG12	2.01	0.91
30:Z:58:ARG:NH1	32:b:241:LEU:HD21	1.82	0.91
30:Z:433:PHE:CE2	33:c:38:ILE:HD11	2.04	0.91
40:j:449:ASP:HB2	47:q:157:LYS:HZ1	1.26	0.91
40:j:469:ASP:CG	44:n:231:TRP:CD1	2.49	0.91
55:y:116:GLN:CD	55:y:119:LEU:HD12	1.96	0.91
20:P:218:LYS:HD3	25:U:18:DG:OP1	1.71	0.91
27:W:342:CYS:HG	27:W:638:GLN:HA	1.33	0.91
29:Y:464:LEU:HD11	29:Y:513:ARG:HH11	1.25	0.91
42:l:148:VAL:HB	44:n:196:LYS:HB3	1.51	0.91
6:B:1130:THR:HG22	6:B:1132:THR:H	1.34	0.91
49:s:179:ASP:N	49:s:181:GLU:OE1	2.04	0.91
3:2:301:GLU:OE1	3:2:304:LYS:CE	2.19	0.91
48:r:234:LEU:CA	48:r:246:ARG:O	2.18	0.90
30:Z:409:TYR:HB3	30:Z:412:PHE:CZ	2.05	0.90
40:j:197:ARG:HG3	40:j:204:LEU:HD23	1.52	0.90
56:z:719:PRO:HG3	56:z:743:TYR:HE1	1.33	0.90
30:Z:122:LEU:HD21	32:b:50:PHE:HD1	1.14	0.90
48:r:160:VAL:HA	48:r:164:GLY:H	1.36	0.90
24:T:230:LYS:CE	26:V:67:DC:H5"	2.01	0.90
30:Z:57:MET:HB3	32:b:51:MET:HE3	1.53	0.90
40:j:197:ARG:CZ	40:j:204:LEU:HD21	2.00	0.90
49:s:128:ALA:O	49:s:131:LYS:N	2.03	0.90
55:y:116:GLN:OE1	55:y:119:LEU:CB	2.18	0.90
3:2:272:ARG:HD2	3:2:936:GLU:HG3	1.53	0.90
8:D:70:ARG:CB	43:m:20:LYS:NZ	2.34	0.90
8:D:141:GLN:CG	43:m:70:ARG:CZ	2.28	0.90
30:Z:57:MET:SD	32:b:51:MET:HG3	2.10	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:198:LYS:CD	43:m:88:LEU:HD22	2.02	0.90
48:r:91:ARG:NH2	53:w:126:SER:OG	2.04	0.90
48:r:221:ARG:HB3	48:r:221:ARG:HH11	1.36	0.90
21:Q:148:MET:HE2	41:k:200:GLU:HG2	1.50	0.90
23:S:135:PHE:HB2	24:T:43:LEU:HB3	1.53	0.90
24:T:226:LYS:HE3	25:U:29:DC:H3'	1.52	0.90
52:v:51:ILE:O	52:v:54:CYS:N	2.04	0.90
27:W:175:TYR:CE1	27:W:459:GLN:HA	2.07	0.90
48:r:61:ARG:O	48:r:65:GLU:HB3	1.71	0.90
30:Z:38:PRO:HB2	30:Z:121:ALA:HB1	1.52	0.90
30:Z:58:ARG:HB3	32:b:229:TRP:CZ3	2.05	0.90
42:l:121:ASP:OD1	44:n:236:TYR:HA	1.72	0.90
43:m:134:TYR:CE1	47:q:153:ASN:OD1	2.24	0.90
50:t:81:LEU:HD22	50:t:119:VAL:HB	1.54	0.90
53:w:128:ARG:NH1	53:w:128:ARG:O	2.04	0.90
8:D:70:ARG:HB2	43:m:20:LYS:HZ1	1.31	0.90
52:v:69:GLU:O	52:v:73:GLN:N	2.05	0.90
27:W:278:GLU:HG2	27:W:483:LEU:HD11	1.54	0.89
40:j:463:HIS:HD2	43:m:128:TYR:CD1	1.90	0.89
48:r:175:ASP:N	48:r:175:ASP:OD1	1.94	0.89
1:0:13:MET:HE2	1:0:405:PHE:CB	2.02	0.89
1:0:790:CYS:CB	44:n:41:ASN:HB2	2.02	0.89
28:X:288:LEU:CD2	28:X:293:ARG:HE	1.85	0.89
46:p:103:ASP:OD1	48:r:944:PHE:HD2	1.09	0.89
48:r:234:LEU:CB	48:r:246:ARG:O	2.20	0.89
49:s:146:GLU:N	49:s:146:GLU:OE2	2.03	0.89
52:v:8:LEU:O	52:v:12:LEU:HB3	1.71	0.89
1:0:15:LEU:HD13	1:0:455:LEU:HD23	1.53	0.89
3:2:915:ARG:CZ	56:z:701:ASN:HA	2.02	0.89
27:W:159:CYS:C	27:W:163:TYR:CD2	2.50	0.89
39:i:78:PRO:CB	40:j:197:ARG:HB2	1.98	0.89
43:m:115:LYS:HE3	45:o:142:VAL:HG12	1.54	0.89
27:W:175:TYR:CZ	27:W:459:GLN:CA	2.55	0.89
48:r:882:ILE:HD13	48:r:914:ILE:HD11	1.55	0.89
5:A:1481:LYS:NZ	48:r:331:ALA:CB	2.35	0.89
28:X:324:ARG:NH1	34:d:97:ASP:OD1	2.06	0.89
40:j:492:GLN:NE2	40:j:507:ARG:HD3	1.88	0.89
48:r:51:LEU:N	52:v:60:ASP:OD1	2.05	0.89
50:t:11:PRO:HB2	55:y:40:ARG:HH12	1.38	0.89
50:t:167:CYS:O	50:t:170:SER:OG	1.90	0.89
54:x:75:SER:O	54:x:78:SER:OG	1.89	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:440:LEU:HD22	33:c:36:GLN:HE21	1.38	0.89
43:m:123:ILE:CD1	47:q:163:LEU:CD1	2.01	0.89
50:t:78:LEU:O	50:t:81:LEU:N	2.06	0.89
5:A:1650:TYR:OH	35:e:216:ASP:C	2.16	0.89
30:Z:46:ARG:NH1	32:b:53:ARG:HD2	1.88	0.89
40:j:598:ARG:NH1	56:z:683:ALA:O	2.05	0.88
46:p:110:TYR:CE2	56:z:649:ILE:HD13	2.08	0.88
48:r:230:PHE:CE1	48:r:296:LEU:HD13	2.07	0.88
30:Z:440:LEU:HD13	33:c:36:GLN:HE21	1.37	0.88
39:i:114:MET:HE2	47:q:159:ILE:CG1	1.95	0.88
44:n:35:LEU:HD23	56:z:642:PHE:HE2	1.37	0.88
48:r:222:VAL:CG2	48:r:234:LEU:O	2.21	0.88
27:W:520:ARG:CA	33:c:22:TYR:CD1	2.52	0.88
31:a:260:ALA:CB	31:a:264:ASP:OD1	2.21	0.88
8:D:70:ARG:HG3	43:m:20:LYS:HE2	0.90	0.88
27:W:85:PHE:CE2	30:Z:336:TYR:CD2	2.51	0.88
27:W:295:TYR:HB3	27:W:333:ALA:O	1.74	0.88
39:i:78:PRO:HG2	40:j:197:ARG:HD3	1.51	0.88
39:i:115:LEU:HD13	45:o:129:VAL:HG13	1.55	0.88
54:x:8:LEU:HD22	54:x:75:SER:HB2	1.52	0.88
55:y:115:LEU:O	55:y:119:LEU:HG	1.72	0.88
27:W:172:HIS:CA	27:W:434:GLU:CD	2.42	0.88
43:m:134:TYR:CE2	47:q:157:LYS:HD2	2.09	0.88
52:v:2:ALA:O	52:v:6:ASP:N	2.05	0.88
27:W:129:VAL:HA	27:W:334:ARG:HH11	1.33	0.88
32:b:268:CYS:HB3	32:b:271:CYS:SG	2.14	0.88
43:m:138:SER:OG	47:q:150:LYS:HD2	1.72	0.88
48:r:669:GLN:CD	56:z:770:THR:HG21	1.99	0.88
49:s:145:SER:N	49:s:146:GLU:OE2	2.06	0.88
52:v:100:ASP:OD1	52:v:103:LYS:NZ	2.07	0.88
30:Z:46:ARG:HH22	32:b:53:ARG:HD2	1.38	0.88
48:r:235:THR:N	48:r:246:ARG:O	2.06	0.88
4:3:123:GLN:NE2	4:3:123:GLN:HA	1.88	0.88
8:D:78:GLU:CD	38:h:51:LEU:CB	2.47	0.88
28:X:293:ARG:NH1	28:X:378:ARG:CA	2.37	0.88
28:X:310:LEU:CD2	28:X:409:THR:HG21	2.04	0.88
40:j:567:SER:HB2	40:j:585:GLY:CA	2.03	0.88
6:B:489:ILE:HD13	6:B:498:PRO:HG3	1.55	0.88
27:W:172:HIS:H	27:W:461:HIS:HE1	1.22	0.88
27:W:274:GLN:HB2	27:W:459:GLN:HE22	1.39	0.88
30:Z:403:PHE:HE2	33:c:54:GLN:CD	1.81	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:374:ASN:ND2	40:j:434:GLN:HE22	1.71	0.88
8:D:114:LEU:HD12	8:D:115:ILE:HG12	1.55	0.87
40:j:463:HIS:CD2	43:m:128:TYR:CD1	2.61	0.87
21:Q:148:MET:HE3	41:k:200:GLU:CD	1.99	0.87
30:Z:38:PRO:HB3	30:Z:121:ALA:HB2	0.89	0.87
31:a:320:ARG:NH2	32:b:182:PHE:HE1	1.73	0.87
24:T:131:GLN:O	24:T:134:GLU:O	1.92	0.87
40:j:598:ARG:HH12	56:z:683:ALA:CA	1.85	0.87
49:s:141:GLY:HA3	49:s:144:SER:HB3	1.56	0.87
56:z:718:VAL:CB	56:z:719:PRO:CD	2.51	0.87
20:P:294:ARG:NH1	25:U:14:DA:OP1	2.07	0.87
40:j:191:ARG:NH2	40:j:196:LEU:CB	2.38	0.87
43:m:122:GLU:HB3	45:o:135:LYS:HZ3	1.05	0.87
54:x:74:ASP:O	54:x:77:PRO:HD2	1.74	0.87
7:C:127:VAL:HG12	7:C:128:ILE:HD12	1.56	0.87
27:W:274:GLN:NE2	27:W:459:GLN:CG	2.36	0.87
40:j:396:ALA:HB1	41:k:73:ARG:HH22	1.39	0.87
42:l:121:ASP:OD2	44:n:237:GLN:CA	2.22	0.87
42:l:121:ASP:OD2	44:n:237:GLN:HB3	1.74	0.87
44:n:34:CYS:SG	48:r:861:LYS:NZ	2.48	0.87
48:r:165:SER:O	48:r:168:ARG:NH1	2.08	0.87
49:s:133:LYS:NZ	49:s:136:GLU:OE1	2.07	0.87
27:W:292:LEU:HG	27:W:294:GLU:OE2	1.70	0.87
40:j:419:ASN:HD21	42:l:73:LEU:HD21	1.37	0.87
53:w:84:ILE:HA	53:w:87:TYR:HB2	1.55	0.87
54:x:15:LEU:HD11	54:x:72:LEU:CD1	2.04	0.87
27:W:351:VAL:CG2	27:W:378:PHE:CD1	2.56	0.87
40:j:197:ARG:CD	40:j:204:LEU:HD23	2.04	0.87
3:2:915:ARG:NH2	56:z:701:ASN:CA	2.38	0.87
27:W:351:VAL:HG22	27:W:378:PHE:CE1	2.09	0.87
28:X:726:GLN:NE2	31:a:223:LEU:HD11	1.89	0.87
40:j:197:ARG:CG	40:j:204:LEU:HD23	2.04	0.87
55:y:64:ALA:O	55:y:66:TYR:N	2.08	0.87
25:U:60:DG:H4'	27:W:528:LYS:HE2	1.55	0.86
27:W:105:GLU:HA	27:W:487:LYS:NZ	1.90	0.86
39:i:114:MET:CG	47:q:155:GLN:CB	2.50	0.86
21:Q:53:LYS:HD2	22:R:166:ILE:HD11	1.56	0.86
29:Y:372:ILE:CG2	31:a:54:ARG:NE	2.33	0.86
29:Y:503:THR:O	29:Y:507:PRO:HG3	1.74	0.86
27:W:351:VAL:HG22	27:W:378:PHE:HD1	1.12	0.86
55:y:76:LEU:O	55:y:80:GLN:N	2.08	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:156:LEU:CD1	44:n:288:LEU:HG	2.05	0.86
56:z:699:SER:HB3	56:z:704:VAL:HG23	1.57	0.86
8:D:78:GLU:CD	38:h:51:LEU:HB2	2.00	0.86
29:Y:507:PRO:HD2	29:Y:508:PHE:N	1.87	0.86
31:a:292:PRO:O	32:b:264:ILE:HD11	1.75	0.86
40:j:464:TRP:CA	40:j:475:VAL:HG23	2.06	0.86
48:r:568:TYR:CZ	48:r:641:LEU:HG	2.10	0.86
48:r:669:GLN:NE2	56:z:770:THR:CG2	2.38	0.86
1:0:124:SER:HB3	1:0:179:TRP:HH2	1.40	0.86
27:W:112:HIS:HD2	30:Z:310:GLU:HG3	0.69	0.86
27:W:173:ASN:OD1	27:W:459:GLN:O	1.94	0.86
35:e:209:ARG:NH1	37:g:53:GLN:NE2	2.23	0.86
49:s:185:GLY:O	49:s:189:GLN:N	2.07	0.86
27:W:109:ARG:HH11	27:W:492:ASN:CA	1.67	0.86
48:r:669:GLN:HG2	56:z:770:THR:HG21	0.87	0.86
27:W:173:ASN:ND2	27:W:434:GLU:CA	2.37	0.86
29:Y:471:LEU:HD13	29:Y:502:VAL:CG1	2.04	0.86
29:Y:524:HIS:ND1	31:a:270:SER:HB3	1.89	0.86
40:j:142:GLN:HE21	40:j:143:THR:HG23	1.41	0.86
30:Z:58:ARG:CZ	32:b:241:LEU:CG	2.54	0.85
30:Z:121:ALA:O	32:b:101:TYR:N	2.08	0.85
40:j:367:HIS:CD2	40:j:438:ILE:HG21	2.11	0.85
49:s:151:TYR:OH	55:y:64:ALA:O	1.93	0.85
50:t:146:ARG:NH2	54:x:97:ASN:OD1	2.09	0.85
40:j:456:GLU:OE1	43:m:138:SER:CA	2.24	0.85
42:l:156:LEU:HD11	44:n:288:LEU:CD1	2.05	0.85
48:r:129:PHE:O	48:r:132:THR:OG1	1.92	0.85
48:r:230:PHE:CE1	48:r:296:LEU:HD11	2.10	0.85
56:z:718:VAL:CB	56:z:719:PRO:HD2	2.04	0.85
4:3:123:GLN:HG2	4:3:160:THR:HG21	1.58	0.85
8:D:78:GLU:OE1	38:h:51:LEU:HB3	1.74	0.85
27:W:473:GLU:OE2	27:W:632:SER:HB3	1.60	0.85
40:j:415:LYS:CD	42:l:116:ARG:HH12	1.89	0.85
8:D:70:ARG:CA	43:m:20:LYS:HZ3	1.90	0.85
18:N:7:ARG:HH22	18:N:37:LEU:HB3	1.41	0.85
27:W:115:GLU:OE2	30:Z:336:TYR:OH	1.94	0.85
40:j:393:PRO:CG	41:k:137:ARG:NH2	2.40	0.85
41:k:198:HIS:HE2	41:k:200:GLU:CD	1.84	0.85
48:r:641:LEU:HD13	48:r:644:PHE:HB2	1.58	0.85
50:t:76:LYS:HA	50:t:79:ARG:HG3	1.57	0.85
27:W:519:TYR:O	33:c:22:TYR:CE1	2.29	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:442:VAL:CG2	33:c:9:LEU:HD13	2.05	0.85
31:a:257:HIS:CG	32:b:248:HIS:HE1	1.95	0.85
52:v:68:PHE:O	52:v:72:ASP:N	2.09	0.85
1:0:361:ILE:HG13	1:0:379:GLY:HA3	1.57	0.85
27:W:110:PRO:O	27:W:494:MET:HE1	1.77	0.85
28:X:216:LYS:CD	28:X:309:VAL:HG22	2.00	0.85
28:X:300:GLU:CB	28:X:304:HIS:NE2	2.39	0.85
40:j:259:VAL:HG12	40:j:343:ILE:HG23	1.57	0.85
48:r:745:VAL:HG21	48:r:805:TYR:HB2	1.56	0.85
52:v:70:TYR:OH	52:v:77:PRO:O	1.93	0.85
55:y:123:GLN:O	55:y:126:ASN:N	2.10	0.85
30:Z:57:MET:HG3	32:b:51:MET:SD	2.17	0.85
30:Z:122:LEU:HD11	32:b:50:PHE:CD1	2.10	0.85
52:v:75:ARG:HH12	53:w:105:LEU:H	1.25	0.85
27:W:172:HIS:HB3	27:W:434:GLU:OE2	1.76	0.85
29:Y:372:ILE:HB	31:a:54:ARG:HD2	1.56	0.85
30:Z:401:LEU:HA	33:c:16:MET:CE	1.99	0.85
42:l:156:LEU:HD11	44:n:288:LEU:HD11	1.59	0.85
48:r:230:PHE:CE2	48:r:296:LEU:CG	2.60	0.85
52:v:103:LYS:O	52:v:107:SER:OG	1.93	0.85
54:x:52:GLU:O	54:x:55:ALA:N	2.09	0.85
56:z:721:LEU:HD11	56:z:736:TRP:CD2	2.11	0.85
20:P:222:THR:HG21	26:V:78:DT:H2"	1.59	0.85
27:W:159:CYS:CB	27:W:163:TYR:HE2	1.88	0.85
27:W:275:GLU:HA	27:W:456:THR:HG23	1.58	0.85
29:Y:495:SER:O	29:Y:499:ARG:HG3	1.76	0.85
30:Z:74:TRP:CZ2	32:b:229:TRP:CZ2	2.64	0.85
1:0:683:GLN:HE22	1:0:723:GLN:HG2	1.41	0.84
39:i:97:VAL:HG23	45:o:147:ASN:HD21	1.41	0.84
40:j:392:MET:CE	41:k:49:GLU:OE2	2.25	0.84
40:j:412:ALA:CB	42:l:76:PHE:CZ	2.29	0.84
42:l:119:TYR:HB3	42:l:122:PHE:HB3	1.59	0.84
56:z:719:PRO:CG	56:z:742:GLN:HE21	1.89	0.84
30:Z:58:ARG:HH22	32:b:240:GLN:HB2	1.42	0.84
39:i:78:PRO:CG	40:j:197:ARG:HB2	2.07	0.84
40:j:307:ILE:HG21	40:j:375:LEU:HD21	1.59	0.84
1:0:812:ARG:NE	46:p:90:ASN:HB3	1.91	0.84
21:Q:77:ARG:HG3	21:Q:78:VAL:H	1.42	0.84
38:h:23:LYS:NZ	40:j:110:CYS:SG	2.49	0.84
43:m:115:LYS:HE2	45:o:142:VAL:HG12	1.57	0.84
50:t:139:MET:HA	50:t:142:GLN:HE21	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:170:LEU:HD21	27:W:175:TYR:HD2	1.02	0.84
48:r:69:LEU:O	48:r:73:LEU:N	2.10	0.84
51:u:132:LEU:O	51:u:136:LYS:N	2.10	0.84
27:W:278:GLU:OE2	27:W:452:ARG:HG2	1.76	0.84
40:j:392:MET:SD	41:k:137:ARG:CD	2.65	0.84
27:W:121:TYR:CE1	27:W:486:PRO:HA	2.13	0.84
27:W:129:VAL:CG2	27:W:334:ARG:HH12	1.89	0.84
49:s:141:GLY:O	49:s:143:ILE:N	2.10	0.84
1:0:795:CYS:O	1:0:836:VAL:CG2	2.23	0.84
40:j:387:LEU:HD11	41:k:44:ASP:HB2	1.60	0.84
46:p:114:ASP:OD2	48:r:915:ARG:NH1	2.09	0.84
48:r:51:LEU:HB3	52:v:60:ASP:HA	1.60	0.84
50:t:158:GLU:O	50:t:161:ILE:N	2.10	0.84
52:v:34:GLN:HA	52:v:37:LEU:HB2	1.59	0.84
54:x:13:ASN:OD1	54:x:17:ASP:OD2	1.94	0.84
40:j:456:GLU:OE1	43:m:139:SER:N	2.10	0.84
49:s:188:GLY:O	49:s:191:ASN:N	2.10	0.84
28:X:300:GLU:HB3	28:X:304:HIS:CE1	2.13	0.83
40:j:419:ASN:HD21	42:l:73:LEU:CD2	1.91	0.83
40:j:492:GLN:NE2	40:j:507:ARG:CD	2.39	0.83
55:y:50:ASN:O	55:y:53:LYS:N	2.10	0.83
1:0:792:THR:HG21	44:n:39:MET:O	1.78	0.83
5:A:419:ILE:HG21	5:A:438:LEU:HD21	1.60	0.83
30:Z:392:ARG:HG2	30:Z:392:ARG:HH11	1.40	0.83
40:j:398:ALA:HB2	41:k:107:ASP:HB3	1.57	0.83
48:r:797:PHE:CE2	48:r:873:PHE:HD1	1.95	0.83
54:x:76:LEU:O	54:x:78:SER:N	2.11	0.83
5:A:1620:PRO:CB	38:h:104:VAL:HG11	2.08	0.83
35:e:164:SER:OG	35:e:167:ARG:CD	2.26	0.83
40:j:394:HIS:CG	41:k:78:ARG:CG	2.58	0.83
40:j:419:ASN:ND2	42:l:73:LEU:HD23	1.93	0.83
5:A:18:ILE:H	5:A:1462:GLN:HE22	1.26	0.83
27:W:85:PHE:CE1	30:Z:336:TYR:CZ	2.65	0.83
29:Y:513:ARG:O	29:Y:516:TYR:CE2	2.30	0.83
31:a:347:GLY:O	32:b:139:LYS:HG2	1.79	0.83
40:j:187:LEU:HD21	40:j:191:ARG:HE	1.44	0.83
40:j:479:ILE:HG21	40:j:529:MET:SD	2.18	0.83
40:j:491:ILE:HD13	40:j:532:HIS:CB	2.07	0.83
8:D:141:GLN:NE2	43:m:70:ARG:NH1	2.26	0.83
30:Z:442:VAL:HG21	33:c:9:LEU:CG	2.07	0.83
40:j:456:GLU:OE1	43:m:138:SER:N	2.11	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:121:ASP:CG	44:n:237:GLN:N	2.28	0.83
55:y:34:LEU:O	55:y:37:LEU:N	2.11	0.83
30:Z:38:PRO:CG	30:Z:121:ALA:HB1	2.06	0.83
30:Z:122:LEU:HD11	32:b:50:PHE:CG	2.13	0.83
35:e:94:MET:HE3	35:e:152:LYS:HD2	1.61	0.83
42:l:148:VAL:CB	44:n:196:LYS:HB3	2.08	0.83
1:0:792:THR:CG2	44:n:40:ARG:O	2.26	0.83
27:W:351:VAL:CG2	27:W:378:PHE:HD1	1.90	0.83
27:W:351:VAL:CG1	27:W:378:PHE:CE1	2.61	0.83
27:W:516:PRO:CG	33:c:18:GLN:CD	2.51	0.83
30:Z:401:LEU:CD1	33:c:57:VAL:HG11	2.05	0.83
40:j:198:LYS:HG3	40:j:203:ILE:CD1	2.09	0.83
45:o:118:LEU:HD11	47:q:146:ASN:OD1	1.77	0.83
54:x:91:TYR:HA	54:x:94:GLU:HG3	1.58	0.83
55:y:80:GLN:C	55:y:85:ARG:HH22	1.87	0.83
55:y:126:ASN:O	55:y:130:GLY:N	2.12	0.83
5:A:757:GLN:HE22	5:A:778:LYS:HD3	1.43	0.83
3:2:175:ARG:NE	3:2:225:ILE:O	2.12	0.83
8:D:70:ARG:HG3	43:m:20:LYS:NZ	1.93	0.83
39:i:84:TYR:CZ	40:j:195:LYS:HB3	2.14	0.83
48:r:94:GLN:O	48:r:97:VAL:N	2.10	0.83
52:v:75:ARG:NH1	53:w:105:LEU:H	1.77	0.83
27:W:128:SER:C	27:W:334:ARG:NH1	2.34	0.82
40:j:198:LYS:NZ	40:j:203:ILE:HD11	1.94	0.82
50:t:77:GLU:H	50:t:77:GLU:CD	1.85	0.82
29:Y:381:ARG:HB3	32:b:256:PHE:CG	2.15	0.82
56:z:719:PRO:CG	56:z:743:TYR:HE1	1.91	0.82
28:X:314:VAL:O	28:X:314:VAL:HG12	1.77	0.82
40:j:419:ASN:ND2	42:l:73:LEU:CD2	2.41	0.82
56:z:699:SER:CB	56:z:704:VAL:HG23	2.09	0.82
27:W:85:PHE:HE2	30:Z:336:TYR:CB	1.92	0.82
29:Y:475:PHE:CZ	29:Y:499:ARG:HG2	2.14	0.82
29:Y:544:LEU:HA	29:Y:547:LYS:HG3	1.60	0.82
30:Z:38:PRO:HG3	30:Z:121:ALA:CB	2.08	0.82
30:Z:401:LEU:HD11	33:c:57:VAL:CB	2.08	0.82
40:j:410:PRO:O	42:l:86:ILE:CG2	2.26	0.82
44:n:282:GLN:HG2	44:n:304:ALA:HB3	1.61	0.82
27:W:85:PHE:CE2	30:Z:336:TYR:CD1	2.66	0.82
27:W:129:VAL:CG2	27:W:334:ARG:NH1	2.43	0.82
27:W:170:LEU:CD2	27:W:175:TYR:CG	2.63	0.82
40:j:393:PRO:HB3	40:j:406:ARG:HH22	1.06	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:199:LEU:CD1	48:r:222:VAL:HG13	2.01	0.82
48:r:204:VAL:HG22	54:x:129:GLN:NE2	1.94	0.82
50:t:24:GLU:H	50:t:24:GLU:CD	1.86	0.82
55:y:116:GLN:O	55:y:119:LEU:N	2.13	0.82
29:Y:411:MET:O	32:b:120:THR:CG2	2.28	0.82
30:Z:61:PHE:CG	32:b:228:LEU:HD12	2.13	0.82
48:r:153:ALA:C	48:r:155:PRO:HD2	2.03	0.82
49:s:181:GLU:O	49:s:184:SER:N	2.13	0.82
55:y:78:LEU:O	55:y:85:ARG:NH1	2.12	0.82
29:Y:414:TYR:CZ	32:b:115:ILE:CD1	2.62	0.82
31:a:256:GLN:HE22	32:b:261:LEU:HD21	1.45	0.82
39:i:84:TYR:OH	40:j:195:LYS:HB3	1.80	0.82
39:i:111:CYS:HA	47:q:159:ILE:HD11	1.61	0.82
40:j:469:ASP:HB2	44:n:231:TRP:NE1	1.93	0.82
48:r:200:ARG:HB3	54:x:126:ALA:HB1	1.62	0.82
27:W:109:ARG:HH12	27:W:492:ASN:N	1.76	0.82
30:Z:403:PHE:HD2	33:c:54:GLN:OE1	1.55	0.82
30:Z:409:TYR:HB3	30:Z:412:PHE:HZ	1.43	0.82
35:e:108:VAL:HG21	37:g:63:MET:HE1	1.59	0.82
40:j:567:SER:OG	40:j:584:ASN:O	1.97	0.82
46:p:86:THR:HG21	56:z:628:ASN:ND2	1.95	0.82
48:r:116:ALA:O	48:r:119:SER:OG	1.96	0.82
5:A:1623:SER:OG	55:y:92:GLN:CD	2.22	0.82
5:A:1623:SER:OG	55:y:92:GLN:HG3	1.78	0.82
10:F:68:THR:HG21	11:G:59:ILE:HD12	1.61	0.82
48:r:674:GLU:OE2	48:r:681:ALA:HB1	1.79	0.82
5:A:72:GLN:HG3	5:A:74:CYS:H	1.42	0.82
27:W:278:GLU:OE2	27:W:452:ARG:CB	2.27	0.82
30:Z:46:ARG:NH2	32:b:53:ARG:HD2	1.95	0.82
40:j:410:PRO:HA	42:l:86:ILE:CG2	2.10	0.82
43:m:140:SER:C	47:q:146:ASN:HB3	2.04	0.82
1:0:13:MET:HE1	1:0:405:PHE:CB	2.07	0.81
5:A:1650:TYR:HE2	35:e:215:GLY:O	1.63	0.81
27:W:159:CYS:HA	27:W:163:TYR:CD2	2.12	0.81
27:W:519:TYR:HD2	33:c:22:TYR:CG	1.97	0.81
30:Z:122:LEU:CD1	32:b:50:PHE:CE1	2.63	0.81
40:j:190:LEU:HG	40:j:194:TRP:CE3	2.14	0.81
48:r:797:PHE:HE2	48:r:873:PHE:CD1	1.97	0.81
55:y:58:TRP:HA	55:y:63:TYR:HD2	1.41	0.81
56:z:715:LEU:HD12	56:z:716:PRO:HD3	1.59	0.81
5:A:1626:SER:H	5:A:1627:PRO:HD3	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:41:CYS:HB2	30:Z:118:LEU:HD21	1.63	0.81
54:x:6:THR:HA	54:x:9:GLN:HG3	1.59	0.81
1:0:394:VAL:HG13	1:0:399:LEU:HA	1.62	0.81
5:A:1650:TYR:CZ	35:e:215:GLY:O	2.33	0.81
28:X:293:ARG:HH11	28:X:377:GLU:C	1.87	0.81
28:X:307:ASN:OD1	28:X:380:ARG:NH1	2.12	0.81
46:p:104:LYS:NZ	48:r:948:LYS:NZ	2.28	0.81
54:x:15:LEU:CD1	54:x:72:LEU:HD11	2.10	0.81
8:D:66:ASN:OD1	43:m:13:THR:HG22	1.80	0.81
30:Z:54:ASN:O	30:Z:58:ARG:HG3	1.81	0.81
40:j:609:VAL:HG12	56:z:682:VAL:HG11	1.62	0.81
53:w:91:GLN:H	53:w:91:GLN:CD	1.86	0.81
28:X:288:LEU:HD21	28:X:293:ARG:HE	1.44	0.81
30:Z:61:PHE:CB	32:b:228:LEU:HD12	2.10	0.81
40:j:491:ILE:HD13	40:j:532:HIS:CA	2.08	0.81
27:W:105:GLU:CG	27:W:487:LYS:NZ	2.43	0.81
27:W:170:LEU:HD22	27:W:175:TYR:CD2	2.13	0.81
52:v:83:GLU:O	52:v:87:ARG:NH1	2.13	0.81
53:w:130:LEU:HA	53:w:134:PRO:HA	1.61	0.81
27:W:516:PRO:HG3	33:c:18:GLN:CB	2.11	0.81
30:Z:41:CYS:CB	30:Z:118:LEU:HD21	2.09	0.81
21:Q:107:LEU:CD1	21:Q:111:ARG:CZ	2.59	0.81
28:X:297:ALA:CA	28:X:300:GLU:CD	2.51	0.81
29:Y:539:TRP:CZ2	29:Y:543:ARG:HD3	2.16	0.81
43:m:123:ILE:HG13	47:q:163:LEU:HD21	1.63	0.81
50:t:135:LEU:O	50:t:138:MET:N	2.13	0.81
54:x:71:VAL:O	54:x:74:ASP:N	2.13	0.81
1:0:792:THR:HG23	44:n:40:ARG:O	1.81	0.81
27:W:171:LYS:HA	27:W:461:HIS:HE1	1.43	0.81
30:Z:57:MET:CG	32:b:51:MET:CE	2.38	0.81
40:j:415:LYS:CD	42:l:116:ARG:NH1	2.41	0.81
48:r:231:GLU:OE1	48:r:251:GLU:HB2	1.80	0.81
48:r:233:THR:HG23	48:r:248:LEU:HB2	1.62	0.81
50:t:77:GLU:OE1	50:t:77:GLU:N	2.12	0.81
54:x:6:THR:C	54:x:9:GLN:HG3	2.06	0.81
1:0:671:SER:CB	46:p:88:ILE:HD11	2.11	0.81
28:X:309:VAL:HG21	28:X:402:ASN:ND2	1.95	0.81
44:n:49:GLU:CD	56:z:629:ILE:HG22	2.06	0.81
55:y:94:ALA:O	55:y:98:ASP:CG	2.24	0.81
29:Y:407:ILE:HD13	32:b:19:PRO:HA	1.63	0.80
29:Y:539:TRP:CH2	29:Y:543:ARG:CD	2.63	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:440:LEU:HD13	33:c:36:GLN:CD	2.00	0.80
39:i:110:THR:HG22	39:i:114:MET:HE2	1.61	0.80
40:j:410:PRO:O	42:l:86:ILE:CD1	2.29	0.80
40:j:546:TRP:CD1	40:j:574:PRO:HA	2.16	0.80
48:r:58:LEU:HD11	48:r:95:LEU:HD21	1.63	0.80
54:x:13:ASN:O	54:x:17:ASP:OD2	1.98	0.80
29:Y:407:ILE:CD1	32:b:19:PRO:HA	2.12	0.80
40:j:487:ILE:HB	44:n:135:ARG:CA	2.04	0.80
44:n:294:PRO:HA	44:n:306:HIS:HB3	1.60	0.80
55:y:124:GLN:O	55:y:128:THR:HG23	1.79	0.80
30:Z:433:PHE:CD2	33:c:38:ILE:HD11	2.15	0.80
40:j:191:ARG:NH1	43:m:88:LEU:HD21	1.96	0.80
48:r:88:PHE:O	48:r:92:THR:OG1	1.99	0.80
3:2:672:ARG:HE	3:2:695:MET:HE2	1.47	0.80
35:e:17:PHE:HE2	48:r:68:VAL:HG11	1.44	0.80
40:j:463:HIS:HD2	43:m:128:TYR:CE1	1.91	0.80
48:r:150:PRO:O	50:t:127:ARG:NH1	2.14	0.80
56:z:702:GLY:O	56:z:727:ALA:CB	2.25	0.80
29:Y:457:ILE:HD13	29:Y:520:ASN:ND2	1.97	0.80
30:Z:58:ARG:HD3	32:b:241:LEU:CD2	2.10	0.80
30:Z:433:PHE:HE1	33:c:42:HIS:CD2	1.95	0.80
30:Z:442:VAL:HB	33:c:9:LEU:HD22	1.64	0.80
1:0:170:LEU:HB3	1:0:173:GLY:H	1.43	0.80
29:Y:381:ARG:HD3	32:b:256:PHE:HB3	1.62	0.80
29:Y:513:ARG:CA	29:Y:516:TYR:HE2	1.95	0.80
29:Y:544:LEU:HA	29:Y:547:LYS:HE3	1.63	0.80
30:Z:122:LEU:HD11	32:b:50:PHE:CD2	2.17	0.80
30:Z:313:TYR:OH	30:Z:390:GLN:NE2	2.14	0.80
5:A:460:ARG:HG3	5:A:501:MET:HE2	1.63	0.80
27:W:342:CYS:SG	27:W:638:GLN:CG	2.69	0.80
30:Z:400:ARG:HG2	33:c:16:MET:HG3	1.63	0.80
39:i:114:MET:SD	47:q:155:GLN:CA	2.70	0.80
42:l:121:ASP:OD2	44:n:237:GLN:CB	2.30	0.80
43:m:134:TYR:HH	47:q:157:LYS:HD2	1.47	0.80
54:x:6:THR:HA	54:x:9:GLN:CD	2.07	0.80
55:y:91:ALA:N	55:y:92:GLN:OE1	2.15	0.80
27:W:172:HIS:H	27:W:461:HIS:CE1	2.00	0.80
42:l:166:GLY:HA2	42:l:170:PRO:HD3	1.64	0.80
48:r:55:ILE:O	48:r:58:LEU:HB3	1.82	0.80
1:0:304:SER:HB3	1:0:350:ARG:HA	1.62	0.80
29:Y:389:ILE:HD11	32:b:259:ARG:HG3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:449:ILE:HG22	29:Y:450:ASN:N	1.97	0.80
44:n:56:PHE:CE2	56:z:621:LEU:HD23	2.16	0.80
49:s:151:TYR:OH	55:y:67:LEU:N	2.15	0.80
1:0:14:ASP:OD1	1:0:14:ASP:N	2.13	0.79
33:c:6:LYS:HA	33:c:6:LYS:HZ2	1.46	0.79
40:j:190:LEU:CD1	40:j:194:TRP:HZ3	1.95	0.79
43:m:122:GLU:CB	45:o:135:LYS:HZ3	1.83	0.79
48:r:51:LEU:O	48:r:54:LEU:N	2.15	0.79
29:Y:440:LEU:HD12	32:b:226:TYR:HE1	1.45	0.79
30:Z:313:TYR:CD2	30:Z:394:TRP:HH2	1.97	0.79
43:m:130:LEU:CA	47:q:160:MET:HE2	1.88	0.79
44:n:128:LEU:HG	45:o:81:ILE:HD11	1.62	0.79
51:u:135:TYR:HB3	54:x:117:LYS:HZ2	1.47	0.79
53:w:103:GLU:N	53:w:106:SER:OG	2.14	0.79
43:m:134:TYR:OH	47:q:157:LYS:CD	2.28	0.79
52:v:38:ASN:HA	52:v:41:LEU:HD13	1.63	0.79
36:f:126:VAL:HG11	36:f:140:LEU:HB2	1.63	0.79
37:g:66:ILE:HG22	37:g:85:GLN:HG3	1.62	0.79
40:j:415:LYS:HD2	42:l:116:ARG:CZ	2.13	0.79
40:j:464:TRP:HZ3	40:j:497:ILE:CD1	1.95	0.79
48:r:232:ALA:HA	48:r:250:LEU:HG	1.64	0.79
48:r:799:GLU:CG	48:r:816:LYS:HE3	2.09	0.79
55:y:118:ALA:O	55:y:121:GLU:N	2.16	0.79
3:2:82:ILE:HG23	3:2:97:LEU:HD23	1.65	0.79
28:X:310:LEU:CD2	28:X:409:THR:CB	2.61	0.79
30:Z:408:LEU:HD13	33:c:44:PHE:CD2	2.08	0.79
40:j:393:PRO:HD2	41:k:137:ARG:HH21	1.47	0.79
43:m:138:SER:OG	47:q:150:LYS:HD3	1.82	0.79
54:x:6:THR:O	54:x:9:GLN:HG3	1.82	0.79
54:x:115:LEU:CD1	54:x:119:GLN:HE22	1.95	0.79
30:Z:442:VAL:HG21	33:c:9:LEU:HB2	1.64	0.79
48:r:169:LEU:HB2	48:r:173:ILE:HA	1.64	0.79
48:r:230:PHE:CD2	48:r:296:LEU:HD13	2.17	0.79
48:r:1220:LEU:HB2	48:r:1299:LEU:HD21	1.65	0.79
30:Z:122:LEU:HD11	32:b:50:PHE:CE1	2.17	0.79
30:Z:442:VAL:CG2	33:c:9:LEU:HB2	2.13	0.79
52:v:77:PRO:O	52:v:80:TYR:N	2.11	0.79
1:0:640:ARG:CB	1:0:641:PRO:HD2	2.12	0.79
29:Y:504:LYS:O	29:Y:507:PRO:CG	2.31	0.79
21:Q:148:MET:CE	41:k:200:GLU:CB	2.60	0.79
21:Q:148:MET:HE1	41:k:200:GLU:HG2	0.80	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:172:HIS:C	27:W:434:GLU:HG2	2.08	0.79
29:Y:486:LEU:O	29:Y:490:VAL:HG23	1.83	0.79
40:j:412:ALA:H	42:l:86:ILE:HD13	1.48	0.79
43:m:130:LEU:CD1	47:q:156:LEU:HD11	2.11	0.79
48:r:52:SER:H	52:v:60:ASP:HA	1.46	0.79
54:x:6:THR:HA	54:x:9:GLN:CG	2.13	0.79
55:y:39:GLN:HE21	55:y:90:ASN:HA	1.46	0.79
40:j:327:VAL:HG23	40:j:328:LYS:H	1.47	0.78
44:n:60:LEU:HD13	56:z:618:CYS:HB3	1.64	0.78
48:r:144:LEU:O	48:r:147:ALA:N	2.15	0.78
50:t:75:LYS:NZ	54:x:79:GLU:OE1	2.16	0.78
52:v:74:GLY:O	52:v:76:ASN:ND2	2.16	0.78
24:T:226:LYS:CE	25:U:29:DC:H3'	2.14	0.78
27:W:159:CYS:CA	27:W:163:TYR:CZ	2.47	0.78
43:m:140:SER:CA	47:q:146:ASN:CB	2.58	0.78
46:p:122:LEU:HD13	48:r:902:GLN:HB2	1.65	0.78
7:C:19:VAL:HG12	7:C:233:VAL:HG22	1.66	0.78
43:m:16:GLN:HG2	43:m:20:LYS:HE3	1.65	0.78
48:r:441:PRO:HA	48:r:451:CYS:HB2	1.65	0.78
27:W:85:PHE:CD2	30:Z:338:PHE:HZ	2.01	0.78
28:X:311:PRO:CD	28:X:410:TYR:OH	2.32	0.78
44:n:310:ARG:HD3	48:r:715:ARG:HH22	1.48	0.78
54:x:115:LEU:O	54:x:118:ILE:N	2.16	0.78
20:P:195:LYS:NZ	24:T:172:ASP:O	2.17	0.78
40:j:615:TRP:CH2	56:z:680:GLY:CA	2.67	0.78
27:W:471:VAL:CG2	27:W:634:ARG:HH21	1.97	0.78
48:r:230:PHE:HE2	48:r:296:LEU:HD22	0.70	0.78
52:v:100:ASP:HA	52:v:103:LYS:HG2	1.66	0.78
27:W:172:HIS:N	27:W:461:HIS:HE1	1.81	0.78
50:t:131:ALA:O	50:t:134:THR:OG1	2.01	0.78
52:v:97:GLY:O	52:v:101:THR:HG23	1.83	0.78
27:W:278:GLU:OE2	27:W:452:ARG:CG	2.31	0.78
43:m:16:GLN:CD	43:m:20:LYS:HE3	2.08	0.78
44:n:56:PHE:CE2	56:z:621:LEU:CD2	2.67	0.78
21:Q:107:LEU:HD12	21:Q:111:ARG:NH1	1.97	0.78
4:3:125:PHE:CD2	4:3:178:ILE:HD12	2.18	0.77
8:D:136:THR:HG21	38:h:61:LYS:HE3	1.64	0.77
17:M:371:ILE:HG12	18:N:55:ARG:HH22	1.49	0.77
48:r:68:VAL:O	48:r:72:LEU:HG	1.84	0.77
27:W:497:GLN:NE2	27:W:685:TYR:CD1	2.30	0.77
40:j:491:ILE:HD12	40:j:532:HIS:HB2	0.78	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:618:LEU:HD21	48:r:725:VAL:HG21	1.66	0.77
42:l:156:LEU:HD11	44:n:288:LEU:HG	1.62	0.77
48:r:232:ALA:HB2	48:r:250:LEU:CD1	2.13	0.77
30:Z:122:LEU:HG	32:b:50:PHE:CZ	2.18	0.77
40:j:491:ILE:HD13	40:j:532:HIS:HB2	1.61	0.77
55:y:39:GLN:NE2	55:y:90:ASN:HA	1.99	0.77
56:z:731:ALA:H	56:z:766:LYS:HZ2	1.32	0.77
1:0:15:LEU:CD1	1:0:455:LEU:CD2	2.62	0.77
8:D:78:GLU:HB2	38:h:51:LEU:HD23	1.63	0.77
29:Y:539:TRP:CH2	29:Y:543:ARG:NE	2.52	0.77
48:r:674:GLU:CD	48:r:681:ALA:CB	2.55	0.77
49:s:121:LEU:O	49:s:124:ALA:HB3	1.83	0.77
29:Y:134:SER:O	29:Y:505:LEU:HD21	1.84	0.77
30:Z:401:LEU:CD1	33:c:57:VAL:CG1	2.57	0.77
46:p:104:LYS:HZ1	48:r:948:LYS:NZ	1.83	0.77
48:r:61:ARG:O	48:r:65:GLU:CB	2.32	0.77
50:t:127:ARG:HD3	54:x:5:LEU:HD22	1.66	0.77
5:A:1625:THR:C	55:y:39:GLN:HG2	2.09	0.77
6:B:832:PRO:HB2	6:B:840:MET:HE1	1.67	0.77
29:Y:415:THR:OG1	32:b:112:VAL:HG11	1.84	0.77
29:Y:496:ASN:O	29:Y:500:PHE:CD2	2.37	0.77
30:Z:433:PHE:HB2	33:c:9:LEU:HD21	1.65	0.77
40:j:191:ARG:HH21	40:j:196:LEU:HB2	1.45	0.77
40:j:617:HIS:H	40:j:617:HIS:CD2	2.03	0.77
49:s:180:LEU:HA	49:s:183:ARG:HB2	1.66	0.77
50:t:143:LYS:N	50:t:146:ARG:HE	1.83	0.77
52:v:101:THR:O	52:v:105:PHE:CB	2.29	0.77
54:x:8:LEU:CD2	54:x:75:SER:HB2	2.14	0.77
55:y:23:GLU:O	55:y:26:GLN:N	2.17	0.77
1:0:17:TYR:CD2	1:0:738:LEU:HD21	2.20	0.77
40:j:394:HIS:ND1	41:k:78:ARG:HG2	1.98	0.77
27:W:105:GLU:CA	27:W:487:LYS:HZ1	1.95	0.77
30:Z:384:PRO:HB2	30:Z:387:ILE:HB	1.67	0.77
48:r:55:ILE:HD12	48:r:55:ILE:H	1.48	0.77
48:r:230:PHE:CZ	48:r:296:LEU:CG	2.66	0.77
52:v:120:ASP:HB3	52:v:124:TYR:CE1	2.20	0.77
55:y:30:ASN:O	55:y:33:TYR:HB3	1.85	0.77
24:T:177:ARG:NH1	25:U:20:DG:OP1	2.17	0.77
27:W:159:CYS:CA	27:W:163:TYR:CD2	2.67	0.77
40:j:190:LEU:CG	40:j:194:TRP:CZ3	2.65	0.77
5:A:1481:LYS:HZ3	48:r:331:ALA:CB	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:151:THR:HG23	21:Q:153:ARG:HD3	1.66	0.77
27:W:342:CYS:SG	27:W:638:GLN:CB	2.73	0.77
42:l:30:MET:HE2	48:r:521:GLN:HE22	1.49	0.77
44:n:306:HIS:NE2	44:n:309:CYS:SG	2.56	0.77
46:p:71:LEU:HD21	56:z:617:LEU:HD11	1.64	0.77
56:z:715:LEU:HD12	56:z:716:PRO:CD	2.15	0.77
3:2:179:HIS:HA	3:2:182:LYS:HG2	1.66	0.76
5:A:942:VAL:HA	5:A:948:ILE:HD11	1.66	0.76
5:A:1165:THR:H	5:A:1168:LYS:HZ3	1.30	0.76
19:O:32:MET:HE2	19:O:45:VAL:HG21	1.65	0.76
28:X:309:VAL:O	28:X:309:VAL:HG12	1.84	0.76
29:Y:475:PHE:CZ	29:Y:499:ARG:CG	2.68	0.76
39:i:115:LEU:CD1	45:o:129:VAL:HG13	2.14	0.76
40:j:207:LEU:HD11	40:j:222:PHE:HB3	1.67	0.76
50:t:151:GLU:O	50:t:154:GLN:HG2	1.85	0.76
52:v:124:TYR:HA	52:v:127:ILE:HB	1.65	0.76
55:y:45:ASP:O	55:y:48:PHE:N	2.17	0.76
20:P:210:THR:OG1	26:V:79:DT:H5'	1.85	0.76
29:Y:507:PRO:CD	29:Y:508:PHE:H	1.95	0.76
31:a:292:PRO:CB	32:b:264:ILE:HG13	2.13	0.76
40:j:415:LYS:HZ3	42:l:123:LEU:CD1	1.95	0.76
48:r:149:LEU:O	49:s:153:HIS:NE2	2.17	0.76
48:r:919:ARG:HD3	48:r:919:ARG:H	1.50	0.76
3:2:915:ARG:NH1	56:z:702:GLY:H	1.82	0.76
32:b:46:ASN:O	32:b:50:PHE:HB2	1.85	0.76
43:m:140:SER:HB2	47:q:146:ASN:HB3	1.59	0.76
48:r:139:LEU:O	48:r:143:ALA:HB3	1.86	0.76
49:s:187:LEU:HA	49:s:190:MET:HE3	1.66	0.76
50:t:20:GLU:OE1	50:t:20:GLU:N	2.17	0.76
27:W:77:TRP:CB	30:Z:338:PHE:CE2	2.68	0.76
5:A:457:ILE:HD11	5:A:515:ILE:HG13	1.66	0.76
8:D:141:GLN:HE21	43:m:70:ARG:HH11	1.28	0.76
13:I:40:ARG:HD3	23:S:172:ASN:H	1.50	0.76
28:X:310:LEU:HD21	28:X:409:THR:OG1	1.84	0.76
52:v:82:LYS:HE2	53:w:96:PHE:HA	1.65	0.76
6:B:65:ILE:HD11	6:B:412:LEU:HG	1.66	0.76
10:F:65:VAL:HG13	10:F:104:ILE:HD11	1.68	0.76
19:O:221:ASN:HB3	19:O:277:ILE:HD11	1.67	0.76
27:W:128:SER:CB	27:W:334:ARG:NH2	2.48	0.76
28:X:338:GLU:HG3	34:d:68:VAL:HG21	1.66	0.76
29:Y:513:ARG:HA	29:Y:516:TYR:CE2	2.13	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:111:CYS:SG	45:o:133:LEU:HG	2.25	0.76
40:j:573:SER:OG	40:j:574:PRO:HD2	1.85	0.76
44:n:56:PHE:CZ	56:z:621:LEU:HD22	1.92	0.76
47:q:72:GLN:H	47:q:74:ARG:HH21	1.33	0.76
50:t:88:ASN:OD1	50:t:89:PHE:N	2.18	0.76
52:v:76:ASN:CG	53:w:104:LYS:HB3	2.10	0.76
54:x:6:THR:CA	54:x:9:GLN:HG3	2.15	0.76
31:a:320:ARG:NH1	32:b:182:PHE:CD1	2.54	0.76
40:j:211:SER:OG	41:k:45:ASN:HB2	1.86	0.76
48:r:1236:GLU:HB3	48:r:1237:PRO:HD2	1.65	0.76
56:z:721:LEU:CD1	56:z:736:TRP:CE2	2.43	0.76
5:A:734:ARG:NH2	13:I:108:MET:SD	2.56	0.76
40:j:190:LEU:HG	40:j:194:TRP:HZ3	1.48	0.76
48:r:669:GLN:CG	56:z:770:THR:HG22	2.16	0.76
50:t:123:ILE:O	50:t:126:TYR:N	2.19	0.76
55:y:92:GLN:CD	55:y:92:GLN:H	1.93	0.76
1:0:124:SER:HB3	1:0:179:TRP:CH2	2.21	0.76
29:Y:464:LEU:HD21	29:Y:509:GLN:OE1	1.85	0.76
30:Z:346:VAL:O	30:Z:394:TRP:CZ3	2.38	0.76
37:g:76:PRO:HG2	37:g:77:ILE:HD12	1.67	0.76
44:n:215:LYS:CE	44:n:232:SER:OG	2.34	0.76
51:u:133:GLN:HA	51:u:136:LYS:HB2	1.68	0.76
40:j:392:MET:HE3	41:k:49:GLU:OE2	1.85	0.76
40:j:534:VAL:HG21	40:j:568:ALA:O	1.85	0.76
50:t:75:LYS:O	50:t:78:LEU:N	2.18	0.76
54:x:62:ILE:O	54:x:65:THR:N	2.19	0.76
27:W:125:ALA:HB2	27:W:486:PRO:HB2	0.83	0.75
27:W:159:CYS:O	27:W:163:TYR:HD2	1.68	0.75
31:a:292:PRO:HB3	32:b:263:GLU:HG3	1.68	0.75
40:j:47:ILE:H	40:j:47:ILE:HD13	1.51	0.75
40:j:552:SER:HB2	48:r:650:THR:HG21	1.68	0.75
48:r:102:LEU:O	48:r:106:ALA:HB2	1.85	0.75
28:X:193:PHE:CZ	28:X:302:ASP:CG	2.64	0.75
30:Z:46:ARG:NH2	32:b:53:ARG:CD	2.41	0.75
52:v:63:VAL:O	52:v:65:LEU:HD12	1.86	0.75
30:Z:97:HIS:HE1	30:Z:112:PRO:HD3	1.50	0.75
30:Z:380:THR:HB	30:Z:381:PRO:HD3	1.67	0.75
30:Z:433:PHE:CD2	33:c:38:ILE:CD1	2.69	0.75
40:j:598:ARG:NH1	56:z:683:ALA:CA	2.47	0.75
43:m:111:GLU:OE2	45:o:146:ILE:CG2	2.35	0.75
48:r:959:LEU:HD12	48:r:1211:LEU:HD21	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:85:HIS:NE2	4:3:97:TRP:CE3	2.54	0.75
5:A:1626:SER:H	5:A:1627:PRO:CD	2.00	0.75
5:A:1650:TYR:OH	35:e:215:GLY:O	2.05	0.75
27:W:170:LEU:CD1	27:W:460:ALA:O	2.35	0.75
31:a:379:LEU:HD11	32:b:138:ALA:CB	2.15	0.75
40:j:387:LEU:HD21	41:k:46:MET:CA	2.16	0.75
40:j:393:PRO:CD	41:k:137:ARG:HH21	1.99	0.75
45:o:118:LEU:CD1	47:q:146:ASN:OD1	2.33	0.75
48:r:208:LEU:HB2	48:r:212:LEU:HD12	1.67	0.75
48:r:222:VAL:O	48:r:233:THR:HA	1.86	0.75
48:r:1320:MET:CE	48:r:1333:LYS:CB	2.58	0.75
52:v:113:LEU:HA	52:v:116:VAL:HG22	1.65	0.75
27:W:171:LYS:HA	27:W:461:HIS:ND1	2.01	0.75
29:Y:411:MET:HG3	32:b:119:MET:CB	2.16	0.75
29:Y:422:LEU:CD1	32:b:224:LEU:HD23	2.16	0.75
37:g:66:ILE:HB	37:g:83:LYS:HZ1	1.52	0.75
44:n:36:LYS:HG3	56:z:643:VAL:HG22	1.68	0.75
48:r:1323:GLU:HG2	48:r:1331:GLN:C	2.07	0.75
55:y:53:LYS:HA	55:y:56:LEU:HD12	1.68	0.75
5:A:1657:TYR:HE1	35:e:61:ARG:HH12	1.31	0.75
11:G:137:ILE:HG12	11:G:170:LEU:HD21	1.67	0.75
42:l:26:ARG:O	42:l:30:MET:HG2	1.87	0.75
2:1:985:GLU:HG2	2:1:1025:LYS:HG2	1.69	0.75
5:A:256:PRO:O	5:A:261:ARG:NH1	2.18	0.75
11:G:59:ILE:HG22	11:G:66:VAL:HG22	1.67	0.75
18:N:82:ARG:HE	18:N:85:THR:HA	1.50	0.75
30:Z:57:MET:CE	32:b:51:MET:CA	2.58	0.75
48:r:159:ASP:O	48:r:164:GLY:N	2.19	0.75
49:s:143:ILE:HG22	49:s:146:GLU:CD	2.12	0.75
49:s:144:SER:N	49:s:146:GLU:OE1	2.19	0.75
52:v:70:TYR:CE2	52:v:80:TYR:HB2	2.22	0.75
5:A:1481:LYS:HZ1	48:r:331:ALA:CB	1.99	0.75
40:j:259:VAL:HG23	40:j:368:LEU:HB3	1.68	0.75
40:j:395:PRO:HD2	40:j:406:ARG:HH12	0.80	0.75
41:k:156:ASN:HD21	41:k:158:ASP:HB2	1.52	0.75
5:A:419:ILE:HG23	5:A:427:ILE:HB	1.66	0.75
24:T:230:LYS:HE2	26:V:67:DC:H5"	1.68	0.75
27:W:109:ARG:HB3	27:W:494:MET:SD	2.27	0.75
40:j:464:TRP:CZ3	40:j:497:ILE:CD1	2.70	0.75
44:n:35:LEU:CD2	56:z:642:PHE:HE2	1.97	0.75
48:r:1387:ILE:H	48:r:1397:GLN:HA	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:95:ILE:O	50:t:96:LEU:HB2	1.85	0.75
55:y:13:GLY:HA2	55:y:16:LEU:HB3	1.69	0.75
4:3:125:PHE:CE1	4:3:140:ARG:HB3	2.21	0.74
8:D:70:ARG:CG	43:m:20:LYS:CE	2.48	0.74
27:W:278:GLU:OE1	27:W:452:ARG:HG2	1.86	0.74
30:Z:35:TYR:HB3	30:Z:114:PHE:HD1	1.50	0.74
48:r:230:PHE:CZ	48:r:296:LEU:HD21	2.22	0.74
48:r:674:GLU:OE2	48:r:681:ALA:HB3	1.86	0.74
52:v:105:PHE:O	52:v:109:LEU:CB	2.34	0.74
1:0:35:LEU:HG	1:0:50:ASP:OD2	1.87	0.74
5:A:540:ASP:HA	6:B:970:HIS:HE2	1.52	0.74
20:P:163:PRO:HB3	20:P:262:CYS:HB2	1.66	0.74
20:P:178:LEU:HD21	20:P:247:PRO:HD2	1.69	0.74
28:X:310:LEU:HD11	28:X:409:THR:OG1	1.86	0.74
30:Z:433:PHE:CZ	33:c:39:ASP:HB2	2.20	0.74
3:2:658:PHE:O	3:2:662:ARG:NH1	2.20	0.74
28:X:592:ARG:HH11	31:a:177:CYS:HA	1.53	0.74
48:r:657:LEU:HD22	48:r:682:ILE:CD1	2.17	0.74
49:s:104:ASP:OD1	49:s:108:GLN:NE2	2.19	0.74
20:P:309:LYS:CD	26:V:83:DA:OP1	2.35	0.74
27:W:351:VAL:CB	27:W:378:PHE:CE1	2.69	0.74
28:X:310:LEU:HD21	28:X:409:THR:HB	1.69	0.74
29:Y:527:GLU:OE1	31:a:268:LYS:HG3	1.88	0.74
48:r:71:ASP:C	48:r:74:PRO:HD2	2.13	0.74
51:u:123:GLU:O	51:u:127:THR:OG1	2.02	0.74
52:v:114:SER:HA	52:v:118:PRO:HB3	1.69	0.74
56:z:743:TYR:HD1	56:z:749:LEU:HD12	1.52	0.74
2:1:434:ARG:HD2	2:1:483:THR:HB	1.69	0.74
3:2:85:PHE:HB3	3:2:130:TRP:HE1	1.53	0.74
5:A:61:ARG:HA	5:A:72:GLN:HB3	1.69	0.74
5:A:68:THR:HA	19:O:12:ARG:HD3	1.69	0.74
21:Q:48:MET:HE2	21:Q:52:LEU:HB2	1.70	0.74
27:W:351:VAL:HG13	27:W:378:PHE:CD1	2.22	0.74
48:r:199:LEU:HD11	48:r:222:VAL:CG1	2.02	0.74
54:x:93:LEU:HA	54:x:96:GLU:HG2	1.69	0.74
5:A:702:ILE:HD12	5:A:752:THR:HG23	1.70	0.74
8:D:142:TYR:CE2	43:m:25:ASP:N	2.55	0.74
17:M:335:VAL:HB	18:N:95:ILE:HA	1.69	0.74
40:j:288:SER:OG	40:j:292:GLN:OE1	2.03	0.74
40:j:463:HIS:CD2	43:m:131:GLU:OE1	2.41	0.74
40:j:544:MET:HE3	45:o:89:ARG:HD3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:609:VAL:CG1	56:z:682:VAL:CG1	2.55	0.74
45:o:101:GLN:HE22	47:q:108:PRO:HD2	1.52	0.74
46:p:156:PRO:HB2	46:p:159:GLN:HB2	1.69	0.74
54:x:13:ASN:O	54:x:17:ASP:CG	2.30	0.74
56:z:718:VAL:HB	56:z:719:PRO:HD3	1.68	0.74
40:j:482:GLN:HB3	40:j:634:ASN:ND2	2.02	0.74
42:l:30:MET:HE2	48:r:521:GLN:NE2	2.03	0.74
49:s:89:ILE:HG12	49:s:93:MET:HE2	1.69	0.74
49:s:128:ALA:HA	49:s:131:LYS:HG2	1.70	0.74
54:x:3:ASP:OD1	54:x:7:GLN:NE2	2.21	0.74
55:y:84:PHE:HB2	55:y:85:ARG:HH11	1.53	0.74
22:R:82:VAL:HG11	24:T:238:GLU:HB3	1.69	0.74
23:S:49:ARG:HH22	23:S:96:GLN:H	1.35	0.74
23:S:115:LYS:NZ	23:S:117:GLY:O	2.20	0.74
27:W:351:VAL:CB	27:W:378:PHE:HE1	2.00	0.74
30:Z:442:VAL:CG2	33:c:9:LEU:HD22	2.17	0.74
30:Z:442:VAL:HG11	33:c:9:LEU:CD2	2.18	0.74
39:i:104:LEU:CD2	45:o:136:LEU:HD22	2.16	0.74
48:r:234:LEU:HA	48:r:246:ARG:O	1.88	0.74
54:x:51:THR:O	54:x:54:TYR:HB2	1.87	0.74
54:x:112:ASP:O	54:x:116:GLU:HG3	1.87	0.74
54:x:115:LEU:HD12	54:x:119:GLN:HE22	1.52	0.74
3:2:417:VAL:O	3:2:421:LEU:HB2	1.87	0.74
13:I:39:CYS:SG	13:I:40:ARG:N	2.60	0.74
29:Y:453:VAL:HG21	29:Y:517:LEU:HD12	1.70	0.74
43:m:130:LEU:HB3	47:q:160:MET:SD	2.28	0.74
52:v:11:HIS:CG	52:v:12:LEU:N	2.55	0.74
8:D:70:ARG:CG	43:m:20:LYS:HZ1	2.00	0.73
8:D:70:ARG:CA	43:m:20:LYS:NZ	2.51	0.73
27:W:112:HIS:HB2	30:Z:310:GLU:CD	2.11	0.73
27:W:128:SER:C	27:W:334:ARG:NH2	2.46	0.73
27:W:523:VAL:CG2	33:c:22:TYR:CE2	2.63	0.73
29:Y:381:ARG:CG	32:b:256:PHE:HB3	2.17	0.73
40:j:190:LEU:CG	40:j:194:TRP:HZ3	2.01	0.73
43:m:115:LYS:HD3	45:o:143:LEU:HD13	1.64	0.73
52:v:98:LYS:HE3	52:v:101:THR:HG21	1.68	0.73
2:1:95:ARG:HG2	2:1:129:VAL:HG13	1.70	0.73
25:U:59:DC:H5"	27:W:629:HIS:NE2	2.04	0.73
27:W:519:TYR:C	33:c:22:TYR:CE1	2.66	0.73
28:X:300:GLU:OE1	28:X:304:HIS:HE1	1.71	0.73
43:m:130:LEU:HD11	47:q:156:LEU:HD11	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:140:SER:CA	47:q:146:ASN:CG	2.60	0.73
49:s:152:ALA:HA	49:s:155:ILE:HB	1.68	0.73
51:u:118:LEU:HA	51:u:121:LEU:HD12	1.69	0.73
52:v:49:GLN:HA	52:v:52:ASP:OD2	1.88	0.73
52:v:99:ILE:O	52:v:103:LYS:HE3	1.88	0.73
27:W:129:VAL:H	27:W:334:ARG:HH22	1.33	0.73
40:j:412:ALA:CB	42:l:186:PRO:HG2	2.13	0.73
48:r:97:VAL:HA	48:r:100:LEU:HG	1.70	0.73
2:1:304:LEU:HD11	2:1:341:PHE:HD2	1.53	0.73
27:W:471:VAL:HG21	27:W:634:ARG:HH21	1.53	0.73
29:Y:381:ARG:HD3	32:b:256:PHE:CB	2.18	0.73
30:Z:61:PHE:HB3	32:b:228:LEU:HD12	1.70	0.73
40:j:191:ARG:NE	43:m:88:LEU:HD11	2.04	0.73
40:j:415:LYS:HG2	40:j:416:ASN:H	1.52	0.73
55:y:116:GLN:NE2	55:y:119:LEU:HD12	2.03	0.73
56:z:715:LEU:HD22	56:z:715:LEU:N	2.03	0.73
2:1:415:ASN:ND2	2:1:471:ASP:OD1	2.22	0.73
8:D:141:GLN:CD	43:m:70:ARG:HH11	1.93	0.73
27:W:516:PRO:HG2	33:c:18:GLN:CD	2.13	0.73
28:X:293:ARG:NH2	28:X:378:ARG:HD3	2.04	0.73
44:n:109:GLN:HE22	45:o:65:VAL:H	1.37	0.73
48:r:1316:CYS:HA	48:r:1319:ILE:HD12	1.70	0.73
5:A:244:ARG:HE	5:A:245:PRO:HD2	1.54	0.73
30:Z:58:ARG:NH2	32:b:241:LEU:HG	2.03	0.73
40:j:479:ILE:CG2	40:j:529:MET:SD	2.77	0.73
48:r:231:GLU:O	48:r:250:LEU:HA	1.87	0.73
48:r:669:GLN:NE2	56:z:770:THR:HG21	2.02	0.73
55:y:14:ASN:OD1	55:y:15:ARG:N	2.19	0.73
55:y:82:GLU:O	55:y:86:LYS:NZ	2.20	0.73
48:r:132:THR:O	48:r:135:ARG:HB3	1.89	0.73
50:t:84:SER:OG	50:t:85:ILE:N	2.14	0.73
5:A:1182:GLN:HA	5:A:1193:VAL:HG11	1.71	0.73
30:Z:61:PHE:HZ	32:b:47:SER:OG	1.72	0.73
30:Z:313:TYR:CZ	30:Z:390:GLN:CG	2.49	0.73
37:g:87:GLN:NE2	37:g:91:GLN:O	2.22	0.73
39:i:99:TYR:HH	40:j:366:ASP:CG	1.90	0.73
40:j:559:PRO:HG2	40:j:583:ARG:HH11	1.53	0.73
48:r:234:LEU:HB3	48:r:247:LEU:HA	1.71	0.73
48:r:567:LYS:NZ	48:r:569:TYR:OH	2.22	0.73
2:1:414:ILE:HD11	2:1:473:LYS:HB3	1.69	0.73
27:W:113:VAL:HB	30:Z:316:TYR:CZ	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:506:CYS:N	29:Y:507:PRO:HD3	2.04	0.73
40:j:393:PRO:CD	41:k:137:ARG:NH2	2.52	0.73
49:s:99:GLU:HB3	49:s:103:ARG:NH2	2.03	0.73
50:t:90:LEU:O	50:t:93:LEU:N	2.21	0.73
54:x:118:ILE:HG13	54:x:119:GLN:HG3	1.69	0.73
27:W:109:ARG:CD	27:W:492:ASN:CG	2.60	0.73
27:W:129:VAL:N	27:W:334:ARG:HH22	1.86	0.73
30:Z:433:PHE:CB	33:c:9:LEU:HD21	2.18	0.73
42:l:76:PHE:CE1	42:l:86:ILE:HG23	2.24	0.73
44:n:53:ILE:CD1	56:z:629:ILE:CD1	2.66	0.73
48:r:160:VAL:O	48:r:163:THR:N	2.22	0.73
51:u:129:ASN:HA	51:u:132:LEU:HG	1.70	0.73
1:0:15:LEU:CD1	1:0:455:LEU:HD23	2.19	0.72
5:A:1657:TYR:CZ	35:e:61:ARG:NH1	2.57	0.72
8:D:70:ARG:HA	43:m:20:LYS:HZ3	1.54	0.72
28:X:297:ALA:CA	28:X:300:GLU:OE2	2.35	0.72
29:Y:422:LEU:HD11	32:b:224:LEU:HD23	1.70	0.72
29:Y:430:THR:HG21	32:b:225:GLN:HB3	1.71	0.72
39:i:78:PRO:HG2	40:j:197:ARG:HD2	0.73	0.72
54:x:75:SER:OG	54:x:76:LEU:N	2.18	0.72
41:k:137:ARG:NH1	41:k:142:LYS:HD3	2.03	0.72
52:v:102:MET:O	52:v:105:PHE:N	2.21	0.72
54:x:18:GLN:HE22	54:x:68:ASP:HB2	1.53	0.72
29:Y:496:ASN:O	29:Y:500:PHE:HD2	1.72	0.72
30:Z:442:VAL:HG21	33:c:9:LEU:CB	2.19	0.72
40:j:640:GLU:OE2	44:n:135:ARG:NH1	2.21	0.72
48:r:514:THR:HG23	48:r:540:ILE:HG23	1.71	0.72
54:x:126:ALA:HA	54:x:129:GLN:HE21	1.52	0.72
56:z:709:LYS:HG3	56:z:720:PRO:HG3	1.70	0.72
27:W:473:GLU:CD	27:W:632:SER:CA	2.57	0.72
40:j:367:HIS:CD2	40:j:438:ILE:CG2	2.72	0.72
40:j:412:ALA:HB1	42:l:76:PHE:HZ	1.51	0.72
43:m:111:GLU:OE2	45:o:146:ILE:HG23	1.89	0.72
5:A:1430:CYS:SG	5:A:1435:THR:OG1	2.47	0.72
8:D:142:TYR:CE2	43:m:21:ARG:O	2.42	0.72
43:m:122:GLU:HB3	45:o:135:LYS:HZ1	0.91	0.72
43:m:133:GLU:HG3	45:o:125:LYS:HE2	1.72	0.72
49:s:109:GLN:NE2	50:t:167:CYS:SG	2.63	0.72
49:s:145:SER:H	49:s:146:GLU:CD	1.98	0.72
54:x:51:THR:HA	54:x:54:TYR:CD2	2.25	0.72
55:y:77:GLU:O	55:y:80:GLN:HG2	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:191:GLU:OE2	6:B:743:ARG:NH1	2.22	0.72
30:Z:122:LEU:HD11	32:b:50:PHE:CZ	2.25	0.72
40:j:410:PRO:O	42:l:86:ILE:HG21	1.89	0.72
40:j:567:SER:HB2	40:j:585:GLY:HA2	1.72	0.72
43:m:115:LYS:HG3	45:o:146:ILE:CD1	2.20	0.72
48:r:130:VAL:HG12	54:x:27:GLN:HB2	1.71	0.72
53:w:103:GLU:O	53:w:107:ASN:N	2.23	0.72
9:E:121:MET:HE1	9:E:125:TYR:HB2	1.72	0.72
17:M:49:LYS:HZ1	18:N:18:SER:HB2	1.54	0.72
22:R:197:LYS:HG3	22:R:198:LYS:HG3	1.72	0.72
30:Z:41:CYS:HB2	30:Z:118:LEU:CD2	2.19	0.72
30:Z:122:LEU:HD11	32:b:50:PHE:CE2	2.25	0.72
35:e:17:PHE:CE2	48:r:68:VAL:HG11	2.25	0.72
50:t:132:ARG:O	50:t:135:LEU:N	2.22	0.72
8:D:70:ARG:CG	43:m:20:LYS:NZ	2.51	0.72
27:W:109:ARG:HH12	27:W:492:ASN:HA	1.21	0.72
27:W:689:VAL:HG12	30:Z:393:LEU:CD1	2.11	0.72
38:h:106:PRO:O	38:h:110:ARG:HG3	1.89	0.72
39:i:78:PRO:CG	40:j:197:ARG:CB	2.68	0.72
40:j:255:ALA:HB2	40:j:301:VAL:HA	1.72	0.72
40:j:317:GLN:O	40:j:319:LYS:N	2.22	0.72
40:j:412:ALA:N	42:l:86:ILE:HD13	2.05	0.72
41:k:147:LYS:NZ	41:k:164:SER:O	2.22	0.72
4:3:25:THR:OG1	4:3:104:MET:O	2.06	0.72
20:P:270:LEU:HD23	20:P:291:LEU:HB2	1.71	0.72
30:Z:442:VAL:HG21	33:c:9:LEU:HD22	1.71	0.72
49:s:122:ALA:HB1	49:s:126:TYR:OH	1.90	0.72
50:t:132:ARG:NH2	54:x:84:ALA:O	2.22	0.72
51:u:125:VAL:HG13	51:u:126:ARG:H	1.54	0.72
52:v:83:GLU:OE2	52:v:84:CYS:N	2.22	0.72
1:0:244:VAL:HG12	1:0:257:THR:HG22	1.71	0.72
8:D:70:ARG:HB2	43:m:20:LYS:NZ	2.02	0.72
21:Q:107:LEU:HD12	21:Q:111:ARG:CZ	2.20	0.72
22:R:131:GLU:HG3	22:R:140:LYS:HA	1.72	0.72
27:W:165:LYS:HG3	27:W:181:HIS:CE1	2.24	0.72
30:Z:58:ARG:HH11	32:b:241:LEU:CD2	2.01	0.72
40:j:398:ALA:CB	41:k:107:ASP:HB3	2.19	0.72
48:r:91:ARG:HH21	53:w:127:LEU:HD22	1.55	0.72
5:A:78:MET:O	6:B:1072:ARG:NH2	2.23	0.71
17:M:42:LEU:HB3	18:N:22:LEU:HG	1.72	0.71
1:0:16:ALA:CB	1:0:454:VAL:O	2.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:171:GLN:NE2	4:3:197:LYS:O	2.20	0.71
5:A:1626:SER:N	5:A:1627:PRO:CD	2.53	0.71
29:Y:381:ARG:HB3	32:b:256:PHE:CD2	2.24	0.71
43:m:115:LYS:CG	45:o:146:ILE:CD1	2.67	0.71
43:m:130:LEU:O	47:q:160:MET:CE	2.12	0.71
49:s:111:GLN:OE1	49:s:112:LYS:N	2.23	0.71
1:0:145:LEU:HD22	1:0:159:PHE:HD1	1.56	0.71
1:0:634:ASN:O	1:0:634:ASN:ND2	2.23	0.71
13:I:60:HIS:CD2	13:I:103:ARG:HE	2.08	0.71
18:N:60:GLY:HA3	18:N:78:ASP:HA	1.72	0.71
29:Y:512:ILE:O	29:Y:516:TYR:CE2	2.43	0.71
30:Z:400:ARG:HD2	33:c:16:MET:HG2	1.71	0.71
40:j:191:ARG:HH22	40:j:196:LEU:HB2	1.55	0.71
40:j:463:HIS:NE2	43:m:128:TYR:HE1	1.88	0.71
48:r:115:CYS:O	48:r:118:ILE:N	2.22	0.71
54:x:22:ALA:HA	54:x:61:LEU:HD13	1.71	0.71
55:y:25:VAL:O	55:y:27:CYS:N	2.23	0.71
5:A:1481:LYS:NZ	48:r:331:ALA:HB2	2.05	0.71
12:H:148:LEU:HD23	12:H:150:PHE:H	1.55	0.71
23:S:111:LYS:HB3	23:S:149:LEU:HD21	1.70	0.71
27:W:170:LEU:HD22	27:W:175:TYR:CE2	2.22	0.71
40:j:482:GLN:HB3	40:j:634:ASN:HD22	1.55	0.71
40:j:569:ILE:HG23	40:j:582:VAL:O	1.89	0.71
40:j:609:VAL:HG11	56:z:682:VAL:CG1	2.17	0.71
48:r:158:ILE:O	48:r:161:LEU:N	2.22	0.71
49:s:94:GLN:HG3	49:s:98:LYS:HE3	1.72	0.71
53:w:103:GLU:O	53:w:106:SER:N	2.23	0.71
3:2:7:LYS:HG3	3:2:49:GLN:HE21	1.56	0.71
27:W:159:CYS:C	27:W:163:TYR:CE2	2.69	0.71
33:c:6:LYS:H	33:c:6:LYS:HD2	1.55	0.71
44:n:166:ILE:HD11	44:n:204:MET:HE1	1.72	0.71
48:r:56:GLU:HB3	52:v:55:ARG:HD3	1.72	0.71
48:r:1387:ILE:O	48:r:1396:THR:C	2.32	0.71
49:s:181:GLU:O	49:s:184:SER:OG	2.05	0.71
29:Y:381:ARG:CD	32:b:256:PHE:HB3	2.20	0.71
30:Z:46:ARG:CZ	32:b:53:ARG:HD2	2.20	0.71
34:d:125:TYR:O	34:d:129:ASN:HB2	1.91	0.71
39:i:27:ASN:HB3	39:i:52:PHE:CG	2.25	0.71
44:n:215:LYS:HE2	44:n:232:SER:OG	1.90	0.71
55:y:60:ASP:HB2	55:y:63:TYR:CD1	2.26	0.71
8:D:78:GLU:HG3	38:h:51:LEU:HD22	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:400:ARG:HB3	33:c:16:MET:SD	2.30	0.71
40:j:336:PHE:HE1	40:j:500:GLU:HG3	1.53	0.71
43:m:131:GLU:N	47:q:160:MET:CE	2.42	0.71
48:r:169:LEU:HD13	48:r:173:ILE:HA	1.71	0.71
1:0:671:SER:HG	46:p:88:ILE:HD11	0.89	0.71
3:2:534:PRO:HD2	3:2:673:MET:HE3	1.72	0.71
5:A:1628:SER:O	5:A:1629:TYR:CD2	2.44	0.71
6:B:488:PRO:O	6:B:490:GLY:N	2.24	0.71
27:W:516:PRO:HG3	33:c:18:GLN:CD	2.14	0.71
29:Y:538:THR:O	29:Y:542:ARG:HG3	1.91	0.71
39:i:87:ARG:NH1	40:j:296:GLU:OE1	2.23	0.71
43:m:16:GLN:CG	43:m:20:LYS:HE3	2.20	0.71
48:r:610:THR:OG1	48:r:611:ASN:OD1	2.09	0.71
50:t:152:ARG:HH12	50:t:156:HIS:HB2	1.55	0.71
6:B:984:CYS:SG	6:B:1046:THR:OG1	2.40	0.71
28:X:305:LEU:CD1	28:X:391:LEU:HD13	2.20	0.71
29:Y:431:ILE:CG2	30:Z:62:LEU:HD11	2.19	0.71
40:j:191:ARG:NH1	40:j:203:ILE:HG21	2.04	0.71
43:m:35:GLU:OE2	43:m:64:ARG:NE	2.22	0.71
43:m:60:GLU:OE2	43:m:64:ARG:NH2	2.23	0.71
3:2:477:TYR:HB3	3:2:489:ARG:HD2	1.72	0.71
20:P:218:LYS:HE2	25:U:18:DG:OP1	1.87	0.71
30:Z:392:ARG:HG2	30:Z:392:ARG:NH1	2.05	0.71
33:c:8:VAL:HB	33:c:45:VAL:O	1.91	0.70
37:g:127:GLN:NE2	43:m:58:ASN:OD1	2.23	0.70
40:j:387:LEU:HD21	41:k:46:MET:HA	1.72	0.70
43:m:140:SER:HB3	47:q:146:ASN:CG	1.85	0.70
48:r:509:ILE:HD11	48:r:645:VAL:HG11	1.72	0.70
53:w:82:ASN:O	53:w:85:THR:N	2.19	0.70
1:0:60:ARG:HH21	1:0:60:ARG:HG2	1.56	0.70
4:3:125:PHE:CD2	4:3:178:ILE:CD1	2.74	0.70
28:X:292:LEU:HD22	28:X:318:ALA:O	1.91	0.70
29:Y:404:PHE:CE1	32:b:123:ASP:O	2.44	0.70
40:j:47:ILE:HD13	40:j:47:ILE:N	2.06	0.70
50:t:143:LYS:H	50:t:146:ARG:HH21	1.39	0.70
53:w:92:ALA:HA	53:w:95:LYS:HD2	1.73	0.70
55:y:32:ASN:O	55:y:35:ASN:N	2.24	0.70
2:1:942:ASP:HB3	2:1:943:PRO:HD3	1.72	0.70
6:B:941:GLN:HE22	6:B:972:ILE:HD13	1.57	0.70
37:g:79:PHE:HB2	37:g:100:ILE:HB	1.72	0.70
39:i:78:PRO:HG3	40:j:197:ARG:HB2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:115:LYS:HG3	45:o:146:ILE:HD12	1.74	0.70
46:p:85:ASN:ND2	56:z:641:THR:HG22	2.02	0.70
48:r:55:ILE:HA	48:r:58:LEU:HD13	1.72	0.70
52:v:62:THR:O	52:v:64:PRO:HD3	1.91	0.70
1:0:510:GLU:OE1	1:0:513:ARG:NH1	2.24	0.70
28:X:533:ASP:OD2	31:a:206:ARG:N	2.24	0.70
29:Y:414:TYR:CB	32:b:116:LYS:HE2	2.11	0.70
40:j:534:VAL:HG11	40:j:568:ALA:O	1.91	0.70
40:j:598:ARG:HH12	56:z:683:ALA:C	1.98	0.70
48:r:882:ILE:HD11	48:r:926:ILE:HD13	1.72	0.70
49:s:130:GLU:O	49:s:134:SER:OG	2.05	0.70
52:v:9:GLU:O	52:v:11:HIS:N	2.24	0.70
27:W:520:ARG:N	33:c:22:TYR:CE1	2.59	0.70
40:j:615:TRP:CZ2	56:z:680:GLY:HA2	2.26	0.70
55:y:112:ARG:HB3	55:y:112:ARG:CZ	2.21	0.70
3:2:417:VAL:HG21	3:2:451:LEU:HG	1.74	0.70
5:A:1657:TYR:CE1	35:e:61:ARG:NH1	2.58	0.70
17:M:355:ASP:N	17:M:368:SER:O	2.23	0.70
30:Z:121:ALA:O	32:b:100:LYS:C	2.35	0.70
52:v:106:LYS:O	52:v:109:LEU:HB3	1.90	0.70
54:x:122:LEU:O	54:x:125:ILE:HG13	1.92	0.70
5:A:389:THR:O	5:A:507:GLN:NE2	2.19	0.70
21:Q:75:ARG:H	21:Q:91:TYR:HB2	1.55	0.70
22:R:234:GLU:OE1	22:R:238:LYS:NZ	2.25	0.70
27:W:503:ALA:CB	27:W:646:ALA:CB	2.66	0.70
29:Y:136:VAL:O	29:Y:501:GLN:OE1	2.07	0.70
31:a:374:PHE:CZ	32:b:141:LEU:CB	2.72	0.70
48:r:181:ASP:OD1	48:r:181:ASP:N	2.22	0.70
49:s:34:LEU:HB3	51:u:98:ARG:HE	1.56	0.70
49:s:72:ARG:HA	49:s:75:GLU:HG3	1.74	0.70
50:t:81:LEU:HD11	50:t:118:HIS:HB3	1.74	0.70
6:B:754:PRO:HB2	6:B:773:PRO:HG2	1.73	0.70
20:P:262:CYS:SG	20:P:263:ASP:N	2.65	0.70
21:Q:107:LEU:CD1	21:Q:111:ARG:HH22	2.05	0.70
27:W:274:GLN:HE22	27:W:459:GLN:CG	1.95	0.70
29:Y:372:ILE:HG21	31:a:54:ARG:NH2	2.05	0.70
41:k:130:VAL:HG13	41:k:149:PHE:HB2	1.73	0.70
48:r:168:ARG:HG2	55:y:74:HIS:CE1	2.27	0.70
50:t:166:ASN:O	50:t:170:SER:N	2.22	0.70
54:x:18:GLN:HE22	54:x:68:ASP:CB	2.03	0.70
29:Y:464:LEU:CD2	29:Y:509:GLN:OE1	2.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:399:PRO:HD3	41:k:107:ASP:OD2	1.92	0.70
40:j:440:LEU:O	40:j:440:LEU:HD23	1.92	0.70
41:k:136:PHE:HB2	41:k:143:ILE:HG23	1.74	0.70
53:w:103:GLU:C	53:w:107:ASN:HB2	2.16	0.70
54:x:102:THR:OG1	54:x:103:CYS:N	2.21	0.70
4:3:23:GLU:OE1	4:3:26:ALA:N	2.21	0.69
21:Q:23:ARG:HD2	21:Q:31:ALA:HB1	1.73	0.69
25:U:57:DC:H42	26:V:37:DG:H1	1.38	0.69
27:W:503:ALA:HB2	27:W:646:ALA:CB	2.13	0.69
40:j:464:TRP:HA	40:j:475:VAL:CG2	2.14	0.69
48:r:657:LEU:CD2	48:r:682:ILE:CD1	2.70	0.69
52:v:67:VAL:HA	52:v:70:TYR:HB3	1.73	0.69
1:O:264:PHE:CD1	3:2:541:ASN:HB2	2.26	0.69
5:A:602:CYS:HB2	5:A:655:ILE:HD11	1.73	0.69
6:B:438:ARG:O	6:B:442:ASP:HB2	1.91	0.69
27:W:275:GLU:CA	27:W:456:THR:HG23	2.22	0.69
29:Y:449:ILE:CG2	29:Y:450:ASN:H	2.05	0.69
54:x:66:ALA:O	54:x:69:ILE:HG12	1.92	0.69
19:O:189:LYS:HE3	25:U:12:DA:OP1	1.92	0.69
29:Y:480:PRO:HD2	29:Y:481:VAL:N	2.07	0.69
48:r:233:THR:CG2	48:r:248:LEU:HB3	2.20	0.69
53:w:91:GLN:OE1	53:w:91:GLN:N	2.24	0.69
54:x:93:LEU:O	54:x:97:ASN:ND2	2.25	0.69
56:z:731:ALA:N	56:z:766:LYS:HZ2	1.88	0.69
5:A:538:VAL:HG12	5:A:539:GLN:H	1.58	0.69
5:A:1629:TYR:C	37:g:13:ILE:CD1	2.51	0.69
21:Q:36:ILE:HD11	22:R:163:LEU:HD22	1.75	0.69
30:Z:57:MET:CE	32:b:51:MET:HG3	2.15	0.69
35:e:43:ILE:HD13	35:e:87:ILE:HG13	1.73	0.69
48:r:136:LEU:O	48:r:139:LEU:N	2.26	0.69
49:s:152:ALA:O	49:s:156:SER:OG	2.06	0.69
52:v:69:GLU:HA	52:v:72:ASP:HB2	1.73	0.69
52:v:112:GLU:HA	52:v:115:LYS:HB2	1.74	0.69
5:A:998:PRO:O	5:A:1059:ARG:NH1	2.25	0.69
6:B:51:ILE:HD12	6:B:160:TYR:CD2	2.27	0.69
27:W:109:ARG:HH11	27:W:492:ASN:HA	0.87	0.69
27:W:172:HIS:N	27:W:461:HIS:CE1	2.59	0.69
27:W:379:LYS:HE2	27:W:386:ASP:CG	2.17	0.69
55:y:84:PHE:HB2	55:y:85:ARG:NH1	2.08	0.69
6:B:873:LEU:HD12	6:B:888:THR:HA	1.73	0.69
27:W:278:GLU:CD	27:W:452:ARG:CG	2.63	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:449:ILE:CG2	29:Y:450:ASN:N	2.56	0.69
42:l:148:VAL:CG2	44:n:196:LYS:HB3	2.22	0.69
43:m:130:LEU:CA	47:q:160:MET:HE3	1.98	0.69
48:r:1411:ALA:HB1	48:r:1413:MET:HE2	1.75	0.69
3:2:898:ASN:HD22	3:2:944:LEU:HD22	1.56	0.69
5:A:364:ARG:HH11	5:A:502:ASN:HD21	1.40	0.69
11:G:10:GLU:HB3	11:G:67:LEU:HD11	1.73	0.69
29:Y:524:HIS:CE1	31:a:270:SER:HB3	2.26	0.69
30:Z:61:PHE:CD2	32:b:228:LEU:CD1	2.43	0.69
40:j:186:GLU:OE1	40:j:291:TRP:CZ3	2.45	0.69
40:j:622:PHE:CE1	48:r:675:GLY:HA3	2.28	0.69
48:r:942:SER:O	48:r:945:ASP:O	2.09	0.69
50:t:141:VAL:O	50:t:144:ARG:HB3	1.92	0.69
56:z:721:LEU:CD2	56:z:736:TRP:CZ3	2.75	0.69
3:2:273:MET:HE2	3:2:815:TRP:HA	1.74	0.69
6:B:347:MET:O	6:B:361:LYS:NZ	2.26	0.69
17:M:337:CYS:HB3	17:M:356:GLY:HA2	1.75	0.69
17:M:349:TRP:HB2	17:M:374:ALA:HB3	1.75	0.69
21:Q:107:LEU:CD1	21:Q:111:ARG:NH2	2.55	0.69
27:W:640:LEU:HD22	27:W:685:TYR:CE2	2.27	0.69
30:Z:122:LEU:HD21	32:b:104:LEU:HD11	1.75	0.69
40:j:191:ARG:HH22	40:j:196:LEU:CB	2.02	0.69
40:j:617:HIS:CE1	48:r:741:PRO:HB2	2.28	0.69
48:r:54:LEU:HD23	53:w:131:ILE:HD12	1.73	0.69
48:r:135:ARG:HH12	50:t:108:LYS:HE2	1.56	0.69
48:r:202:ARG:HG2	48:r:243:VAL:N	2.07	0.69
48:r:1265:VAL:HG12	48:r:1267:PRO:HD3	1.73	0.69
52:v:66:GLU:O	52:v:69:GLU:N	2.26	0.69
55:y:64:ALA:C	55:y:66:TYR:H	2.01	0.69
55:y:82:GLU:OE1	55:y:82:GLU:N	2.26	0.69
8:D:129:GLN:HG3	38:h:65:HIS:ND1	2.06	0.69
23:S:46:ARG:HA	23:S:100:LEU:HD21	1.75	0.69
27:W:274:GLN:CA	27:W:459:GLN:HE21	1.86	0.69
27:W:295:TYR:CD2	27:W:333:ALA:O	2.45	0.69
27:W:640:LEU:CD2	27:W:685:TYR:OH	2.41	0.69
40:j:198:LYS:HB2	43:m:88:LEU:HD21	1.66	0.69
40:j:415:LYS:CG	42:l:116:ARG:HH12	2.06	0.69
40:j:546:TRP:CZ2	40:j:643:MET:HG2	2.28	0.69
43:m:115:LYS:HG2	45:o:139:TRP:HZ3	1.57	0.69
44:n:53:ILE:HD11	56:z:629:ILE:HD11	1.75	0.69
48:r:151:SER:OG	49:s:156:SER:O	2.11	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:21:GLN:O	52:v:21:GLN:NE2	2.26	0.69
2:1:755:ASN:HA	2:1:758:LYS:HD3	1.75	0.69
5:A:100:LEU:HD23	5:A:193:ARG:HE	1.58	0.69
29:Y:374:LEU:HB2	31:a:54:ARG:HG2	1.74	0.69
30:Z:122:LEU:CD1	32:b:50:PHE:CD1	2.76	0.69
30:Z:433:PHE:HE2	33:c:38:ILE:CG1	2.06	0.69
40:j:612:ASP:OD1	40:j:614:LYS:N	2.25	0.69
48:r:1421:ARG:HG2	48:r:1425:MET:HE1	1.75	0.69
27:W:124:TYR:OH	27:W:291:LEU:O	2.10	0.68
29:Y:415:THR:OG1	32:b:112:VAL:CG1	2.41	0.68
40:j:514:LEU:HD12	40:j:520:GLU:HB3	1.75	0.68
40:j:549:LEU:HB3	48:r:711:ARG:HD2	1.75	0.68
40:j:553:ASN:O	40:j:568:ALA:HB2	1.93	0.68
41:k:55:GLU:OE2	41:k:73:ARG:NE	2.26	0.68
5:A:79:THR:HG21	19:O:43:ASP:HB3	1.75	0.68
5:A:1622:TYR:HH	37:g:118:ARG:HH12	1.41	0.68
27:W:351:VAL:CG2	27:W:378:PHE:CE1	2.76	0.68
35:e:40:ILE:HG12	35:e:90:VAL:HG22	1.76	0.68
35:e:164:SER:HG	35:e:167:ARG:HD3	1.58	0.68
43:m:133:GLU:CD	45:o:125:LYS:CE	2.65	0.68
1:O:15:LEU:HD12	1:O:453:SER:HB3	1.76	0.68
13:I:29:ASP:HB2	13:I:36:LEU:HD13	1.76	0.68
27:W:295:TYR:HE1	27:W:461:HIS:HB3	1.57	0.68
29:Y:498:GLU:O	29:Y:502:VAL:CG2	2.33	0.68
30:Z:433:PHE:CD1	33:c:42:HIS:NE2	2.62	0.68
37:g:61:ASN:O	37:g:86:ARG:NH1	2.25	0.68
40:j:409:GLY:CA	42:l:74:SER:OG	2.41	0.68
40:j:567:SER:HB2	40:j:585:GLY:HA3	1.72	0.68
48:r:93:ARG:O	48:r:97:VAL:HG23	1.93	0.68
51:u:125:VAL:O	51:u:129:ASN:HB2	1.92	0.68
52:v:79:LEU:O	52:v:83:GLU:HG3	1.93	0.68
54:x:3:ASP:OD2	54:x:4:ARG:NH1	2.26	0.68
5:A:57:LEU:O	5:A:261:ARG:NH2	2.26	0.68
28:X:591:GLY:H	31:a:207:VAL:HG21	0.97	0.68
29:Y:431:ILE:HG21	30:Z:62:LEU:HD11	1.75	0.68
29:Y:503:THR:O	29:Y:507:PRO:CG	2.41	0.68
52:v:101:THR:HB	54:x:26:LEU:HD23	1.75	0.68
1:O:812:ARG:NH1	46:p:90:ASN:O	2.27	0.68
18:N:58:PHE:HB3	18:N:81:PHE:HD1	1.59	0.68
27:W:85:PHE:CD2	30:Z:338:PHE:CE2	2.69	0.68
42:l:21:VAL:HG21	42:l:128:THR:HG22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:40:ARG:HD3	55:y:42:TYR:HE2	1.58	0.68
8:D:78:GLU:CD	38:h:51:LEU:HB3	2.15	0.68
21:Q:148:MET:HE3	41:k:200:GLU:CB	2.23	0.68
35:e:226:PHE:HB3	35:e:231:THR:HG22	1.75	0.68
40:j:203:ILE:HD12	43:m:88:LEU:HD21	1.74	0.68
41:k:55:GLU:CG	41:k:73:ARG:HG2	2.17	0.68
49:s:123:THR:HA	49:s:126:TYR:CD2	2.28	0.68
52:v:99:ILE:O	52:v:102:MET:HB2	1.94	0.68
52:v:120:ASP:O	52:v:124:TYR:N	2.27	0.68
4:3:147:ASN:O	4:3:186:ARG:NH2	2.27	0.68
5:A:967:ARG:NH2	5:A:1326:GLY:O	2.26	0.68
5:A:1098:PRO:HG2	5:A:1386:ILE:HD12	1.75	0.68
21:Q:48:MET:HA	21:Q:48:MET:HE3	1.75	0.68
28:X:591:GLY:HA2	31:a:207:VAL:HB	1.73	0.68
29:Y:471:LEU:HD22	29:Y:502:VAL:HG21	1.76	0.68
34:d:295:ARG:HD2	35:e:163:GLY:HA3	1.76	0.68
40:j:412:ALA:H	42:l:86:ILE:CD1	2.05	0.68
48:r:135:ARG:O	48:r:138:SER:OG	2.12	0.68
49:s:86:GLN:HA	49:s:89:ILE:HG22	1.75	0.68
51:u:117:GLN:O	51:u:120:SER:OG	2.12	0.68
7:C:7:PRO:O	15:K:104:ARG:NH1	2.27	0.68
27:W:77:TRP:CE3	30:Z:341:MET:HE1	2.29	0.68
27:W:171:LYS:CA	27:W:461:HIS:CE1	2.71	0.68
31:a:320:ARG:NH2	32:b:182:PHE:CE1	2.57	0.68
40:j:336:PHE:HZ	40:j:500:GLU:CB	2.07	0.68
48:r:666:ILE:HG21	48:r:684:LEU:HD22	1.76	0.68
52:v:15:PHE:O	52:v:19:ILE:HG13	1.94	0.68
1:0:832:LEU:H	1:0:832:LEU:CD2	2.00	0.68
3:2:73:VAL:HG23	3:2:74:SER:H	1.57	0.68
20:P:257:ASN:HD22	25:U:15:DA:H5'	1.59	0.68
20:P:295:MET:HE2	20:P:298:PRO:HG2	1.74	0.68
24:T:86:GLN:HE22	24:T:115:GLU:HB2	1.57	0.68
30:Z:61:PHE:CE1	32:b:228:LEU:HD11	2.28	0.68
39:i:44:LEU:O	39:i:48:GLN:HG2	1.94	0.68
40:j:478:LEU:HD23	40:j:478:LEU:C	2.18	0.68
48:r:165:SER:C	48:r:167:PRO:HD3	2.19	0.68
52:v:3:GLU:HA	52:v:6:ASP:HB2	1.76	0.68
52:v:70:TYR:HE2	52:v:80:TYR:HB2	1.57	0.68
52:v:82:LYS:O	52:v:85:LEU:HB3	1.94	0.68
7:C:54:ALA:HB3	7:C:160:ARG:HB2	1.75	0.68
8:D:141:GLN:HE21	43:m:70:ARG:NH1	1.89	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:51:LEU:HB3	23:S:99:LEU:HD13	1.74	0.68
23:S:96:GLN:HG3	23:S:97:PRO:HD2	1.76	0.68
27:W:295:TYR:CB	27:W:333:ALA:O	2.42	0.68
29:Y:510:GLU:CD	29:Y:526:GLU:OE2	2.36	0.68
30:Z:41:CYS:SG	30:Z:114:PHE:HE1	2.12	0.68
30:Z:61:PHE:CE2	32:b:228:LEU:HD22	2.29	0.68
35:e:125:LEU:HD21	35:e:195:ASP:HB3	1.75	0.68
42:l:174:ALA:O	42:l:178:ASN:N	2.27	0.68
43:m:115:LYS:HE3	45:o:142:VAL:O	1.94	0.68
48:r:156:TYR:O	48:r:160:VAL:N	2.21	0.68
50:t:74:HIS:O	50:t:126:TYR:OH	2.10	0.68
52:v:53:LYS:O	52:v:56:GLN:NE2	2.27	0.68
1:0:138:HIS:HB2	1:0:220:PHE:CD2	2.28	0.67
24:T:170:LYS:HG3	24:T:171:GLU:HG2	1.75	0.67
28:X:305:LEU:HD21	28:X:391:LEU:HD13	1.75	0.67
40:j:463:HIS:NE2	43:m:128:TYR:CE1	2.60	0.67
52:v:83:GLU:CD	52:v:84:CYS:H	2.02	0.67
54:x:7:GLN:N	54:x:7:GLN:OE1	2.25	0.67
54:x:15:LEU:O	54:x:19:PHE:CD2	2.47	0.67
1:0:832:LEU:HD22	1:0:832:LEU:N	2.05	0.67
12:H:60:ILE:HD11	12:H:123:MET:HE1	1.75	0.67
20:P:168:ILE:HG23	20:P:258:MET:HB3	1.76	0.67
30:Z:46:ARG:CZ	32:b:53:ARG:CB	2.41	0.67
30:Z:313:TYR:CE2	30:Z:394:TRP:HZ2	2.10	0.67
46:p:84:GLN:HE22	46:p:95:SER:HB2	1.59	0.67
48:r:230:PHE:HZ	48:r:296:LEU:HD21	1.58	0.67
56:z:719:PRO:HB3	56:z:742:GLN:NE2	2.00	0.67
27:W:85:PHE:HZ	30:Z:336:TYR:CD1	1.99	0.67
28:X:300:GLU:CB	28:X:304:HIS:HE2	2.06	0.67
28:X:310:LEU:HG	28:X:405:THR:HG22	1.74	0.67
30:Z:123:LEU:CA	32:b:100:LYS:HG2	2.25	0.67
39:i:114:MET:HE2	47:q:159:ILE:CD1	2.13	0.67
40:j:410:PRO:CA	42:l:86:ILE:HG22	2.21	0.67
40:j:491:ILE:CD1	40:j:532:HIS:N	2.57	0.67
44:n:49:GLU:OE1	56:z:629:ILE:HG22	1.88	0.67
54:x:21:ASN:O	54:x:24:GLY:N	2.28	0.67
54:x:74:ASP:C	54:x:77:PRO:HD2	2.17	0.67
54:x:86:GLN:O	54:x:89:SER:OG	2.11	0.67
3:2:915:ARG:HH12	56:z:702:GLY:H	1.40	0.67
21:Q:20:TYR:O	21:Q:23:ARG:NH2	2.27	0.67
33:c:6:LYS:HZ2	33:c:6:LYS:CA	2.07	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:140:SER:CB	47:q:146:ASN:CA	2.35	0.67
44:n:107:LEU:HD13	46:p:164:ILE:HG23	1.76	0.67
48:r:173:ILE:HD12	48:r:173:ILE:H	1.58	0.67
48:r:792:ALA:O	48:r:796:ILE:HG22	1.93	0.67
50:t:136:ARG:NH1	54:x:89:SER:OG	2.27	0.67
52:v:40:LYS:HA	52:v:43:PHE:CD2	2.29	0.67
1:0:115:ALA:HB3	1:0:834:TRP:CE3	2.30	0.67
4:3:123:GLN:CG	4:3:160:THR:HG21	2.25	0.67
28:X:307:ASN:CB	28:X:308:PRO:CD	2.71	0.67
30:Z:97:HIS:CE1	30:Z:112:PRO:HD3	2.28	0.67
37:g:123:VAL:HG22	38:h:56:LEU:HD21	1.75	0.67
40:j:190:LEU:HD12	40:j:291:TRP:CD1	2.29	0.67
48:r:64:SER:HA	48:r:67:MET:HG2	1.76	0.67
48:r:123:ASP:O	48:r:127:ILE:HG12	1.95	0.67
49:s:109:GLN:C	49:s:113:GLN:HE21	2.02	0.67
49:s:187:LEU:O	49:s:190:MET:N	2.27	0.67
52:v:23:GLY:HA2	52:v:26:VAL:HG12	1.74	0.67
52:v:124:TYR:HD1	52:v:127:ILE:HB	1.60	0.67
1:0:19:CYS:HB3	1:0:750:LEU:HB2	1.76	0.67
3:2:602:ILE:HD11	3:2:642:MET:HE3	1.76	0.67
5:A:220:ARG:NH1	22:R:227:SER:OG	2.24	0.67
29:Y:527:GLU:OE1	31:a:268:LYS:CG	2.42	0.67
30:Z:442:VAL:HG21	33:c:9:LEU:CD2	2.24	0.67
49:s:179:ASP:C	49:s:183:ARG:HE	2.02	0.67
54:x:3:ASP:CG	54:x:4:ARG:HD3	2.20	0.67
1:0:832:LEU:N	1:0:832:LEU:HD13	2.08	0.67
5:A:67:ARG:HD2	19:O:46:ILE:HG22	1.76	0.67
5:A:344:LYS:HG2	5:A:345:GLY:H	1.59	0.67
7:C:143:VAL:HG13	7:C:145:GLN:HG2	1.75	0.67
8:D:141:GLN:CB	43:m:70:ARG:CZ	2.73	0.67
23:S:110:PHE:HB3	23:S:148:PRO:HA	1.77	0.67
28:X:487:ARG:HE	28:X:724:MET:HG2	1.59	0.67
36:f:238:LEU:HB3	36:f:245:LEU:HB2	1.76	0.67
48:r:202:ARG:HD3	48:r:243:VAL:CA	2.25	0.67
17:M:357:ILE:HG23	17:M:366:ILE:HG22	1.75	0.67
30:Z:440:LEU:CD2	33:c:36:GLN:HE21	1.91	0.67
35:e:209:ARG:HH12	37:g:53:GLN:NE2	1.92	0.67
50:t:119:VAL:O	50:t:122:LEU:HB3	1.95	0.67
51:u:133:GLN:O	51:u:137:SER:N	2.28	0.67
54:x:53:GLU:O	54:x:57:LEU:HG	1.95	0.67
54:x:67:LYS:HA	54:x:70:ASP:OD2	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:285:LEU:HD23	6:B:298:MET:HE1	1.76	0.67
20:P:161:ILE:H	20:P:325:PHE:HE2	1.43	0.67
21:Q:24:GLY:HA2	22:R:209:GLN:HG2	1.75	0.67
48:r:221:ARG:HH11	48:r:221:ARG:CB	2.08	0.67
48:r:568:TYR:CE2	48:r:641:LEU:HG	2.29	0.67
50:t:89:PHE:O	50:t:92:LEU:HB2	1.94	0.67
50:t:105:ARG:N	50:t:108:LYS:H	1.92	0.67
52:v:96:LYS:NZ	53:w:83:LEU:HD11	2.09	0.67
54:x:105:GLU:O	54:x:108:VAL:N	2.28	0.67
55:y:82:GLU:OE1	55:y:83:HIS:N	2.28	0.67
6:B:601:VAL:HG23	6:B:616:THR:HG22	1.74	0.67
22:R:141:PRO:HB2	22:R:144:ASN:HB3	1.76	0.67
28:X:293:ARG:HH22	28:X:378:ARG:HD3	1.59	0.67
40:j:464:TRP:HZ3	40:j:497:ILE:HD12	1.60	0.67
48:r:1247:LEU:HG	48:r:1267:PRO:HG3	1.76	0.67
49:s:107:ILE:HA	49:s:110:LEU:HD12	1.76	0.67
52:v:22:LEU:HD21	52:v:40:LYS:HB3	1.76	0.67
54:x:82:THR:O	54:x:86:GLN:NE2	2.28	0.67
40:j:371:LEU:HD21	40:j:434:GLN:HB3	1.77	0.66
52:v:65:LEU:C	52:v:68:PHE:HB2	2.20	0.66
55:y:31:PRO:O	55:y:32:ASN:C	2.37	0.66
55:y:56:LEU:O	55:y:59:LYS:NZ	2.28	0.66
55:y:91:ALA:C	55:y:94:ALA:H	2.02	0.66
3:2:196:LEU:HD13	3:2:199:LEU:HD22	1.77	0.66
33:c:5:LEU:HD12	33:c:5:LEU:N	2.11	0.66
35:e:158:LEU:HD12	35:e:173:VAL:HB	1.76	0.66
37:g:65:GLY:O	37:g:86:ARG:N	2.21	0.66
44:n:215:LYS:HB3	44:n:219:GLU:HG3	1.77	0.66
49:s:191:ASN:HA	49:s:194:SER:C	2.21	0.66
50:t:146:ARG:HH12	54:x:97:ASN:HB3	1.58	0.66
54:x:116:GLU:HA	54:x:119:GLN:OE1	1.95	0.66
5:A:621:ILE:HG12	12:H:27:ARG:HH12	1.60	0.66
7:C:67:ARG:NH2	14:J:3:ILE:O	2.26	0.66
27:W:112:HIS:CG	30:Z:310:GLU:OE2	2.48	0.66
31:a:249:LEU:HB2	32:b:289:PHE:HE1	1.61	0.66
46:p:104:LYS:NZ	48:r:948:LYS:HZ2	1.92	0.66
50:t:143:LYS:N	50:t:146:ARG:HH21	1.93	0.66
52:v:65:LEU:O	52:v:68:PHE:HB2	1.95	0.66
52:v:75:ARG:HD2	53:w:105:LEU:HD23	1.77	0.66
6:B:223:SER:O	6:B:233:SER:OG	2.13	0.66
8:D:78:GLU:OE2	38:h:48:SER:HA	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:108:ILE:HG13	11:G:109:SER:H	1.60	0.66
30:Z:41:CYS:CB	30:Z:118:LEU:CD2	2.73	0.66
30:Z:346:VAL:O	30:Z:394:TRP:HZ3	1.76	0.66
42:l:147:CYS:SG	42:l:148:VAL:N	2.68	0.66
43:m:140:SER:OG	47:q:146:ASN:HA	1.95	0.66
48:r:168:ARG:CZ	55:y:73:LEU:HD11	2.26	0.66
48:r:1293:PRO:HB3	48:r:1295:LYS:HZ3	1.60	0.66
55:y:43:PHE:C	55:y:44:LYS:HD2	2.19	0.66
2:1:842:GLN:O	2:1:846:CYS:N	2.29	0.66
25:U:60:DG:C4'	27:W:528:LYS:HE2	2.25	0.66
30:Z:433:PHE:CZ	33:c:42:HIS:CD2	2.82	0.66
40:j:619:ARG:HH21	48:r:744:HIS:CE1	2.13	0.66
50:t:112:LEU:O	50:t:115:LEU:N	2.29	0.66
50:t:143:LYS:CA	50:t:146:ARG:HE	2.08	0.66
1:0:515:THR:HG23	1:0:517:ALA:H	1.59	0.66
2:1:102:ILE:HD11	2:1:137:LEU:HG	1.76	0.66
2:1:1034:LEU:HD23	2:1:1038:ARG:HE	1.60	0.66
3:2:165:LEU:HD22	3:2:221:LEU:HD12	1.77	0.66
3:2:568:LYS:HD2	3:2:570:VAL:HG22	1.76	0.66
3:2:953:SER:O	3:2:957:LYS:HG2	1.96	0.66
9:E:54:ARG:NH2	9:E:107:GLN:OE1	2.29	0.66
21:Q:72:ILE:HG22	21:Q:94:ILE:HA	1.78	0.66
27:W:159:CYS:HB3	27:W:163:TYR:HE2	1.60	0.66
29:Y:440:LEU:HD12	32:b:226:TYR:CE1	2.28	0.66
29:Y:527:GLU:OE1	31:a:268:LYS:CB	2.43	0.66
37:g:25:ASN:O	37:g:28:SER:OG	2.09	0.66
39:i:97:VAL:HG23	45:o:147:ASN:ND2	2.11	0.66
40:j:592:ILE:HD12	40:j:627:TRP:HZ2	1.61	0.66
50:t:151:GLU:O	50:t:155:LYS:HG2	1.96	0.66
52:v:11:HIS:CE1	52:v:12:LEU:HB2	2.30	0.66
1:0:589:ASP:HB2	1:0:698:ILE:HD11	1.78	0.66
6:B:463:ARG:HE	6:B:466:VAL:HG21	1.61	0.66
30:Z:46:ARG:HH12	32:b:53:ARG:CD	2.05	0.66
30:Z:61:PHE:CZ	32:b:47:SER:OG	2.45	0.66
30:Z:313:TYR:CD2	30:Z:394:TRP:CZ2	2.83	0.66
48:r:86:VAL:O	48:r:90:SER:OG	2.14	0.66
48:r:93:ARG:NH2	52:v:19:ILE:O	2.27	0.66
54:x:105:GLU:O	54:x:108:VAL:HG22	1.96	0.66
56:z:721:LEU:HD21	56:z:736:TRP:CE3	2.30	0.66
1:0:338:LYS:HD3	1:0:340:ARG:HH21	1.60	0.66
3:2:170:SER:HA	3:2:174:ASN:HB3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:41:LEU:HD23	8:D:65:LEU:HD22	1.78	0.66
21:Q:136:PHE:O	21:Q:137:THR:OG1	2.13	0.66
31:a:249:LEU:HD12	32:b:268:CYS:HA	1.78	0.66
40:j:563:ILE:HG12	40:j:587:GLU:HG3	1.76	0.66
44:n:303:GLU:OE1	44:n:303:GLU:N	2.29	0.66
48:r:654:PHE:CE2	48:r:680:HIS:HB2	2.31	0.66
54:x:112:ASP:N	54:x:112:ASP:OD1	2.25	0.66
1:O:166:PRO:HB3	1:O:175:PRO:HB3	1.78	0.66
6:B:196:ALA:HB2	6:B:395:LEU:HD13	1.78	0.66
22:R:158:HIS:O	22:R:162:GLY:N	2.29	0.66
27:W:379:LYS:HE2	27:W:386:ASP:OD1	1.96	0.66
28:X:307:ASN:OD1	28:X:380:ARG:CZ	2.43	0.66
30:Z:122:LEU:CD1	32:b:50:PHE:CZ	2.78	0.66
36:f:177:ARG:NH2	36:f:235:SER:O	2.29	0.66
40:j:336:PHE:CZ	40:j:500:GLU:HB2	2.31	0.66
48:r:234:LEU:HB3	48:r:246:ARG:O	1.95	0.66
50:t:158:GLU:O	50:t:161:ILE:HG22	1.96	0.66
54:x:54:TYR:HA	54:x:57:LEU:HD12	1.76	0.66
2:1:475:ALA:O	2:1:479:ASN:HB2	1.95	0.65
30:Z:122:LEU:CD2	32:b:50:PHE:HE1	2.03	0.65
30:Z:403:PHE:CE2	33:c:54:GLN:CD	2.61	0.65
40:j:410:PRO:C	42:l:86:ILE:HB	2.21	0.65
41:k:27:VAL:HG21	41:k:35:LEU:HD13	1.78	0.65
41:k:37:HIS:HD2	43:m:92:PRO:HA	1.60	0.65
48:r:301:LEU:HD13	48:r:361:ILE:HG13	1.79	0.65
48:r:793:HIS:O	48:r:796:ILE:HG23	1.97	0.65
48:r:890:MET:HB2	48:r:893:LEU:HD21	1.78	0.65
52:v:11:HIS:NE2	52:v:12:LEU:HB2	2.11	0.65
1:O:795:CYS:SG	1:O:836:VAL:HG21	2.36	0.65
27:W:519:TYR:CD2	33:c:22:TYR:CG	2.84	0.65
28:X:468:PRO:HA	28:X:473:PHE:HB3	1.78	0.65
30:Z:440:LEU:CD1	33:c:36:GLN:HE21	1.90	0.65
40:j:43:LEU:HD13	48:r:191:THR:HG21	1.77	0.65
40:j:367:HIS:NE2	40:j:438:ILE:CG2	2.60	0.65
40:j:410:PRO:HB2	41:k:111:SER:HB3	1.78	0.65
41:k:143:ILE:HD13	41:k:171:LEU:HD12	1.78	0.65
48:r:122:LEU:HD13	52:v:91:LYS:HB2	1.79	0.65
54:x:69:ILE:O	54:x:73:ILE:HG12	1.95	0.65
5:A:126:ILE:HD13	5:A:129:ILE:HD11	1.77	0.65
6:B:634:LEU:HB3	6:B:661:VAL:HG12	1.78	0.65
24:T:30:GLN:O	24:T:34:ALA:HB2	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:318:PRO:CD	27:W:501:TYR:OH	2.42	0.65
40:j:592:ILE:HD12	40:j:627:TRP:CZ2	2.31	0.65
42:l:121:ASP:OD1	44:n:236:TYR:CA	2.44	0.65
53:w:90:GLU:O	53:w:93:TYR:HB3	1.96	0.65
56:z:703:THR:HB	56:z:725:VAL:O	1.95	0.65
1:0:129:ASP:OD1	1:0:129:ASP:N	2.23	0.65
1:0:812:ARG:HH21	46:p:90:ASN:CB	2.03	0.65
3:2:971:THR:HG21	3:2:982:ALA:HB2	1.78	0.65
5:A:1620:PRO:HB2	38:h:104:VAL:HG11	1.78	0.65
20:P:294:ARG:CZ	25:U:14:DA:OP1	2.44	0.65
24:T:87:SER:OG	24:T:88:VAL:N	2.29	0.65
27:W:471:VAL:HB	27:W:634:ARG:HE	0.70	0.65
36:f:218:LEU:HD12	36:f:252:MET:HE1	1.77	0.65
40:j:546:TRP:CE2	40:j:643:MET:HG2	2.31	0.65
44:n:96:PRO:HG2	48:r:1334:TRP:CB	2.26	0.65
48:r:102:LEU:O	48:r:106:ALA:CB	2.44	0.65
3:2:436:LEU:HD22	3:2:491:LEU:HD21	1.78	0.65
29:Y:421:VAL:HG22	32:b:39:ASP:HB3	1.79	0.65
37:g:85:GLN:HB2	37:g:93:ILE:HG13	1.78	0.65
38:h:60:ASN:O	38:h:64:LYS:HG2	1.96	0.65
40:j:487:ILE:HG13	40:j:543:VAL:HG22	1.78	0.65
48:r:247:LEU:C	48:r:247:LEU:HD12	2.22	0.65
49:s:103:ARG:CZ	51:u:121:LEU:HD13	2.26	0.65
50:t:128:PRO:O	50:t:131:ALA:HB3	1.96	0.65
55:y:36:PHE:O	55:y:40:ARG:CB	2.42	0.65
5:A:94:VAL:HG21	5:A:314:VAL:HG11	1.78	0.65
6:B:776:ILE:HD11	14:J:8:PHE:CE2	2.32	0.65
22:R:227:SER:HB3	22:R:230:GLU:HB2	1.77	0.65
31:a:254:PHE:HE2	32:b:274:ILE:CG2	2.08	0.65
41:k:50:THR:HG22	41:k:51:PHE:H	1.61	0.65
50:t:76:LYS:N	50:t:77:GLU:OE1	2.29	0.65
52:v:121:MET:O	52:v:124:TYR:HB2	1.95	0.65
1:0:806:MET:SD	1:0:810:PRO:HG2	2.36	0.65
18:N:2:ALA:HB1	18:N:41:ASP:HB3	1.77	0.65
22:R:144:ASN:HA	22:R:173:GLU:HB2	1.78	0.65
27:W:282:LYS:HE2	27:W:478:VAL:HG11	1.78	0.65
28:X:311:PRO:HD3	28:X:410:TYR:OH	1.96	0.65
52:v:13:GLU:O	52:v:16:VAL:HG22	1.97	0.65
55:y:125:GLN:O	55:y:128:THR:OG1	2.13	0.65
27:W:85:PHE:HZ	30:Z:336:TYR:CE1	2.07	0.65
35:e:113:HIS:CD2	35:e:308:PRO:HD3	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:546:TRP:HD1	40:j:574:PRO:HA	1.60	0.65
49:s:134:SER:O	49:s:137:LYS:N	2.30	0.65
55:y:110:ARG:CB	55:y:110:ARG:HH11	2.09	0.65
56:z:689:PHE:HZ	56:z:777:ALA:HB2	1.62	0.65
20:P:242:GLN:HB2	20:P:248:ALA:HB3	1.79	0.65
29:Y:372:ILE:CG2	31:a:54:ARG:NH2	2.60	0.65
29:Y:476:TRP:HB2	31:a:307:ILE:O	1.97	0.65
30:Z:58:ARG:HH21	32:b:237:GLN:HB3	1.62	0.65
40:j:608:ASP:HB3	56:z:693:LEU:CD2	2.11	0.65
43:m:134:TYR:CE2	47:q:157:LYS:CD	2.80	0.65
48:r:150:PRO:HG3	54:x:9:GLN:HE22	1.62	0.65
49:s:140:LYS:O	49:s:144:SER:OG	2.12	0.65
55:y:25:VAL:O	55:y:26:GLN:C	2.39	0.65
5:A:353:ASN:HD22	6:B:1073:GLN:HG3	1.62	0.65
11:G:123:SER:C	38:h:167:ARG:NH2	2.55	0.65
25:U:59:DC:H5"	27:W:629:HIS:HE2	1.62	0.65
27:W:469:THR:HB	27:W:634:ARG:HB3	1.79	0.65
40:j:191:ARG:HE	43:m:88:LEU:HD11	1.61	0.65
40:j:387:LEU:O	41:k:46:MET:SD	2.49	0.65
48:r:188:LYS:HA	48:r:188:LYS:CE	2.26	0.65
49:s:95:VAL:HA	49:s:98:LYS:HD2	1.78	0.65
55:y:64:ALA:O	55:y:67:LEU:N	2.26	0.65
40:j:186:GLU:HG3	40:j:228:THR:HG23	1.79	0.64
47:q:36:ILE:O	47:q:40:THR:HG23	1.97	0.64
48:r:666:ILE:CG2	48:r:684:LEU:HD22	2.27	0.64
48:r:706:LEU:HD11	48:r:727:ALA:HB2	1.79	0.64
48:r:950:VAL:HG23	48:r:951:GLU:H	1.62	0.64
50:t:105:ARG:N	50:t:107:GLU:HG2	2.12	0.64
52:v:84:CYS:HA	52:v:87:ARG:HG2	1.78	0.64
53:w:126:SER:OG	53:w:127:LEU:N	2.30	0.64
54:x:53:GLU:OE2	54:x:54:TYR:N	2.30	0.64
2:1:585:ILE:HA	2:1:589:LEU:HD12	1.79	0.64
3:2:271:LYS:HA	3:2:276:ILE:HD12	1.79	0.64
5:A:397:PHE:HB3	10:F:87:THR:HB	1.79	0.64
27:W:85:PHE:CE2	30:Z:336:TYR:CB	2.73	0.64
33:c:5:LEU:O	33:c:5:LEU:HD13	1.98	0.64
37:g:68:TYR:CZ	37:g:83:LYS:HD3	2.32	0.64
40:j:627:TRP:CZ3	40:j:638:LYS:HB3	2.32	0.64
54:x:92:LYS:HA	54:x:95:GLU:OE1	1.97	0.64
12:H:55:LYS:HD3	12:H:150:PHE:HE2	1.63	0.64
29:Y:407:ILE:HG21	32:b:19:PRO:HB2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:46:ARG:HH22	32:b:53:ARG:HG3	1.55	0.64
33:c:5:LEU:HD13	33:c:5:LEU:C	2.22	0.64
40:j:612:ASP:OD1	40:j:613:ASN:N	2.31	0.64
41:k:37:HIS:CD2	43:m:92:PRO:HA	2.32	0.64
48:r:486:MET:HA	48:r:488:ARG:N	2.11	0.64
1:0:236:ALA:H	1:0:266:ARG:NH1	1.96	0.64
2:1:496:VAL:HA	2:1:499:ILE:HG22	1.78	0.64
5:A:1160:ARG:NH2	5:A:1350:LYS:O	2.30	0.64
5:A:1362:ILE:HD11	5:A:1381:GLU:HG3	1.78	0.64
27:W:493:TRP:CE2	27:W:683:GLN:HB3	2.32	0.64
29:Y:372:ILE:O	31:a:54:ARG:CG	2.38	0.64
29:Y:411:MET:O	32:b:120:THR:HG23	1.97	0.64
48:r:212:LEU:HD11	48:r:289:LEU:HD21	1.78	0.64
55:y:39:GLN:NE2	55:y:89:VAL:O	2.30	0.64
27:W:165:LYS:CG	27:W:181:HIS:NE2	2.49	0.64
48:r:135:ARG:HD2	50:t:109:LEU:CD2	2.20	0.64
49:s:122:ALA:O	49:s:125:VAL:N	2.31	0.64
50:t:137:VAL:HA	50:t:140:GLU:HB2	1.79	0.64
56:z:743:TYR:CD1	56:z:749:LEU:HD12	2.31	0.64
1:0:17:TYR:CE2	1:0:738:LEU:CD2	2.79	0.64
8:D:73:ARG:O	8:D:76:ASN:ND2	2.30	0.64
20:P:218:LYS:HD3	25:U:18:DG:P	2.37	0.64
21:Q:76:MET:HE3	21:Q:88:ARG:HD2	1.80	0.64
28:X:193:PHE:CE2	28:X:302:ASP:OD2	2.51	0.64
33:c:39:ASP:HB3	33:c:42:HIS:H	1.63	0.64
40:j:393:PRO:HG2	41:k:137:ARG:HH21	1.62	0.64
41:k:60:LEU:HB3	41:k:68:PHE:HB3	1.80	0.64
42:l:63:MET:HE1	42:l:79:PHE:HB2	1.78	0.64
44:n:36:LYS:HG2	56:z:643:VAL:HG22	1.75	0.64
49:s:148:ILE:HA	49:s:151:TYR:HD2	1.61	0.64
49:s:179:ASP:OD1	49:s:180:LEU:N	2.25	0.64
50:t:106:GLU:HA	50:t:109:LEU:CD2	2.27	0.64
54:x:121:ALA:O	54:x:124:ASP:HB2	1.98	0.64
55:y:37:LEU:O	55:y:42:TYR:HD2	1.81	0.64
17:M:333:ASN:HA	17:M:359:ASN:HB3	1.80	0.64
21:Q:111:ARG:HD3	21:Q:188:TYR:OH	1.97	0.64
27:W:347:SER:OG	27:W:377:GLN:NE2	2.31	0.64
29:Y:480:PRO:HD2	29:Y:481:VAL:H	1.62	0.64
42:l:111:GLU:OE2	42:l:113:ARG:NE	2.30	0.64
48:r:168:ARG:HH22	55:y:73:LEU:HD21	1.60	0.64
54:x:62:ILE:C	54:x:65:THR:HG1	2.04	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:526:GLU:O	3:2:530:GLN:NE2	2.31	0.64
15:K:8:GLU:HG2	15:K:13:PHE:CE1	2.33	0.64
29:Y:507:PRO:CD	29:Y:508:PHE:N	2.56	0.64
40:j:336:PHE:HZ	40:j:500:GLU:HB2	1.62	0.64
41:k:141:MET:HA	41:k:173:VAL:HG22	1.79	0.64
48:r:168:ARG:NH1	55:y:73:LEU:HD11	2.13	0.64
48:r:676:ASP:O	48:r:678:PHE:N	2.30	0.64
40:j:191:ARG:CZ	43:m:88:LEU:HD21	2.28	0.64
50:t:143:LYS:HA	50:t:146:ARG:HE	1.62	0.64
5:A:1620:PRO:CG	38:h:104:VAL:HG11	2.28	0.64
8:D:75:LYS:HE3	8:D:142:TYR:HA	1.80	0.64
27:W:121:TYR:CZ	27:W:486:PRO:C	2.76	0.64
30:Z:121:ALA:O	32:b:100:LYS:HA	1.97	0.64
30:Z:352:GLN:OE1	30:Z:398:ARG:HB3	1.98	0.64
30:Z:433:PHE:HB3	33:c:9:LEU:CD2	2.28	0.64
38:h:154:ILE:HG12	43:m:34:THR:HG22	1.80	0.64
48:r:169:LEU:CD2	48:r:176:LYS:H	2.11	0.64
48:r:683:ARG:HH12	48:r:707:ASP:CB	2.11	0.64
49:s:109:GLN:HA	49:s:112:LYS:HE2	1.80	0.64
52:v:32:SER:O	52:v:34:GLN:NE2	2.31	0.64
5:A:337:LYS:O	5:A:341:GLN:HB3	1.98	0.63
5:A:589:LYS:NZ	5:A:638:GLY:O	2.29	0.63
5:A:640:LEU:HD23	5:A:645:LEU:HD22	1.80	0.63
5:A:1229:GLU:O	5:A:1233:GLU:HG2	1.98	0.63
7:C:59:LEU:HD12	7:C:151:VAL:HG12	1.79	0.63
19:O:12:ARG:HG3	19:O:13:VAL:H	1.63	0.63
24:T:226:LYS:HG2	25:U:30:DG:OP1	1.98	0.63
27:W:175:TYR:HH	27:W:459:GLN:HA	1.54	0.63
28:X:300:GLU:OE1	28:X:304:HIS:CE1	2.50	0.63
28:X:314:VAL:O	28:X:314:VAL:CG1	2.46	0.63
30:Z:406:GLY:O	33:c:7:GLY:O	2.16	0.63
31:a:292:PRO:C	32:b:264:ILE:HD11	2.23	0.63
49:s:108:GLN:O	49:s:112:LYS:HG2	1.97	0.63
54:x:3:ASP:OD2	54:x:4:ARG:HD3	1.98	0.63
54:x:118:ILE:HG13	54:x:119:GLN:N	2.12	0.63
55:y:46:LYS:HE2	55:y:46:LYS:H	1.62	0.63
2:1:324:GLY:HA3	2:1:328:GLN:HB3	1.79	0.63
2:1:590:PRO:O	2:1:593:PHE:N	2.30	0.63
27:W:170:LEU:HD23	27:W:175:TYR:HA	1.79	0.63
28:X:300:GLU:CB	28:X:304:HIS:CE1	2.81	0.63
29:Y:503:THR:O	29:Y:507:PRO:CD	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:400:ARG:HD2	33:c:16:MET:CG	2.28	0.63
30:Z:442:VAL:CG1	33:c:9:LEU:HD22	2.28	0.63
40:j:571:VAL:HG22	40:j:581:SER:OG	1.98	0.63
44:n:215:LYS:NZ	44:n:232:SER:OG	2.31	0.63
46:p:85:ASN:HD22	56:z:641:THR:HG23	1.58	0.63
48:r:65:GLU:O	48:r:68:VAL:HB	1.98	0.63
48:r:73:LEU:HB3	48:r:74:PRO:HD3	1.79	0.63
48:r:174:ARG:HG2	48:r:178:ILE:HG23	1.79	0.63
48:r:328:ARG:NH1	48:r:329:TYR:O	2.31	0.63
49:s:179:ASP:O	49:s:183:ARG:NE	2.30	0.63
50:t:11:PRO:HB2	55:y:40:ARG:NH1	2.11	0.63
2:1:675:VAL:HG13	2:1:676:LEU:HD13	1.80	0.63
3:2:175:ARG:HG2	3:2:225:ILE:HG23	1.80	0.63
3:2:553:LYS:HZ3	3:2:557:LEU:HD22	1.62	0.63
5:A:1030:SER:OG	9:E:162:ARG:NE	2.28	0.63
9:E:47:LYS:O	9:E:52:ARG:NH2	2.31	0.63
21:Q:15:LYS:NZ	21:Q:94:ILE:O	2.31	0.63
27:W:689:VAL:O	30:Z:393:LEU:HG	1.99	0.63
30:Z:433:PHE:HB3	33:c:9:LEU:HD22	1.81	0.63
35:e:30:ARG:HH21	35:e:35:ASN:HB2	1.63	0.63
39:i:107:VAL:HG12	47:q:162:GLN:HB3	1.81	0.63
40:j:35:SER:HB3	40:j:38:GLN:HG2	1.80	0.63
40:j:392:MET:SD	41:k:137:ARG:NE	2.71	0.63
49:s:132:LEU:HA	49:s:135:ILE:HG22	1.79	0.63
50:t:142:GLN:C	50:t:146:ARG:HE	2.05	0.63
55:y:39:GLN:NE2	55:y:90:ASN:CA	2.61	0.63
1:0:671:SER:HG	46:p:88:ILE:CD1	1.83	0.63
3:2:176:ALA:HB1	3:2:968:LEU:HD22	1.80	0.63
5:A:1650:TYR:CD1	35:e:216:ASP:OD1	2.51	0.63
9:E:10:LEU:HD12	9:E:52:ARG:HD2	1.80	0.63
9:E:81:LYS:HE2	9:E:111:THR:HG22	1.79	0.63
17:M:28:ILE:HG12	18:N:39:GLN:HG3	1.81	0.63
27:W:167:LYS:CG	27:W:294:GLU:CG	2.67	0.63
30:Z:334:MET:HE2	30:Z:342:VAL:HG11	1.81	0.63
33:c:17:LYS:NZ	33:c:39:ASP:O	2.32	0.63
43:m:130:LEU:HB3	47:q:160:MET:HE2	0.92	0.63
48:r:454:ILE:HG12	48:r:465:LEU:HD11	1.81	0.63
2:1:472:TYR:OH	2:1:526:ASN:ND2	2.31	0.63
5:A:1650:TYR:CE1	35:e:216:ASP:OD1	2.52	0.63
23:S:137:ALA:H	24:T:39:GLU:HG3	1.62	0.63
29:Y:449:ILE:HG22	29:Y:450:ASN:H	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:41:CYS:HB3	30:Z:118:LEU:HD21	1.79	0.63
38:h:18:GLN:HG3	38:h:62:VAL:HG21	1.80	0.63
40:j:410:PRO:CA	42:l:86:ILE:CG2	2.77	0.63
48:r:169:LEU:HD23	48:r:175:ASP:CG	2.23	0.63
48:r:1211:LEU:O	48:r:1215:ILE:HG13	1.97	0.63
55:y:85:ARG:HD3	55:y:85:ARG:N	2.14	0.63
1:0:478:LEU:HG	1:0:491:ILE:HG21	1.79	0.63
3:2:20:ASP:OD1	3:2:20:ASP:N	2.31	0.63
3:2:932:VAL:HG11	3:2:966:VAL:HB	1.81	0.63
4:3:45:GLU:OE2	4:3:50:GLY:HA2	1.99	0.63
6:B:802:ASP:HB3	7:C:173:HIS:CD2	2.34	0.63
19:O:145:VAL:HG21	19:O:198:ILE:HG12	1.80	0.63
27:W:173:ASN:CG	27:W:434:GLU:HA	2.22	0.63
28:X:316:GLN:CG	28:X:373:ARG:NH2	2.59	0.63
39:i:17:ILE:HD11	39:i:59:VAL:HA	1.79	0.63
40:j:449:ASP:HB2	47:q:157:LYS:CE	2.28	0.63
45:o:42:SER:HA	45:o:46:ASP:HB2	1.81	0.63
47:q:71:TYR:HB3	47:q:74:ARG:HE	1.64	0.63
48:r:114:LYS:O	48:r:118:ILE:HG12	1.98	0.63
55:y:48:PHE:O	55:y:52:LEU:HG	1.98	0.63
56:z:731:ALA:N	56:z:766:LYS:NZ	2.47	0.63
5:A:220:ARG:HH12	22:R:227:SER:HG	1.44	0.63
27:W:105:GLU:CG	27:W:487:LYS:HZ3	2.03	0.63
29:Y:394:TYR:OH	32:b:168:GLU:HB2	1.99	0.63
30:Z:412:PHE:CE2	30:Z:441:MET:HE2	2.34	0.63
37:g:99:TYR:HB2	37:g:106:TYR:HB2	1.79	0.63
50:t:115:LEU:O	50:t:118:HIS:HB2	1.99	0.63
50:t:143:LYS:HG2	50:t:146:ARG:NH2	2.13	0.63
52:v:111:GLN:O	52:v:114:SER:OG	2.13	0.63
52:v:118:PRO:C	52:v:124:TYR:HE2	2.07	0.63
54:x:102:THR:O	54:x:105:GLU:HG2	1.99	0.63
54:x:127:GLN:O	54:x:130:LEU:HG	1.98	0.63
55:y:46:LYS:H	55:y:46:LYS:CE	2.12	0.63
55:y:97:ILE:HD12	55:y:97:ILE:O	1.98	0.63
5:A:196:LEU:HB3	5:A:311:GLN:HE21	1.64	0.63
22:R:78:LEU:HD21	22:R:124:LEU:HD22	1.79	0.63
39:i:98:ASP:OD1	45:o:147:ASN:ND2	2.32	0.63
40:j:336:PHE:CZ	40:j:500:GLU:CB	2.81	0.63
40:j:419:ASN:HD22	42:l:73:LEU:HD23	1.64	0.63
43:m:140:SER:HA	47:q:146:ASN:CG	2.24	0.63
48:r:478:MET:HG3	48:r:492:TRP:CD2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:804:ASN:OD1	48:r:805:TYR:N	2.31	0.63
49:s:102:LYS:O	49:s:105:SER:OG	2.17	0.63
50:t:83:MET:HA	50:t:86:LEU:HD13	1.79	0.63
50:t:130:GLN:HB3	54:x:5:LEU:HD21	1.81	0.63
54:x:16:ALA:O	54:x:19:PHE:N	2.31	0.63
54:x:66:ALA:O	54:x:69:ILE:N	2.31	0.63
2:1:636:THR:HB	2:1:638:GLN:HG2	1.79	0.63
6:B:724:TYR:HB3	6:B:728:MET:HE3	1.80	0.63
6:B:1136:GLU:HG3	6:B:1143:LYS:HE2	1.81	0.63
17:M:363:ARG:NH2	17:M:364:ASP:O	2.31	0.63
30:Z:433:PHE:CE2	33:c:38:ILE:CG1	2.82	0.63
48:r:61:ARG:NH1	48:r:65:GLU:HB2	2.14	0.63
49:s:69:LEU:HA	49:s:72:ARG:HG2	1.80	0.63
2:1:837:SER:HB3	2:1:843:LEU:HD21	1.81	0.62
5:A:479:TRP:O	5:A:483:ARG:NH2	2.31	0.62
5:A:539:GLN:NE2	6:B:791:GLU:H	1.96	0.62
24:T:46:ALA:HB2	24:T:57:THR:HG23	1.80	0.62
30:Z:433:PHE:HE1	33:c:42:HIS:HD2	1.33	0.62
45:o:126:ASP:HA	45:o:129:VAL:HG12	1.81	0.62
48:r:55:ILE:C	48:r:58:LEU:HB3	2.24	0.62
48:r:89:ALA:O	48:r:93:ARG:HG3	1.98	0.62
48:r:552:VAL:HG22	48:r:553:GLU:N	2.14	0.62
54:x:115:LEU:HD12	54:x:116:GLU:N	2.14	0.62
1:0:273:ARG:HB3	1:0:276:LYS:HE3	1.81	0.62
3:2:176:ALA:HB2	3:2:965:LYS:HE2	1.81	0.62
4:3:42:PRO:HB2	4:3:228:LEU:HD22	1.79	0.62
5:A:122:ASN:O	5:A:127:LYS:NZ	2.31	0.62
11:G:125:PRO:O	38:h:167:ARG:NH1	2.21	0.62
27:W:106:PRO:HD2	27:W:490:GLU:CD	2.20	0.62
27:W:125:ALA:CB	27:W:486:PRO:CB	2.53	0.62
27:W:455:LEU:HD22	27:W:483:LEU:HG	1.81	0.62
29:Y:407:ILE:HD13	32:b:19:PRO:CA	2.28	0.62
30:Z:408:LEU:HD23	33:c:5:LEU:HD11	1.81	0.62
37:g:78:LEU:HG	37:g:101:ILE:HG12	1.81	0.62
40:j:464:TRP:CD2	40:j:475:VAL:HG21	2.34	0.62
40:j:615:TRP:CZ2	56:z:680:GLY:CA	2.82	0.62
48:r:963:LEU:HD12	48:r:1177:LEU:HD11	1.80	0.62
49:s:114:LEU:HB3	54:x:118:ILE:HD12	1.81	0.62
1:0:168:LEU:HD21	1:0:248:VAL:H	1.62	0.62
1:0:570:ASN:OD1	1:0:570:ASN:N	2.29	0.62
5:A:1313:GLN:O	5:A:1332:GLN:NE2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:803:ARG:NH2	6:B:951:GLN:OE1	2.33	0.62
17:M:368:SER:HB3	17:M:369:LYS:HE3	1.80	0.62
21:Q:100:VAL:O	21:Q:104:LYS:HG2	1.99	0.62
27:W:173:ASN:N	27:W:434:GLU:HG2	2.14	0.62
27:W:520:ARG:N	33:c:22:TYR:CD1	2.67	0.62
40:j:410:PRO:O	42:l:86:ILE:HD12	1.99	0.62
40:j:440:LEU:HD23	40:j:440:LEU:C	2.25	0.62
40:j:464:TRP:CD2	40:j:475:VAL:CG2	2.82	0.62
41:k:55:GLU:HG2	41:k:73:ARG:CG	2.20	0.62
43:m:123:ILE:CG1	47:q:163:LEU:HD21	2.28	0.62
48:r:451:CYS:SG	48:r:452:LEU:N	2.66	0.62
48:r:713:GLN:O	48:r:719:THR:HB	1.98	0.62
48:r:1209:ARG:NH2	48:r:1259:GLN:OE1	2.32	0.62
50:t:10:LEU:HG	50:t:11:PRO:HD2	1.82	0.62
52:v:49:GLN:HB3	52:v:53:LYS:HZ3	1.64	0.62
1:0:601:THR:HG22	1:0:603:GLU:H	1.65	0.62
3:2:404:GLN:OE1	3:2:412:ARG:NH2	2.33	0.62
4:3:85:HIS:NE2	4:3:97:TRP:HE3	1.97	0.62
5:A:1128:ILE:HG23	5:A:1414:ILE:HG23	1.82	0.62
18:N:66:ARG:NH2	20:P:185:LEU:O	2.29	0.62
31:a:379:LEU:HD11	32:b:138:ALA:HB1	1.79	0.62
35:e:134:LEU:HD11	35:e:192:VAL:HA	1.80	0.62
40:j:183:PHE:HD1	40:j:228:THR:OG1	1.81	0.62
40:j:191:ARG:HH11	40:j:203:ILE:HD12	1.60	0.62
40:j:491:ILE:HD12	40:j:532:HIS:CG	2.29	0.62
46:p:110:TYR:CE2	56:z:649:ILE:CD1	2.73	0.62
50:t:76:LYS:HA	50:t:79:ARG:CG	2.29	0.62
52:v:70:TYR:CE2	52:v:77:PRO:HA	2.34	0.62
1:0:812:ARG:NH2	46:p:90:ASN:HB2	2.09	0.62
2:1:995:TYR:CD2	2:1:1030:ILE:HG12	2.34	0.62
5:A:939:VAL:HA	5:A:942:VAL:HG12	1.82	0.62
5:A:1050:CYS:SG	5:A:1051:SER:N	2.71	0.62
6:B:298:MET:HE2	13:I:14:ILE:HG12	1.81	0.62
15:K:63:VAL:HG22	15:K:71:ILE:HG22	1.81	0.62
27:W:371:VAL:CG1	27:W:407:ILE:CG2	2.74	0.62
28:X:310:LEU:HG	28:X:405:THR:CG2	2.29	0.62
29:Y:440:LEU:CD1	32:b:226:TYR:CE1	2.81	0.62
30:Z:400:ARG:CG	33:c:16:MET:HG3	2.30	0.62
37:g:86:ARG:HG2	37:g:92:VAL:HG22	1.81	0.62
38:h:4:GLU:N	38:h:7:GLN:OE1	2.32	0.62
40:j:434:GLN:NE2	40:j:470:VAL:HG23	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:n:77:VAL:HB	46:p:57:VAL:HG12	1.82	0.62
48:r:683:ARG:HH12	48:r:707:ASP:HB2	1.64	0.62
49:s:118:GLU:O	49:s:121:LEU:N	2.32	0.62
52:v:98:LYS:C	52:v:101:THR:HG1	2.04	0.62
6:B:280:SER:HB3	6:B:283:ASP:HB2	1.81	0.62
31:a:116:LYS:HE2	31:a:119:GLU:HG2	1.80	0.62
31:a:320:ARG:CZ	32:b:182:PHE:CD1	2.83	0.62
40:j:336:PHE:HZ	40:j:500:GLU:CA	2.12	0.62
40:j:571:VAL:CG2	40:j:581:SER:OG	2.48	0.62
43:m:123:ILE:HD13	47:q:166:LEU:HD22	1.81	0.62
47:q:139:ARG:HG2	47:q:140:ARG:HH11	1.64	0.62
50:t:81:LEU:O	50:t:85:ILE:HG12	2.00	0.62
50:t:165:GLN:O	50:t:168:LEU:HG	2.00	0.62
52:v:33:SER:O	52:v:36:GLY:N	2.32	0.62
54:x:60:ALA:O	54:x:61:LEU:C	2.39	0.62
54:x:70:ASP:N	54:x:70:ASP:OD1	2.19	0.62
54:x:107:VAL:HA	54:x:110:ARG:HE	1.65	0.62
1:0:61:MET:HE3	1:0:75:SER:HB3	1.80	0.62
2:1:1013:GLU:HG3	2:1:1157:PRO:HG3	1.79	0.62
4:3:153:LEU:HG	4:3:154:PRO:HD2	1.80	0.62
21:Q:107:LEU:HD12	21:Q:111:ARG:NH2	2.14	0.62
29:Y:381:ARG:O	32:b:256:PHE:CE1	2.53	0.62
43:m:121:ASP:OD2	44:n:186:THR:OG1	2.12	0.62
46:p:104:LYS:NZ	48:r:948:LYS:HZ1	1.96	0.62
50:t:30:LEU:HG	50:t:31:ALA:H	1.65	0.62
53:w:87:TYR:O	53:w:89:LEU:N	2.32	0.62
3:2:762:LEU:O	3:2:766:GLU:HG2	2.00	0.62
23:S:31:PHE:HB2	24:T:91:GLN:HB2	1.81	0.62
24:T:236:LYS:NZ	24:T:238:GLU:OE2	2.32	0.62
27:W:278:GLU:OE1	27:W:452:ARG:CG	2.48	0.62
27:W:469:THR:CB	27:W:634:ARG:HH11	2.08	0.62
29:Y:457:ILE:CD1	29:Y:520:ASN:HD22	2.07	0.62
39:i:114:MET:HE1	47:q:159:ILE:HD12	1.53	0.62
42:l:175:VAL:HA	42:l:178:ASN:HB2	1.82	0.62
48:r:122:LEU:HA	48:r:125:GLN:OE1	2.00	0.62
48:r:168:ARG:HG2	55:y:74:HIS:ND1	2.14	0.62
52:v:100:ASP:OD1	52:v:100:ASP:N	2.29	0.62
54:x:85:LEU:H	54:x:85:LEU:HD12	1.64	0.62
54:x:128:SER:O	54:x:132:THR:OG1	2.16	0.62
1:0:835:ARG:HH11	1:0:835:ARG:HG3	1.64	0.62
3:2:945:GLN:HB2	3:2:949:PHE:HD2	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:10:LEU:HD13	9:E:58:LEU:HD21	1.80	0.62
40:j:191:ARG:NE	43:m:88:LEU:CD1	2.63	0.62
43:m:115:LYS:HE2	45:o:142:VAL:CG1	2.29	0.62
48:r:304:GLN:HE21	48:r:370:LEU:HD11	1.63	0.62
6:B:245:GLN:HG2	6:B:252:ILE:HG13	1.82	0.62
29:Y:440:LEU:O	32:b:244:PRO:HB3	2.00	0.62
30:Z:123:LEU:HA	32:b:100:LYS:HG2	1.79	0.62
34:d:265:MET:SD	34:d:268:ARG:NE	2.73	0.62
35:e:13:GLU:OE1	35:e:32:LYS:NZ	2.32	0.62
37:g:112:GLY:HA3	38:h:70:LEU:HB3	1.80	0.62
38:h:26:LEU:HD11	40:j:102:LEU:HD12	1.82	0.62
40:j:198:LYS:HG3	40:j:202:LYS:O	1.99	0.62
47:q:83:ARG:O	47:q:86:SER:OG	2.17	0.62
49:s:180:LEU:N	49:s:183:ARG:HH21	1.98	0.62
52:v:41:LEU:HA	52:v:44:ILE:HD12	1.81	0.62
53:w:84:ILE:C	53:w:87:TYR:H	2.06	0.62
5:A:601:ASN:HD21	5:A:992:LYS:HG3	1.65	0.61
9:E:7:THR:HB	9:E:52:ARG:NH2	2.15	0.61
24:T:44:ARG:O	24:T:57:THR:OG1	2.18	0.61
24:T:121:SER:O	24:T:123:ASN:N	2.33	0.61
30:Z:122:LEU:CG	32:b:50:PHE:CD1	2.77	0.61
40:j:181:ARG:HB3	40:j:185:SER:HB2	1.82	0.61
43:m:130:LEU:HD12	47:q:156:LEU:HD11	1.81	0.61
44:n:125:SER:OG	47:q:56:ARG:NH1	2.33	0.61
44:n:196:LYS:HD3	44:n:217:TYR:CE2	2.35	0.61
46:p:85:ASN:HD21	56:z:640:ARG:HG2	1.64	0.61
49:s:94:GLN:O	49:s:97:GLU:HB3	2.00	0.61
54:x:24:GLY:HA2	54:x:27:GLN:HE21	1.65	0.61
55:y:24:PHE:O	55:y:28:LEU:HG	2.00	0.61
55:y:88:LEU:C	55:y:90:ASN:H	2.07	0.61
4:3:181:SER:HB3	4:3:223:VAL:HA	1.82	0.61
5:A:133:SER:HB3	5:A:136:GLN:HB2	1.82	0.61
6:B:611:GLU:OE2	6:B:613:ARG:NH1	2.33	0.61
28:X:23:SER:HB2	28:X:757:ALA:HB2	1.82	0.61
35:e:284:ILE:HA	35:e:288:GLN:HE21	1.64	0.61
40:j:374:ASN:ND2	40:j:434:GLN:NE2	2.46	0.61
40:j:406:ARG:HB3	41:k:82:PRO:HG3	1.81	0.61
40:j:415:LYS:HZ2	42:l:123:LEU:HD11	1.62	0.61
44:n:192:VAL:HB	44:n:200:VAL:HG22	1.82	0.61
49:s:98:LYS:O	49:s:102:LYS:HB2	1.99	0.61
54:x:125:ILE:O	54:x:129:GLN:HG3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:812:ARG:HH21	46:p:90:ASN:ND2	1.97	0.61
3:2:182:LYS:HB2	3:2:186:ALA:HA	1.82	0.61
5:A:1086:MET:SD	6:B:1095:ILE:HG23	2.41	0.61
6:B:188:ASN:OD1	6:B:913:GLN:NE2	2.33	0.61
18:N:23:ILE:HG12	18:N:28:ILE:HG22	1.81	0.61
24:T:177:ARG:CZ	25:U:20:DG:OP1	2.48	0.61
40:j:187:LEU:HD21	40:j:191:ARG:NE	2.12	0.61
40:j:449:ASP:CB	47:q:157:LYS:NZ	2.55	0.61
40:j:555:VAL:HG22	48:r:646:ALA:HB1	1.81	0.61
42:l:156:LEU:HD11	44:n:288:LEU:CD2	2.30	0.61
48:r:221:ARG:HB3	48:r:221:ARG:NH1	2.13	0.61
54:x:87:ALA:O	54:x:90:LEU:N	2.34	0.61
3:2:562:ASN:OD1	3:2:563:ASN:N	2.33	0.61
5:A:1279:MET:HE1	23:S:170:VAL:HA	1.82	0.61
27:W:471:VAL:CG2	27:W:634:ARG:NH2	2.63	0.61
28:X:307:ASN:CB	28:X:308:PRO:HD3	2.11	0.61
34:d:307:GLN:OE1	36:f:247:GLN:NE2	2.30	0.61
35:e:79:ASP:OD1	35:e:80:ALA:N	2.33	0.61
35:e:132:TRP:CD1	36:f:1:MET:HE3	2.35	0.61
48:r:175:ASP:O	48:r:179:PRO:HD2	1.99	0.61
48:r:431:ILE:H	48:r:437:ALA:HB3	1.65	0.61
49:s:133:LYS:O	49:s:137:LYS:HG2	1.99	0.61
49:s:147:GLU:O	49:s:151:TYR:HB2	1.99	0.61
50:t:95:ILE:HG23	50:t:96:LEU:HB3	1.82	0.61
52:v:87:ARG:O	52:v:90:ALA:N	2.34	0.61
55:y:31:PRO:HA	55:y:34:LEU:HD13	1.80	0.61
55:y:72:CYS:O	55:y:75:MET:HB2	2.00	0.61
3:2:16:GLU:O	3:2:18:TRP:N	2.34	0.61
3:2:640:LEU:HD13	3:2:683:THR:HG21	1.81	0.61
5:A:432:HIS:CD2	5:A:433:PRO:HD2	2.35	0.61
6:B:114:ARG:NH2	6:B:176:GLU:OE2	2.33	0.61
8:D:78:GLU:CG	38:h:51:LEU:HD22	2.29	0.61
35:e:213:LEU:HD13	35:e:225:ILE:HG12	1.83	0.61
49:s:37:LEU:HD12	49:s:72:ARG:HH12	1.65	0.61
50:t:75:LYS:O	50:t:78:LEU:HB3	2.00	0.61
53:w:146:GLY:N	53:w:148:MET:HE3	2.15	0.61
54:x:105:GLU:HA	54:x:108:VAL:HG13	1.82	0.61
54:x:128:SER:O	54:x:131:LYS:HG3	2.00	0.61
4:3:180:PHE:HE1	4:3:198:ALA:HB3	1.65	0.61
5:A:383:SER:HB3	15:K:2:ASN:HD21	1.65	0.61
5:A:632:ASN:HB2	5:A:992:LYS:NZ	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:177:LEU:CD2	34:d:8:ARG:O	2.48	0.61
27:W:347:SER:HA	27:W:374:TRP:CZ2	2.34	0.61
29:Y:372:ILE:HG22	31:a:54:ARG:CZ	2.06	0.61
40:j:466:ASN:O	43:m:120:ARG:NH1	2.33	0.61
44:n:174:PRO:HB2	44:n:175:GLU:OE1	2.01	0.61
50:t:89:PHE:HA	50:t:92:LEU:HD12	1.83	0.61
54:x:96:GLU:O	54:x:99:GLU:HG3	2.00	0.61
55:y:90:ASN:HB2	55:y:92:GLN:CD	2.26	0.61
1:0:243:LYS:NZ	1:0:258:GLU:OE2	2.21	0.61
2:1:338:LEU:O	2:1:342:VAL:HG12	2.01	0.61
3:2:698:TRP:CG	3:2:699:ASN:H	2.19	0.61
4:3:22:ILE:HG12	4:3:145:ILE:HD12	1.82	0.61
5:A:362:SER:HB3	6:B:1084:LEU:HD12	1.81	0.61
6:B:1061:SER:H	6:B:1081:ASP:HB2	1.64	0.61
8:D:32:LEU:HB2	8:D:36:GLU:HG2	1.81	0.61
20:P:166:GLN:HG3	26:V:81:DA:H4'	1.81	0.61
21:Q:25:PHE:O	22:R:217:GLN:NE2	2.33	0.61
24:T:94:THR:HG22	24:T:109:ILE:HG22	1.83	0.61
27:W:503:ALA:HB3	27:W:646:ALA:HB2	1.78	0.61
29:Y:506:CYS:N	29:Y:507:PRO:CD	2.62	0.61
29:Y:524:HIS:HB2	31:a:269:PRO:O	2.00	0.61
29:Y:527:GLU:OE1	31:a:268:LYS:HB3	2.00	0.61
33:c:6:LYS:HA	33:c:6:LYS:NZ	2.16	0.61
40:j:393:PRO:CG	41:k:137:ARG:HH21	2.11	0.61
40:j:412:ALA:HB3	42:l:186:PRO:CB	2.29	0.61
48:r:797:PHE:CZ	48:r:873:PHE:HA	2.36	0.61
50:t:16:GLN:HG3	50:t:17:TYR:CD1	2.36	0.61
50:t:130:GLN:HG2	54:x:5:LEU:HD11	1.83	0.61
52:v:116:VAL:O	52:v:118:PRO:HD3	2.00	0.61
55:y:78:LEU:O	55:y:81:TYR:N	2.32	0.61
1:0:61:MET:HG2	1:0:76:ILE:O	2.01	0.61
2:1:1245:LEU:HD22	2:1:1281:VAL:HG11	1.81	0.61
5:A:221:VAL:HA	5:A:224:ILE:HD12	1.82	0.61
6:B:992:ASN:HD21	14:J:43:TYR:HE1	1.49	0.61
8:D:141:GLN:NE2	38:h:47:ASP:OD1	2.32	0.61
22:R:121:THR:O	22:R:125:VAL:HG23	2.01	0.61
24:T:184:LEU:HA	24:T:187:LEU:HG	1.83	0.61
48:r:174:ARG:O	48:r:178:ILE:N	2.34	0.61
48:r:918:PHE:CE2	48:r:1211:LEU:HB2	2.36	0.61
54:x:61:LEU:O	54:x:65:THR:HG23	2.00	0.61
55:y:78:LEU:HB3	55:y:84:PHE:CD2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1156:ASP:OD1	5:A:1157:ILE:N	2.33	0.61
6:B:118:LEU:HD23	6:B:913:GLN:HB3	1.82	0.61
40:j:598:ARG:NH1	56:z:683:ALA:C	2.57	0.61
48:r:169:LEU:HB2	48:r:173:ILE:CA	2.31	0.61
50:t:32:PRO:O	55:y:18:PHE:HE1	1.84	0.61
4:3:170:VAL:HG12	4:3:198:ALA:HB2	1.83	0.61
20:P:294:ARG:NH2	25:U:14:DA:OP1	2.34	0.61
21:Q:177:LEU:HG	34:d:8:ARG:O	2.01	0.61
23:S:100:LEU:HD22	23:S:110:PHE:CZ	2.36	0.61
28:X:617:ALA:HA	28:X:676:LEU:O	2.01	0.61
42:l:121:ASP:OD1	44:n:237:GLN:N	2.32	0.61
43:m:115:LYS:HG2	45:o:139:TRP:CZ3	2.35	0.61
48:r:374:HIS:HD2	48:r:377:PRO:HG3	1.64	0.61
49:s:33:ALA:HB1	49:s:72:ARG:HB2	1.83	0.61
49:s:132:LEU:O	49:s:135:ILE:N	2.34	0.61
50:t:136:ARG:HD2	54:x:90:LEU:HD12	1.83	0.61
52:v:96:LYS:HZ3	53:w:83:LEU:HD11	1.64	0.61
55:y:74:HIS:O	55:y:77:GLU:HB2	1.99	0.61
1:0:827:CYS:SG	1:0:828:LEU:N	2.74	0.60
2:1:86:ALA:HB1	2:1:92:LEU:HD23	1.82	0.60
2:1:372:LEU:HD23	2:1:402:LEU:HD11	1.83	0.60
3:2:925:GLN:NE2	3:2:959:SER:OG	2.34	0.60
5:A:979:LEU:HD11	5:A:1044:HIS:HD2	1.66	0.60
5:A:1623:SER:CB	55:y:92:GLN:HE21	2.14	0.60
20:P:257:ASN:ND2	20:P:314:GLY:HA2	2.16	0.60
28:X:193:PHE:HE2	28:X:302:ASP:OD2	1.84	0.60
40:j:469:ASP:HB2	44:n:231:TRP:CE2	2.35	0.60
48:r:1257:THR:O	48:r:1259:GLN:N	2.33	0.60
20:P:209:THR:O	20:P:237:TYR:OH	2.19	0.60
22:R:130:ILE:HG12	24:T:236:LYS:HZ2	1.66	0.60
27:W:170:LEU:O	27:W:461:HIS:ND1	2.29	0.60
36:f:215:THR:HA	36:f:252:MET:HE3	1.83	0.60
48:r:134:ASP:O	48:r:137:ALA:N	2.34	0.60
49:s:106:ASP:HA	49:s:109:GLN:HG2	1.81	0.60
50:t:17:TYR:OH	55:y:20:LEU:HD13	2.01	0.60
52:v:64:PRO:O	52:v:68:PHE:N	2.27	0.60
52:v:118:PRO:O	52:v:124:TYR:HE2	1.85	0.60
5:A:560:VAL:HG23	5:A:591:ILE:HD11	1.81	0.60
6:B:180:ASP:OD1	6:B:472:ARG:NH2	2.34	0.60
8:D:76:ASN:ND2	8:D:79:THR:HB	2.11	0.60
8:D:78:GLU:OE1	38:h:47:ASP:O	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:336:VAL:HG21	18:N:9:THR:HG22	1.82	0.60
40:j:384:LYS:HE3	47:q:177:ARG:HH12	1.67	0.60
48:r:359:ILE:HG13	48:r:372:ILE:HG22	1.83	0.60
48:r:528:HIS:CD2	48:r:609:ARG:HH21	2.20	0.60
48:r:660:GLU:HG2	48:r:758:GLY:O	2.01	0.60
48:r:835:LEU:HD12	48:r:852:LEU:HD12	1.84	0.60
49:s:106:ASP:CG	49:s:109:GLN:HE21	2.09	0.60
1:0:138:HIS:HB2	1:0:220:PHE:HD2	1.66	0.60
2:1:403:TYR:CZ	2:1:425:MET:HE2	2.36	0.60
5:A:295:GLN:O	22:R:218:LYS:NZ	2.25	0.60
5:A:1650:TYR:CE1	35:e:216:ASP:CA	2.77	0.60
6:B:246:GLY:HA3	23:S:166:ARG:HH22	1.66	0.60
18:N:76:LEU:HD12	18:N:95:ILE:HD13	1.82	0.60
20:P:167:ASN:ND2	26:V:79:DT:C1'	2.56	0.60
20:P:169:VAL:HG21	25:U:15:DA:H2	1.66	0.60
25:U:57:DC:H2''	25:U:58:DT:H5''	1.83	0.60
27:W:165:LYS:HD2	27:W:181:HIS:CE1	2.36	0.60
28:X:322:SER:HB3	34:d:99:LEU:HB3	1.83	0.60
40:j:395:PRO:HD2	40:j:406:ARG:CZ	2.24	0.60
40:j:537:VAL:HG21	40:j:582:VAL:HG21	1.84	0.60
48:r:428:ASN:OD1	48:r:429:SER:N	2.34	0.60
50:t:91:ASP:O	50:t:94:ASP:N	2.33	0.60
55:y:90:ASN:HB2	55:y:92:GLN:NE2	2.16	0.60
2:1:63:ILE:O	2:1:67:ILE:HG13	2.00	0.60
2:1:389:LEU:HG	2:1:435:LYS:HG3	1.82	0.60
2:1:1286:THR:O	2:1:1322:LYS:NZ	2.33	0.60
5:A:1170:THR:HG23	13:I:58:ILE:HG21	1.83	0.60
6:B:249:LYS:HE2	6:B:252:ILE:HG12	1.84	0.60
21:Q:177:LEU:CD2	34:d:9:CYS:HA	2.26	0.60
27:W:519:TYR:CD2	33:c:22:TYR:CD2	2.89	0.60
28:X:16:TYR:HE2	28:X:730:ARG:HE	1.48	0.60
28:X:309:VAL:O	28:X:309:VAL:CG1	2.49	0.60
30:Z:122:LEU:CG	32:b:50:PHE:CZ	2.80	0.60
36:f:86:TYR:OH	36:f:158:LEU:O	2.18	0.60
40:j:211:SER:OG	41:k:45:ASN:HB3	1.93	0.60
41:k:198:HIS:NE2	41:k:200:GLU:OE2	2.31	0.60
48:r:167:PRO:HD2	48:r:168:ARG:HD2	1.82	0.60
54:x:120:SER:OG	54:x:121:ALA:N	2.33	0.60
55:y:26:GLN:HE22	55:y:68:LYS:N	1.99	0.60
1:0:142:LYS:O	1:0:143:LEU:HB2	2.01	0.60
5:A:521:VAL:HG13	5:A:522:PRO:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:198:GLU:OE2	6:B:524:LYS:NZ	2.34	0.60
6:B:273:PHE:HA	6:B:276:LEU:HD12	1.83	0.60
21:Q:36:ILE:HG21	21:Q:48:MET:HE1	1.84	0.60
22:R:171:ILE:HD13	22:R:177:ASN:HB3	1.83	0.60
22:R:174:ALA:HB1	22:R:180:LYS:HZ1	1.67	0.60
24:T:115:GLU:HG2	24:T:116:CYS:H	1.66	0.60
29:Y:136:VAL:CB	29:Y:505:LEU:CD1	2.79	0.60
31:a:282:PRO:O	31:a:282:PRO:HD2	2.01	0.60
40:j:325:ILE:HB	40:j:332:ILE:HG23	1.83	0.60
40:j:327:VAL:HA	48:r:402:ILE:HD13	1.84	0.60
40:j:534:VAL:HG11	40:j:568:ALA:C	2.26	0.60
45:o:75:THR:HG21	48:r:834:SER:OG	2.02	0.60
49:s:141:GLY:C	49:s:143:ILE:H	2.01	0.60
49:s:143:ILE:O	49:s:145:SER:N	2.34	0.60
56:z:678:LEU:HD11	56:z:769:VAL:HG21	1.84	0.60
56:z:689:PHE:CZ	56:z:777:ALA:HB2	2.36	0.60
56:z:715:LEU:HD13	56:z:716:PRO:HD3	1.80	0.60
1:0:16:ALA:HB2	1:0:454:VAL:O	2.01	0.60
1:0:786:HIS:H	56:z:636:HIS:CD2	2.20	0.60
3:2:955:LEU:HA	3:2:958:VAL:HG22	1.84	0.60
5:A:408:ARG:NH1	5:A:414:PRO:O	2.33	0.60
20:P:222:THR:CG2	26:V:78:DT:H2"	2.29	0.60
21:Q:107:LEU:HD13	21:Q:111:ARG:HH12	0.47	0.60
27:W:493:TRP:HE1	27:W:683:GLN:NE2	2.00	0.60
29:Y:475:PHE:CZ	29:Y:499:ARG:HG3	2.36	0.60
29:Y:504:LYS:O	29:Y:507:PRO:HG2	2.00	0.60
36:f:68:CYS:HB3	36:f:80:VAL:HG22	1.84	0.60
42:l:152:ASP:O	44:n:278:GLN:HB3	2.01	0.60
44:n:32:PHE:HB3	56:z:646:MET:CE	2.31	0.60
48:r:209:PRO:HD3	48:r:290:GLN:HE21	1.65	0.60
48:r:797:PHE:CD1	48:r:797:PHE:C	2.80	0.60
52:v:100:ASP:O	52:v:103:LYS:N	2.35	0.60
52:v:104:LYS:HB2	52:v:108:LEU:HD23	1.84	0.60
3:2:348:LEU:HD13	3:2:360:THR:HG21	1.84	0.60
18:N:80:GLU:HB2	18:N:82:ARG:HD3	1.83	0.60
27:W:85:PHE:CE2	30:Z:338:PHE:CZ	2.90	0.60
29:Y:464:LEU:HD12	29:Y:513:ARG:HH11	1.55	0.60
29:Y:499:ARG:O	29:Y:503:THR:HG23	2.01	0.60
29:Y:503:THR:O	29:Y:507:PRO:HD3	2.02	0.60
29:Y:504:LYS:HB3	29:Y:508:PHE:HE2	1.67	0.60
35:e:118:MET:HE2	35:e:203:LEU:HD22	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:25:ASP:OD1	36:f:28:ARG:NH2	2.35	0.60
39:i:104:LEU:HD22	45:o:136:LEU:CD2	2.28	0.60
40:j:47:ILE:H	40:j:47:ILE:CD1	2.10	0.60
40:j:169:LYS:HA	40:j:172:THR:HG23	1.84	0.60
40:j:464:TRP:CZ3	40:j:497:ILE:HD11	2.36	0.60
48:r:222:VAL:O	48:r:233:THR:CB	2.49	0.60
48:r:232:ALA:CA	48:r:250:LEU:CG	2.75	0.60
48:r:254:VAL:O	48:r:254:VAL:HG12	2.01	0.60
48:r:1278:LEU:O	48:r:1282:GLU:HG2	2.00	0.60
3:2:572:MET:HE3	3:2:573:LYS:H	1.67	0.60
5:A:1622:TYR:HH	37:g:118:ARG:NH1	1.92	0.60
27:W:171:LYS:CA	27:W:461:HIS:HE1	2.12	0.60
28:X:300:GLU:HB2	28:X:304:HIS:HE2	1.65	0.60
29:Y:411:MET:C	32:b:120:THR:CG2	2.74	0.60
36:f:175:LYS:NZ	36:f:185:GLU:OE2	2.29	0.60
37:g:70:LEU:HD11	37:g:73:ALA:HB2	1.84	0.60
40:j:491:ILE:HD11	40:j:532:HIS:HA	0.67	0.60
40:j:609:VAL:HG11	56:z:682:VAL:HG21	1.84	0.60
44:n:53:ILE:CD1	56:z:629:ILE:HD11	2.30	0.60
48:r:169:LEU:HB3	48:r:175:ASP:OD2	2.02	0.60
50:t:132:ARG:HH22	54:x:84:ALA:C	2.08	0.60
1:0:132:VAL:HG21	1:0:182:VAL:HB	1.84	0.60
3:2:23:TRP:HE1	3:2:27:MET:HE2	1.67	0.60
5:A:890:ARG:CZ	5:A:1023:VAL:HG12	2.32	0.60
28:X:308:PRO:HD2	28:X:308:PRO:O	2.01	0.60
29:Y:394:TYR:CG	32:b:130:GLU:OE2	2.37	0.60
29:Y:411:MET:HE3	32:b:34:LEU:HD23	1.84	0.60
46:p:85:ASN:ND2	56:z:641:THR:CG2	2.57	0.60
49:s:127:GLN:OE1	49:s:127:GLN:N	2.35	0.60
49:s:183:ARG:C	49:s:185:GLY:H	2.10	0.60
1:0:792:THR:CG2	44:n:40:ARG:C	2.75	0.59
3:2:598:ALA:O	3:2:601:SER:N	2.33	0.59
3:2:949:PHE:HE1	3:2:952:VAL:HB	1.67	0.59
4:3:198:ALA:O	4:3:224:ARG:NH1	2.30	0.59
5:A:753:GLY:O	5:A:757:GLN:HG3	2.02	0.59
6:B:711:ILE:HD11	6:B:717:ASN:HD22	1.67	0.59
8:D:141:GLN:HG3	43:m:70:ARG:NH2	2.08	0.59
28:X:300:GLU:O	28:X:304:HIS:NE2	2.34	0.59
28:X:613:HIS:CE1	31:a:206:ARG:HG2	2.36	0.59
28:X:726:GLN:NE2	31:a:223:LEU:CD1	2.56	0.59
30:Z:58:ARG:HH11	32:b:241:LEU:HD21	1.59	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:137:ASP:OD1	35:e:139:LYS:NZ	2.35	0.59
36:f:48:LEU:HD23	36:f:276:LYS:HE3	1.83	0.59
40:j:341:LEU:HD11	40:j:368:LEU:HD21	1.84	0.59
40:j:499:VAL:HG23	40:j:499:VAL:O	2.01	0.59
43:m:122:GLU:CA	45:o:135:LYS:HZ1	2.13	0.59
48:r:308:LEU:O	48:r:312:THR:HG23	2.01	0.59
49:s:185:GLY:O	49:s:186:LEU:C	2.45	0.59
50:t:82:ASN:HA	50:t:85:ILE:HG12	1.84	0.59
52:v:8:LEU:O	52:v:12:LEU:CB	2.46	0.59
55:y:53:LYS:HD2	55:y:56:LEU:HD12	1.84	0.59
6:B:1142:ASN:HD21	6:B:1145:GLN:HB2	1.67	0.59
22:R:77:VAL:O	22:R:81:ILE:HG12	2.01	0.59
27:W:121:TYR:OH	27:W:486:PRO:C	2.45	0.59
27:W:640:LEU:HD21	27:W:685:TYR:CZ	2.37	0.59
29:Y:512:ILE:O	29:Y:516:TYR:CZ	2.54	0.59
30:Z:440:LEU:HD13	33:c:38:ILE:CG2	2.15	0.59
41:k:194:LYS:HE2	41:k:198:HIS:ND1	2.16	0.59
43:m:115:LYS:CB	45:o:146:ILE:HD12	2.31	0.59
43:m:122:GLU:C	45:o:135:LYS:NZ	2.60	0.59
44:n:223:THR:OG1	44:n:224:GLU:N	2.35	0.59
48:r:93:ARG:HE	52:v:19:ILE:HG22	1.67	0.59
48:r:162:THR:O	48:r:163:THR:OG1	2.18	0.59
54:x:58:PHE:HA	54:x:61:LEU:HG	1.83	0.59
56:z:731:ALA:H	56:z:766:LYS:NZ	1.99	0.59
1:0:671:SER:CB	46:p:88:ILE:CD1	2.75	0.59
1:0:807:LEU:HD13	1:0:835:ARG:NH1	2.17	0.59
3:2:25:ILE:O	3:2:29:LYS:HG3	2.03	0.59
3:2:915:ARG:NH2	56:z:701:ASN:HB3	2.17	0.59
6:B:295:PRO:O	6:B:299:GLU:HG2	2.02	0.59
17:M:45:LEU:HD13	18:N:22:LEU:HD21	1.84	0.59
23:S:180:ARG:HG3	23:S:181:ARG:HH21	1.66	0.59
30:Z:120:ILE:O	32:b:99:GLY:O	2.20	0.59
30:Z:433:PHE:CB	33:c:9:LEU:CD2	2.80	0.59
40:j:617:HIS:CD2	40:j:617:HIS:N	2.70	0.59
45:o:92:GLU:OE1	47:q:38:GLN:HG3	2.02	0.59
48:r:51:LEU:HB3	52:v:60:ASP:CA	2.30	0.59
48:r:211:GLN:HG2	48:r:293:TYR:CG	2.36	0.59
48:r:797:PHE:CE2	48:r:873:PHE:CD1	2.82	0.59
1:0:13:MET:HG3	1:0:457:LEU:CD2	2.32	0.59
5:A:757:GLN:OE1	5:A:778:LYS:HB3	2.02	0.59
6:B:933:ASP:OD2	6:B:1050:ARG:NH2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:96:VAL:HG22	12:H:116:VAL:HG22	1.83	0.59
19:O:108:SER:OG	19:O:109:SER:N	2.34	0.59
28:X:310:LEU:CD2	28:X:409:THR:CG2	2.69	0.59
29:Y:464:LEU:HG	29:Y:513:ARG:CZ	2.33	0.59
29:Y:475:PHE:CE2	29:Y:499:ARG:CG	2.71	0.59
39:i:114:MET:HG2	47:q:155:GLN:CG	2.30	0.59
40:j:618:LEU:CD2	48:r:725:VAL:HG21	2.32	0.59
41:k:137:ARG:HH12	41:k:142:LYS:HD3	1.66	0.59
43:m:140:SER:HA	47:q:146:ASN:HB3	1.82	0.59
44:n:281:CYS:HA	44:n:304:ALA:HB1	1.83	0.59
48:r:207:ASP:HB2	48:r:287:LYS:HE2	1.84	0.59
50:t:162:GLU:HA	50:t:165:GLN:HB3	1.83	0.59
53:w:84:ILE:O	53:w:88:ASN:N	2.35	0.59
54:x:71:VAL:O	54:x:72:LEU:C	2.41	0.59
56:z:697:HIS:CD2	56:z:705:HIS:HD2	2.10	0.59
56:z:721:LEU:HD21	56:z:736:TRP:CZ3	2.37	0.59
1:O:480:TYR:O	1:O:484:THR:HG22	2.02	0.59
1:O:812:ARG:NH1	46:p:92:GLN:HE21	1.98	0.59
2:1:863:ASP:OD2	2:1:962:ARG:HB3	2.02	0.59
3:2:145:GLY:HA2	3:2:149:GLY:H	1.68	0.59
4:3:143:LEU:HD22	4:3:181:SER:HB2	1.85	0.59
6:B:274:ARG:HG2	6:B:279:VAL:HA	1.84	0.59
21:Q:77:ARG:HG3	21:Q:78:VAL:N	2.16	0.59
28:X:339:TYR:OH	28:X:343:ARG:NH2	2.35	0.59
40:j:314:GLU:HA	40:j:317:GLN:HB2	1.84	0.59
48:r:233:THR:O	48:r:248:LEU:CG	2.50	0.59
48:r:640:VAL:HG13	48:r:641:LEU:HD23	1.84	0.59
52:v:74:GLY:C	53:w:105:LEU:HB3	2.27	0.59
52:v:127:ILE:O	52:v:130:GLU:HB3	2.02	0.59
4:3:68:LEU:HD11	4:3:101:ILE:HD11	1.84	0.59
5:A:1208:SER:HB3	5:A:1261:ILE:HG23	1.84	0.59
5:A:1323:THR:HG23	5:A:1326:GLY:H	1.67	0.59
12:H:30:CYS:HB2	12:H:39:LEU:HD21	1.84	0.59
15:K:47:LYS:HD3	15:K:61:TYR:HD1	1.67	0.59
24:T:196:TYR:HB2	24:T:232:THR:HG23	1.85	0.59
27:W:167:LYS:HD3	27:W:294:GLU:HG3	1.83	0.59
28:X:309:VAL:HG23	28:X:402:ASN:CG	2.28	0.59
29:Y:417:LYS:NZ	32:b:42:MET:HE3	2.17	0.59
40:j:550:SER:OG	48:r:713:GLN:HG2	2.02	0.59
48:r:66:LEU:O	48:r:70:THR:OG1	2.14	0.59
48:r:520:LEU:HD13	48:r:522:LEU:HD21	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:179:ASP:N	49:s:182:MET:H	2.01	0.59
50:t:22:THR:O	50:t:24:GLU:N	2.35	0.59
50:t:83:MET:O	50:t:87:ILE:HG12	2.03	0.59
55:y:42:TYR:O	55:y:44:LYS:N	2.35	0.59
55:y:94:ALA:O	55:y:98:ASP:CB	2.51	0.59
18:N:66:ARG:HB2	18:N:73:THR:HB	1.84	0.59
23:S:45:ALA:HA	24:T:8:ASP:O	2.02	0.59
27:W:105:GLU:HG3	27:W:122:SER:HB3	1.85	0.59
27:W:109:ARG:C	27:W:494:MET:SD	2.85	0.59
27:W:128:SER:OG	27:W:334:ARG:NE	2.36	0.59
28:X:231:VAL:HB	28:X:454:VAL:HG12	1.83	0.59
28:X:728:PHE:HE2	28:X:733:GLN:HE21	1.51	0.59
30:Z:61:PHE:O	32:b:225:GLN:CD	2.46	0.59
33:c:8:VAL:CG2	33:c:47:ALA:HA	2.29	0.59
38:h:119:GLU:HA	38:h:122:LYS:HG2	1.84	0.59
39:i:99:TYR:HE1	40:j:366:ASP:OD1	1.85	0.59
40:j:191:ARG:HG2	40:j:196:LEU:CD1	2.09	0.59
40:j:609:VAL:HG13	56:z:682:VAL:HG11	1.74	0.59
48:r:245:TRP:N	48:r:245:TRP:CD1	2.71	0.59
48:r:412:LYS:O	48:r:415:GLU:HG3	2.02	0.59
48:r:467:LEU:HD23	48:r:470:LEU:HD13	1.84	0.59
52:v:29:PHE:CZ	52:v:31:PRO:HA	2.38	0.59
52:v:45:VAL:HA	52:v:48:LEU:HD23	1.82	0.59
54:x:81:SER:O	54:x:81:SER:OG	2.11	0.59
1:0:265:MET:C	1:0:267:CYS:H	2.10	0.59
2:1:366:ILE:HB	2:1:369:ARG:HD3	1.84	0.59
3:2:167:LYS:O	3:2:171:SER:N	2.35	0.59
4:3:173:ILE:HG13	4:3:178:ILE:HD11	1.84	0.59
6:B:216:ALA:HB2	6:B:241:ALA:HA	1.82	0.59
6:B:626:LEU:HD23	6:B:662:VAL:HG22	1.84	0.59
6:B:924:ARG:NH1	7:C:62:GLU:OE1	2.35	0.59
8:D:136:THR:HG21	38:h:61:LYS:CE	2.30	0.59
27:W:109:ARG:HD3	27:W:492:ASN:ND2	2.16	0.59
40:j:368:LEU:HA	40:j:371:LEU:HB2	1.83	0.59
43:m:134:TYR:CZ	47:q:157:LYS:CD	2.73	0.59
48:r:222:VAL:O	48:r:233:THR:CA	2.51	0.59
50:t:15:MET:N	55:y:24:PHE:HE2	2.01	0.59
50:t:156:HIS:O	50:t:159:ARG:HG3	2.03	0.59
55:y:60:ASP:HB2	55:y:63:TYR:HB2	1.85	0.59
2:1:1199:SER:O	2:1:1201:SER:N	2.36	0.59
3:2:964:PRO:HG3	3:2:989:LEU:HG	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:256:PRO:HD2	5:A:280:LEU:HD11	1.84	0.59
27:W:640:LEU:HD22	27:W:685:TYR:HE2	1.64	0.59
29:Y:506:CYS:SG	29:Y:529:LEU:CD1	2.91	0.59
33:c:8:VAL:HG21	33:c:47:ALA:CA	2.29	0.59
39:i:114:MET:HE1	47:q:159:ILE:CB	2.26	0.59
40:j:198:LYS:CG	40:j:203:ILE:HD13	2.18	0.59
48:r:794:LEU:HD23	48:r:794:LEU:N	2.17	0.59
52:v:71:ILE:C	52:v:74:GLY:H	2.10	0.59
52:v:106:LYS:O	52:v:110:ILE:HG12	2.03	0.59
54:x:73:ILE:O	54:x:76:LEU:HB2	2.03	0.59
55:y:79:LEU:HA	55:y:85:ARG:NH1	2.18	0.59
56:z:693:LEU:HD23	56:z:693:LEU:H	1.66	0.59
56:z:719:PRO:CG	56:z:743:TYR:CE1	2.74	0.59
1:0:628:LEU:HD21	1:0:645:PHE:HB3	1.85	0.59
2:1:1014:MET:SD	2:1:1017:ARG:NH2	2.74	0.59
3:2:510:GLU:HA	3:2:513:LEU:HB2	1.85	0.59
5:A:426:ARG:NH2	5:A:447:GLU:OE2	2.35	0.59
5:A:521:VAL:HG23	5:A:535:MET:HE1	1.85	0.59
5:A:1173:THR:HG22	13:I:56:ASN:O	2.03	0.59
18:N:88:ILE:H	18:N:88:ILE:HD12	1.68	0.59
19:O:169:ARG:HE	19:O:209:ILE:HG23	1.68	0.59
20:P:206:GLU:HB3	20:P:207:PRO:HD3	1.85	0.59
24:T:81:HIS:CG	24:T:82:PRO:HD2	2.37	0.59
27:W:182:PRO:HB3	27:W:268:VAL:HG21	1.84	0.59
29:Y:384:HIS:HD2	32:b:259:ARG:NH1	2.00	0.59
30:Z:54:ASN:ND2	32:b:237:GLN:CG	2.66	0.59
30:Z:401:LEU:HD11	33:c:57:VAL:HB	1.83	0.59
37:g:40:PHE:HD2	37:g:105:ILE:HG12	1.68	0.59
40:j:314:GLU:CD	40:j:427:LEU:H	2.11	0.59
40:j:412:ALA:HB2	42:l:86:ILE:HD13	1.83	0.59
49:s:148:ILE:O	49:s:151:TYR:HB3	2.03	0.59
50:t:17:TYR:CZ	55:y:17:ARG:HD2	2.38	0.59
55:y:32:ASN:OD1	55:y:32:ASN:N	2.29	0.59
56:z:715:LEU:HB3	56:z:716:PRO:HD2	0.64	0.59
2:1:656:LEU:O	2:1:693:ARG:NH2	2.32	0.58
3:2:177:LEU:HA	3:2:180:ILE:HB	1.85	0.58
5:A:513:ALA:HB2	10:F:90:LEU:HD21	1.85	0.58
9:E:29:THR:HG23	9:E:32:GLU:H	1.66	0.58
27:W:159:CYS:SG	27:W:163:TYR:OH	2.55	0.58
39:i:27:ASN:HB3	39:i:52:PHE:CD2	2.38	0.58
46:p:104:LYS:HD2	48:r:945:ASP:OD2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:16:GLN:NE2	50:t:17:TYR:HD1	2.01	0.58
1:0:460:SER:O	1:0:462:GLY:N	2.35	0.58
4:3:85:HIS:CD2	4:3:97:TRP:CD2	2.90	0.58
5:A:275:ASP:HB2	5:A:336:LEU:HB3	1.85	0.58
20:P:192:TYR:HB2	20:P:200:VAL:HG23	1.85	0.58
27:W:170:LEU:HB2	27:W:461:HIS:HA	1.85	0.58
31:a:320:ARG:NH1	32:b:182:PHE:HD1	1.99	0.58
40:j:370:VAL:HG22	47:q:173:MET:HE2	1.85	0.58
41:k:19:MET:HG2	41:k:177:ALA:HA	1.84	0.58
43:m:133:GLU:CG	45:o:125:LYS:HE2	2.33	0.58
50:t:76:LYS:O	50:t:79:ARG:HB2	2.03	0.58
1:0:227:VAL:HG23	1:0:244:VAL:HG23	1.84	0.58
1:0:284:LYS:HB3	1:0:356:LEU:HD11	1.86	0.58
1:0:807:LEU:HD13	1:0:835:ARG:HH12	1.68	0.58
2:1:608:PHE:HE1	2:1:652:LEU:HD21	1.66	0.58
5:A:551:ARG:HH12	12:H:27:ARG:HH21	1.50	0.58
5:A:1628:SER:C	5:A:1629:TYR:CD2	2.81	0.58
6:B:344:GLN:HE22	6:B:355:ASP:HA	1.67	0.58
10:F:53:THR:HG21	10:F:108:ARG:HD3	1.85	0.58
17:M:336:VAL:HG23	17:M:357:ILE:HB	1.84	0.58
17:M:339:TYR:HB3	18:N:97:ALA:HB1	1.85	0.58
20:P:257:ASN:HD21	20:P:314:GLY:HA2	1.68	0.58
27:W:519:TYR:CE2	33:c:22:TYR:CD2	2.90	0.58
40:j:619:ARG:HH21	48:r:744:HIS:HE1	1.50	0.58
40:j:626:GLN:NE2	40:j:628:ASN:OD1	2.31	0.58
49:s:147:GLU:OE1	49:s:147:GLU:N	2.35	0.58
49:s:179:ASP:CG	49:s:180:LEU:H	2.12	0.58
55:y:49:VAL:O	55:y:52:LEU:HB2	2.03	0.58
2:1:856:LYS:HD2	2:1:857:TYR:CE1	2.38	0.58
3:2:725:ASP:HB3	3:2:728:SER:H	1.66	0.58
5:A:1650:TYR:HE2	35:e:177:TRP:HE1	1.50	0.58
18:N:66:ARG:HH21	20:P:188:ARG:NH2	2.01	0.58
22:R:163:LEU:HG	22:R:201:LEU:HD21	1.85	0.58
25:U:5:DG:N2	26:V:90:DC:O2	2.36	0.58
28:X:333:LEU:HD13	28:X:397:LEU:HD11	1.84	0.58
28:X:533:ASP:CG	31:a:206:ARG:H	2.11	0.58
29:Y:524:HIS:HB2	31:a:269:PRO:C	2.28	0.58
35:e:26:VAL:HG22	35:e:41:LYS:HG3	1.84	0.58
38:h:149:ASN:O	38:h:153:LYS:HG2	2.03	0.58
48:r:231:GLU:HG3	48:r:251:GLU:O	2.04	0.58
48:r:1219:HIS:O	48:r:1223:ILE:HG12	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:100:ASP:HA	52:v:103:LYS:CG	2.33	0.58
4:3:25:THR:OG1	4:3:106:GLY:N	2.35	0.58
4:3:65:GLN:HB3	4:3:128:PHE:CZ	2.39	0.58
4:3:141:VAL:HG21	4:3:226:LEU:HD21	1.85	0.58
5:A:769:MET:HE1	6:B:970:HIS:HA	1.84	0.58
5:A:1481:LYS:NZ	48:r:331:ALA:HB1	2.15	0.58
5:A:1624:PRO:CD	38:h:107:ASP:OD2	2.51	0.58
6:B:718:GLN:HG2	6:B:720:PRO:HD2	1.85	0.58
7:C:45:ILE:HD11	7:C:82:LEU:HD22	1.86	0.58
8:D:70:ARG:HA	43:m:20:LYS:NZ	2.17	0.58
22:R:192:VAL:HG21	22:R:203:PHE:HB3	1.86	0.58
28:X:297:ALA:HA	28:X:300:GLU:CG	2.33	0.58
29:Y:381:ARG:O	32:b:256:PHE:CZ	2.56	0.58
41:k:188:ASN:O	41:k:192:GLN:NE2	2.33	0.58
42:l:78:LEU:HD11	42:l:194:MET:HG3	1.85	0.58
47:q:174:LEU:O	47:q:178:ASN:N	2.37	0.58
48:r:221:ARG:HD2	48:r:223:LYS:HZ2	1.68	0.58
48:r:368:LYS:HD3	48:r:369:PRO:HD2	1.85	0.58
48:r:1315:ASP:OD2	48:r:1435:ILE:N	2.36	0.58
55:y:73:LEU:HG	55:y:74:HIS:H	1.68	0.58
1:0:572:PRO:HG2	1:0:574:LYS:HG2	1.86	0.58
2:1:794:TRP:HD1	2:1:795:LYS:HD2	1.68	0.58
2:1:1072:ILE:HD13	2:1:1149:ILE:HG12	1.84	0.58
2:1:1248:VAL:HG11	2:1:1277:MET:HE1	1.86	0.58
6:B:231:PRO:O	6:B:232:THR:HG22	2.03	0.58
20:P:167:ASN:HB3	26:V:80:DT:O2	2.04	0.58
38:h:128:ALA:HB2	40:j:147:ILE:HD13	1.84	0.58
40:j:198:LYS:HD2	43:m:88:LEU:CD2	2.29	0.58
48:r:169:LEU:HD22	48:r:173:ILE:O	2.04	0.58
48:r:693:ILE:HG23	48:r:697:THR:OG1	2.03	0.58
48:r:877:ALA:HB3	48:r:1179:HIS:CE1	2.38	0.58
1:0:147:VAL:HG23	1:0:148:GLU:H	1.68	0.58
3:2:301:GLU:OE1	3:2:304:LYS:HE2	2.01	0.58
4:3:45:GLU:OE1	4:3:51:PRO:HD2	2.03	0.58
5:A:220:ARG:NH2	22:R:226:ASP:H	2.02	0.58
5:A:295:GLN:OE1	5:A:296:ASN:ND2	2.37	0.58
6:B:834:ARG:HG3	6:B:835:GLU:H	1.69	0.58
7:C:48:ASP:OD2	16:L:58:ARG:NH2	2.36	0.58
17:M:320:VAL:HB	20:P:236:LYS:HE3	1.86	0.58
27:W:516:PRO:CG	33:c:18:GLN:OE1	2.50	0.58
30:Z:401:LEU:HD23	33:c:16:MET:CE	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:216:PHE:CD1	40:j:217:PRO:HD2	2.38	0.58
40:j:415:LYS:CG	40:j:416:ASN:H	2.15	0.58
42:l:68:ASN:OD1	42:l:69:SER:N	2.35	0.58
44:n:111:TYR:HE1	46:p:136:HIS:HB2	1.67	0.58
45:o:104:VAL:HG13	45:o:105:GLN:HE21	1.68	0.58
48:r:68:VAL:O	48:r:70:THR:N	2.36	0.58
48:r:202:ARG:HD3	48:r:243:VAL:C	2.28	0.58
48:r:230:PHE:HA	48:r:251:GLU:O	2.03	0.58
52:v:117:PHE:HB2	52:v:119:GLU:CG	2.25	0.58
54:x:60:ALA:HA	54:x:63:ALA:HB3	1.86	0.58
2:1:98:CYS:O	2:1:102:ILE:HG12	2.03	0.58
2:1:357:HIS:CD2	2:1:397:LYS:HG2	2.38	0.58
5:A:1657:TYR:OH	35:e:158:LEU:HA	2.03	0.58
20:P:222:THR:HG21	26:V:78:DT:C2'	2.30	0.58
24:T:230:LYS:NZ	26:V:67:DC:H5''	2.19	0.58
27:W:105:GLU:CG	27:W:487:LYS:CE	2.77	0.58
27:W:640:LEU:CD2	27:W:685:TYR:CE2	2.86	0.58
28:X:300:GLU:O	28:X:304:HIS:CD2	2.57	0.58
29:Y:499:ARG:NH2	29:Y:535:LYS:HE3	2.18	0.58
31:a:292:PRO:HG3	32:b:263:GLU:O	2.04	0.58
40:j:410:PRO:C	42:l:86:ILE:CG2	2.76	0.58
48:r:230:PHE:HZ	48:r:296:LEU:HD11	1.51	0.58
49:s:148:ILE:HA	49:s:151:TYR:HB3	1.85	0.58
53:w:91:GLN:HB3	53:w:95:LYS:HE3	1.86	0.58
2:1:633:VAL:HG22	2:1:635:GLN:H	1.68	0.58
3:2:680:GLN:O	3:2:681:THR:OG1	2.16	0.58
3:2:718:VAL:HG12	3:2:767:LEU:HD13	1.86	0.58
4:3:94:PHE:HA	4:3:97:TRP:HD1	1.69	0.58
5:A:1304:ILE:HG13	5:A:1305:SER:H	1.69	0.58
8:D:90:LYS:HZ3	8:D:130:ILE:HD12	1.68	0.58
24:T:178:ALA:O	24:T:180:LYS:NZ	2.27	0.58
27:W:170:LEU:HD11	27:W:175:TYR:HE2	1.69	0.58
27:W:493:TRP:CG	27:W:683:GLN:O	2.56	0.58
28:X:345:ARG:HH21	34:d:1:MET:CB	2.16	0.58
31:a:256:GLN:HE22	32:b:252:ARG:HH11	1.52	0.58
40:j:415:LYS:HG2	40:j:416:ASN:N	2.18	0.58
48:r:1222:ARG:HH11	48:r:1223:ILE:HD13	1.69	0.58
52:v:18:ASN:O	52:v:21:GLN:HB3	2.04	0.58
54:x:52:GLU:HG2	54:x:55:ALA:HB3	1.86	0.58
54:x:96:GLU:O	54:x:99:GLU:N	2.35	0.58
56:z:721:LEU:CD1	56:z:736:TRP:CZ3	2.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:z:728:ASP:HB3	56:z:732:GLN:HG3	1.85	0.58
1:0:13:MET:HE2	1:0:405:PHE:CG	2.38	0.58
5:A:1206:ARG:HD2	5:A:1266:GLU:HA	1.86	0.58
24:T:134:GLU:C	24:T:136:SER:H	2.11	0.58
27:W:351:VAL:CA	27:W:378:PHE:CE1	2.57	0.58
30:Z:123:LEU:N	32:b:100:LYS:HG2	2.18	0.58
34:d:108:ASN:OD1	34:d:112:ASN:ND2	2.36	0.58
41:k:47:GLU:OE2	41:k:48:PRO:HD2	2.04	0.58
48:r:552:VAL:HG22	48:r:553:GLU:H	1.67	0.58
49:s:110:LEU:O	49:s:113:GLN:HB2	2.04	0.58
50:t:105:ARG:HA	50:t:108:LYS:HG2	1.86	0.58
50:t:166:ASN:HA	50:t:169:ALA:HB3	1.85	0.58
52:v:79:LEU:HA	52:v:82:LYS:HB2	1.86	0.58
1:0:781:HIS:O	1:0:784:ARG:NH2	2.36	0.57
1:0:790:CYS:HB2	44:n:40:ARG:C	2.29	0.57
2:1:390:ALA:HA	2:1:393:LEU:HD23	1.86	0.57
3:2:141:ARG:HH22	3:2:151:PRO:HB3	1.68	0.57
8:D:87:LEU:HA	8:D:90:LYS:HE3	1.85	0.57
19:O:14:THR:HB	19:O:19:PRO:HA	1.85	0.57
21:Q:137:THR:HB	21:Q:140:GLU:OE1	2.04	0.57
30:Z:442:VAL:HG11	33:c:9:LEU:HD22	1.85	0.57
31:a:374:PHE:CD2	32:b:142:CYS:HB3	2.39	0.57
37:g:36:ARG:NH1	37:g:37:SER:H	2.01	0.57
41:k:145:VAL:HG12	41:k:169:VAL:HG12	1.86	0.57
46:p:104:LYS:HZ2	48:r:948:LYS:NZ	2.01	0.57
48:r:154:ILE:N	48:r:155:PRO:HD2	2.19	0.57
49:s:147:GLU:O	49:s:148:ILE:C	2.46	0.57
52:v:78:GLN:O	52:v:81:THR:OG1	2.21	0.57
52:v:99:ILE:HB	52:v:103:LYS:HZ1	1.69	0.57
52:v:108:LEU:HD13	54:x:59:ALA:HA	1.86	0.57
55:y:123:GLN:HA	55:y:126:ASN:OD1	2.04	0.57
55:y:125:GLN:C	55:y:128:THR:HG1	2.11	0.57
3:2:302:GLU:HG3	3:2:354:ARG:NH2	2.19	0.57
3:2:334:VAL:HG11	3:2:372:LEU:HD22	1.86	0.57
5:A:1430:CYS:HG	5:A:1435:THR:HG1	1.47	0.57
7:C:68:LEU:HD11	7:C:120:LEU:HD11	1.86	0.57
7:C:99:VAL:HG21	7:C:128:ILE:HD13	1.86	0.57
9:E:117:SER:O	9:E:121:MET:HB2	2.04	0.57
20:P:166:GLN:O	26:V:80:DT:H4'	2.03	0.57
23:S:167:ARG:HG2	23:S:168:ASN:H	1.69	0.57
27:W:165:LYS:HD2	27:W:181:HIS:HE1	1.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:143:ARG:NH2	28:X:162:ASP:OD2	2.37	0.57
30:Z:313:TYR:OH	30:Z:390:GLN:CB	2.50	0.57
32:b:166:ALA:HB2	32:b:196:LEU:HD12	1.86	0.57
37:g:30:LEU:HA	37:g:33:PHE:CD2	2.40	0.57
38:h:139:GLN:O	38:h:142:SER:OG	2.20	0.57
40:j:101:ASN:O	40:j:104:SER:OG	2.22	0.57
40:j:328:LYS:O	40:j:329:ASN:ND2	2.37	0.57
40:j:391:MET:HG3	40:j:400:PHE:HD1	1.68	0.57
40:j:434:GLN:CD	40:j:470:VAL:HG23	2.28	0.57
43:m:122:GLU:CA	45:o:135:LYS:NZ	2.68	0.57
43:m:130:LEU:C	47:q:160:MET:HE2	2.03	0.57
48:r:192:LEU:HD11	48:r:219:ASN:HB2	1.86	0.57
53:w:84:ILE:O	53:w:87:TYR:N	2.33	0.57
56:z:726:PRO:HD3	56:z:734:PRO:HA	1.86	0.57
2:1:510:PRO:HG2	2:1:954:ILE:HG23	1.86	0.57
2:1:584:PHE:HE1	2:1:604:LEU:HD22	1.69	0.57
3:2:220:THR:O	3:2:224:SER:N	2.37	0.57
3:2:301:GLU:CD	3:2:304:LYS:HE3	2.29	0.57
4:3:23:GLU:OE1	4:3:25:THR:N	2.37	0.57
4:3:179:HIS:HB2	4:3:224:ARG:HB3	1.86	0.57
12:H:55:LYS:HD3	12:H:150:PHE:CE2	2.39	0.57
15:K:47:LYS:HD3	15:K:61:TYR:CD1	2.40	0.57
21:Q:70:LYS:HE2	22:R:226:ASP:HA	1.86	0.57
24:T:170:LYS:HG3	24:T:171:GLU:N	2.20	0.57
28:X:192:TYR:OH	28:X:196:ARG:NH2	2.37	0.57
40:j:569:ILE:HG12	40:j:583:ARG:HG3	1.85	0.57
43:m:115:LYS:HD2	45:o:146:ILE:CD1	2.28	0.57
48:r:212:LEU:CD2	48:r:224:PHE:HD2	2.16	0.57
49:s:148:ILE:HA	49:s:151:TYR:CD2	2.39	0.57
51:u:68:LEU:HB3	51:u:90:LEU:HD21	1.85	0.57
54:x:67:LYS:O	54:x:70:ASP:HB2	2.04	0.57
56:z:688:LYS:HB2	56:z:712:ASP:HB2	1.84	0.57
1:0:18:VAL:O	1:0:18:VAL:HG13	2.03	0.57
1:0:484:THR:O	4:3:78:PRO:HD3	2.05	0.57
3:2:289:CYS:HB3	3:2:309:THR:HG23	1.87	0.57
3:2:601:SER:O	3:2:605:ILE:HG12	2.05	0.57
17:M:13:LEU:O	17:M:17:VAL:HG23	2.04	0.57
24:T:153:TYR:O	24:T:155:PRO:HD3	2.04	0.57
27:W:689:VAL:CB	30:Z:393:LEU:HD11	2.23	0.57
32:b:38:ILE:HG21	32:b:115:ILE:HD13	1.86	0.57
40:j:483:GLY:O	40:j:485:GLU:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:37:HIS:CD2	43:m:95:ASN:HD21	2.23	0.57
48:r:707:ASP:OD2	56:z:684:ARG:HD3	2.04	0.57
52:v:9:GLU:O	52:v:10:GLU:C	2.47	0.57
55:y:73:LEU:O	55:y:74:HIS:C	2.47	0.57
55:y:116:GLN:HA	55:y:119:LEU:HD12	1.84	0.57
3:2:289:CYS:SG	3:2:313:ILE:HG13	2.45	0.57
6:B:787:GLY:HA2	6:B:790:GLN:HE21	1.69	0.57
6:B:1035:ARG:NH1	6:B:1036:LYS:O	2.38	0.57
7:C:59:LEU:HD13	7:C:63:PHE:CE2	2.39	0.57
20:P:204:ILE:HG12	20:P:237:TYR:CZ	2.40	0.57
27:W:170:LEU:CD1	27:W:175:TYR:CE2	2.87	0.57
28:X:84:ILE:HG13	28:X:108:ALA:HB2	1.87	0.57
28:X:292:LEU:HD11	28:X:317:GLU:O	2.04	0.57
31:a:145:LEU:HD11	31:a:169:ILE:HD13	1.87	0.57
36:f:85:MET:HE3	36:f:89:ARG:HE	1.69	0.57
40:j:469:ASP:CB	44:n:231:TRP:CD1	2.88	0.57
48:r:139:LEU:O	48:r:143:ALA:CB	2.52	0.57
50:t:90:LEU:HA	50:t:93:LEU:HD12	1.85	0.57
56:z:710:LEU:HB2	56:z:776:TRP:CZ3	2.39	0.57
56:z:766:LYS:O	56:z:766:LYS:HG3	2.05	0.57
3:2:199:LEU:HA	3:2:202:ILE:HG22	1.86	0.57
4:3:166:THR:O	4:3:170:VAL:HG23	2.05	0.57
5:A:1223:ASP:OD1	5:A:1224:ARG:N	2.37	0.57
5:A:1628:SER:O	5:A:1629:TYR:CG	2.57	0.57
6:B:845:TYR:CD1	6:B:865:VAL:HG11	2.39	0.57
8:D:78:GLU:CB	38:h:51:LEU:HD23	2.34	0.57
19:O:18:HIS:HE1	19:O:37:CYS:HB2	1.69	0.57
22:R:149:LYS:HA	22:R:152:LEU:HD12	1.87	0.57
24:T:7:LEU:HG	24:T:9:LEU:H	1.70	0.57
29:Y:136:VAL:CB	29:Y:505:LEU:HD12	2.33	0.57
31:a:337:GLU:O	31:a:340:ASN:ND2	2.37	0.57
35:e:258:HIS:HB3	35:e:269:LEU:HD21	1.85	0.57
37:g:67:GLU:N	37:g:84:GLN:O	2.37	0.57
40:j:320:SER:OG	40:j:322:VAL:O	2.23	0.57
49:s:131:LYS:O	49:s:135:ILE:HB	2.05	0.57
49:s:186:LEU:O	49:s:189:GLN:HB2	2.04	0.57
50:t:76:LYS:CA	50:t:79:ARG:HG3	2.32	0.57
54:x:13:ASN:C	54:x:17:ASP:OD2	2.47	0.57
1:0:501:GLN:OE1	1:0:543:ARG:NH2	2.37	0.57
3:2:509:SER:OG	3:2:510:GLU:N	2.38	0.57
5:A:1475:LEU:HD22	11:G:66:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1624:PRO:HB2	5:A:1627:PRO:HD2	1.86	0.57
8:D:103:LEU:HD12	8:D:114:LEU:HD13	1.87	0.57
27:W:129:VAL:HG22	27:W:334:ARG:NH1	2.18	0.57
29:Y:476:TRP:CB	31:a:307:ILE:O	2.53	0.57
40:j:318:ILE:HD12	40:j:318:ILE:H	1.69	0.57
42:l:76:PHE:CE1	42:l:86:ILE:HG12	2.39	0.57
43:m:111:GLU:OE2	45:o:146:ILE:HG21	2.03	0.57
43:m:122:GLU:C	45:o:135:LYS:HZ2	2.13	0.57
48:r:165:SER:H	48:r:168:ARG:HH12	1.51	0.57
56:z:743:TYR:CD2	56:z:753:HIS:HB2	2.39	0.57
2:1:759:ASN:O	2:1:763:GLU:HG2	2.04	0.57
3:2:174:ASN:O	3:2:178:LEU:N	2.38	0.57
4:3:45:GLU:HA	4:3:48:ASN:O	2.04	0.57
4:3:82:VAL:HG21	4:3:120:THR:HG21	1.86	0.57
5:A:597:PRO:HD3	5:A:668:PHE:CD1	2.40	0.57
5:A:1481:LYS:HZ1	48:r:331:ALA:HB2	1.63	0.57
6:B:686:GLU:HG3	6:B:687:VAL:H	1.70	0.57
20:P:197:PHE:CD1	26:V:77:DT:C5'	2.82	0.57
28:X:284:GLU:OE2	28:X:287:ARG:NH2	2.37	0.57
41:k:58:PHE:HB3	41:k:123:PHE:HB3	1.86	0.57
44:n:53:ILE:HD12	56:z:626:LEU:HD23	1.85	0.57
48:r:108:ASN:OD1	48:r:108:ASN:N	2.27	0.57
50:t:16:GLN:O	50:t:19:LYS:N	2.34	0.57
50:t:91:ASP:OD1	50:t:92:LEU:N	2.37	0.57
50:t:144:ARG:O	50:t:147:LEU:HG	2.05	0.57
54:x:18:GLN:O	54:x:20:CYS:N	2.37	0.57
2:1:168:ALA:HB2	2:1:204:LEU:HD21	1.87	0.57
2:1:407:GLU:HG3	2:1:408:TYR:H	1.69	0.57
3:2:941:GLY:O	3:2:945:GLN:HG2	2.05	0.57
4:3:182:ILE:HG12	4:3:222:LEU:HD11	1.86	0.57
5:A:987:ILE:HG23	5:A:1060:LEU:HD11	1.87	0.57
8:D:57:LEU:HD13	8:D:62:MET:HG3	1.87	0.57
23:S:19:PRO:O	23:S:22:THR:OG1	2.22	0.57
27:W:167:LYS:HD3	27:W:294:GLU:CB	2.35	0.57
31:a:360:CYS:SG	31:a:361:ALA:N	2.77	0.57
40:j:507:ARG:HE	44:n:252:HIS:HA	1.68	0.57
50:t:123:ILE:O	50:t:124:ASN:C	2.48	0.57
54:x:62:ILE:O	54:x:63:ALA:C	2.48	0.57
1:0:18:VAL:O	1:0:18:VAL:HG22	2.05	0.57
1:0:639:LEU:HD22	1:0:643:HIS:HE1	1.69	0.57
1:0:807:LEU:CD1	1:0:835:ARG:NH1	2.67	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:464:ASN:ND2	2:1:466:SER:O	2.38	0.57
2:1:559:LEU:HB3	2:1:563:LEU:HD22	1.87	0.57
4:3:63:GLY:O	4:3:132:ARG:NH1	2.37	0.57
5:A:722:ASN:HB3	5:A:724:GLU:HG2	1.87	0.57
5:A:917:GLU:HG2	5:A:956:PHE:HZ	1.70	0.57
11:G:124:ASN:O	11:G:126:PRO:HD3	2.05	0.57
17:M:18:ILE:HG13	17:M:46:TRP:CZ2	2.40	0.57
22:R:148:LYS:HG3	22:R:149:LYS:HE2	1.87	0.57
31:a:271:PHE:O	31:a:285:THR:CG2	2.46	0.57
37:g:101:ILE:HB	37:g:106:TYR:HE1	1.69	0.57
40:j:491:ILE:HD13	40:j:532:HIS:N	2.17	0.57
48:r:201:HIS:HE2	49:s:111:GLN:CG	2.13	0.57
52:v:40:LYS:O	52:v:44:ILE:HG13	2.05	0.57
1:0:288:ARG:O	1:0:289:ASP:HB3	2.03	0.56
3:2:506:THR:HG23	3:2:507:TYR:CD1	2.40	0.56
5:A:906:LEU:HD13	5:A:977:VAL:HG21	1.87	0.56
8:D:78:GLU:CG	38:h:51:LEU:CD2	2.83	0.56
29:Y:524:HIS:NE2	31:a:270:SER:CB	2.67	0.56
39:i:10:ARG:HH11	39:i:70:LEU:HD22	1.69	0.56
40:j:336:PHE:CE1	40:j:500:GLU:CG	2.83	0.56
40:j:539:GLN:O	40:j:543:VAL:HG23	2.05	0.56
44:n:109:GLN:HE22	45:o:64:TYR:HD1	1.52	0.56
47:q:109:ILE:HG13	47:q:111:VAL:HG22	1.88	0.56
48:r:209:PRO:HG2	48:r:211:GLN:HE21	1.70	0.56
48:r:669:GLN:HG2	56:z:770:THR:HG22	1.65	0.56
48:r:1313:LEU:O	48:r:1317:VAL:HG23	2.03	0.56
49:s:181:GLU:C	49:s:184:SER:H	2.13	0.56
54:x:98:HIS:HD1	54:x:98:HIS:H	1.51	0.56
2:1:829:PHE:O	2:1:833:GLU:HG2	2.05	0.56
5:A:659:GLU:OE1	5:A:989:ASN:ND2	2.38	0.56
6:B:83:ARG:HB3	6:B:133:ILE:HG23	1.88	0.56
35:e:58:THR:HG23	35:e:157:GLY:HA3	1.87	0.56
39:i:114:MET:HA	47:q:155:GLN:NE2	2.19	0.56
40:j:289:PRO:HG2	40:j:292:GLN:CD	2.30	0.56
40:j:314:GLU:OE1	40:j:428:LEU:N	2.37	0.56
42:l:144:TYR:OH	44:n:238:VAL:HG21	2.05	0.56
48:r:232:ALA:CA	48:r:250:LEU:HG	2.33	0.56
50:t:15:MET:HG3	50:t:16:GLN:H	1.68	0.56
52:v:87:ARG:O	52:v:91:LYS:HG2	2.05	0.56
55:y:95:LYS:O	55:y:99:GLU:N	2.37	0.56
1:0:13:MET:HG3	1:0:457:LEU:HD23	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:78:SER:HA	1:0:108:TRP:CZ2	2.41	0.56
1:0:607:ASP:N	1:0:607:ASP:OD1	2.36	0.56
2:1:13:VAL:HG13	2:1:75:ARG:HH22	1.71	0.56
2:1:633:VAL:HG13	2:1:634:ALA:H	1.70	0.56
2:1:1072:ILE:HD12	2:1:1129:VAL:HG21	1.87	0.56
3:2:82:ILE:HG21	3:2:101:MET:HE3	1.88	0.56
3:2:468:PHE:HB3	3:2:500:LEU:HD21	1.85	0.56
9:E:87:ILE:HD12	9:E:118:LEU:HD23	1.87	0.56
18:N:84:VAL:HG23	18:N:85:THR:H	1.71	0.56
19:O:128:ILE:HG23	19:O:183:VAL:HG11	1.87	0.56
20:P:193:ASN:HD21	20:P:195:LYS:HB2	1.69	0.56
20:P:271:GLU:N	20:P:271:GLU:OE2	2.37	0.56
22:R:86:LYS:NZ	22:R:140:LYS:HD2	2.20	0.56
24:T:18:VAL:O	24:T:111:VAL:N	2.31	0.56
24:T:103:LYS:NZ	24:T:105:SER:O	2.38	0.56
27:W:278:GLU:HG2	27:W:483:LEU:CD1	2.31	0.56
28:X:17:ILE:HD11	28:X:744:LEU:HD21	1.87	0.56
28:X:316:GLN:HG3	28:X:373:ARG:HH22	1.65	0.56
29:Y:527:GLU:CD	31:a:268:LYS:HG3	2.30	0.56
40:j:259:VAL:HB	40:j:343:ILE:HD12	1.85	0.56
40:j:402:HIS:C	40:j:404:ARG:H	2.14	0.56
40:j:591:LYS:HD3	40:j:593:MET:HE3	1.87	0.56
48:r:134:ASP:O	48:r:135:ARG:C	2.49	0.56
48:r:163:THR:OG1	48:r:163:THR:O	2.16	0.56
48:r:222:VAL:O	48:r:233:THR:HB	2.06	0.56
48:r:689:PRO:HA	48:r:698:GLN:HE22	1.70	0.56
49:s:188:GLY:C	49:s:191:ASN:H	2.12	0.56
54:x:21:ASN:C	54:x:24:GLY:H	2.12	0.56
55:y:60:ASP:HB2	55:y:63:TYR:CG	2.41	0.56
55:y:82:GLU:C	55:y:86:LYS:HZ3	2.08	0.56
1:0:132:VAL:CG1	1:0:216:ALA:HB3	2.36	0.56
1:0:508:HIS:O	1:0:512:THR:HG23	2.05	0.56
1:0:568:PHE:CE2	1:0:570:ASN:HB3	2.41	0.56
2:1:222:CYS:SG	2:1:1210:ALA:HA	2.46	0.56
2:1:404:PRO:O	2:1:406:LYS:NZ	2.33	0.56
2:1:827:ALA:O	2:1:831:VAL:HG23	2.05	0.56
3:2:952:VAL:HG13	3:2:955:LEU:HD12	1.87	0.56
21:Q:177:LEU:HD23	34:d:8:ARG:O	2.05	0.56
22:R:148:LYS:HB3	22:R:183:LYS:HE3	1.87	0.56
23:S:20:LYS:HD3	24:T:39:GLU:HB3	1.85	0.56
27:W:167:LYS:CE	27:W:294:GLU:HG3	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:300:GLU:HB2	28:X:304:HIS:NE2	2.20	0.56
30:Z:35:TYR:CB	30:Z:114:PHE:HD1	2.19	0.56
30:Z:69:ALA:O	30:Z:73:LEU:HB2	2.04	0.56
30:Z:121:ALA:O	32:b:100:LYS:CA	2.53	0.56
30:Z:433:PHE:CE2	33:c:38:ILE:HG13	2.40	0.56
40:j:197:ARG:NH2	40:j:204:LEU:HD21	2.21	0.56
48:r:465:LEU:HB2	48:r:479:GLU:OE2	2.06	0.56
50:t:145:GLN:O	50:t:149:THR:HG22	2.05	0.56
52:v:105:PHE:CD1	54:x:62:ILE:HD11	2.40	0.56
2:1:730:HIS:HD2	2:1:977:LEU:HD13	1.71	0.56
3:2:953:SER:HA	3:2:956:VAL:HG12	1.88	0.56
6:B:66:ASP:HA	6:B:85:LEU:HD23	1.88	0.56
21:Q:14:LEU:HD11	21:Q:194:THR:HG23	1.87	0.56
22:R:99:LEU:HD23	22:R:114:LYS:HZ2	1.71	0.56
29:Y:492:LYS:O	29:Y:495:SER:OG	2.22	0.56
30:Z:124:GLY:HA2	32:b:98:ASP:O	2.06	0.56
30:Z:336:TYR:HB2	30:Z:343:VAL:HB	1.88	0.56
32:b:165:LYS:NZ	32:b:167:ALA:O	2.37	0.56
32:b:197:ASP:O	32:b:216:LYS:NZ	2.39	0.56
37:g:55:LEU:HB3	37:g:59:HIS:CG	2.41	0.56
38:h:135:ALA:O	38:h:138:LYS:HG2	2.05	0.56
40:j:580:ILE:HG22	40:j:594:VAL:HG23	1.87	0.56
44:n:37:ASP:OD1	44:n:37:ASP:N	2.37	0.56
50:t:83:MET:O	50:t:86:LEU:HB2	2.04	0.56
50:t:136:ARG:O	50:t:139:MET:HG2	2.06	0.56
50:t:159:ARG:HH12	50:t:160:VAL:HB	1.70	0.56
2:1:756:LEU:O	2:1:760:VAL:HG23	2.06	0.56
5:A:1211:LEU:HD11	5:A:1258:ARG:HB2	1.87	0.56
9:E:16:THR:HG21	9:E:135:LEU:O	2.05	0.56
11:G:7:LEU:HB2	11:G:72:TYR:CZ	2.41	0.56
11:G:89:VAL:HA	11:G:99:THR:HG22	1.88	0.56
17:M:344:ARG:HD2	20:P:203:ARG:NH1	2.19	0.56
22:R:89:HIS:NE2	22:R:138:ALA:O	2.38	0.56
28:X:71:ILE:HB	28:X:231:VAL:HG22	1.88	0.56
29:Y:457:ILE:CD1	29:Y:520:ASN:ND2	2.66	0.56
29:Y:504:LYS:HA	29:Y:507:PRO:CG	2.36	0.56
30:Z:41:CYS:CB	30:Z:114:PHE:CE1	2.89	0.56
32:b:285:CYS:SG	32:b:287:THR:OG1	2.64	0.56
36:f:72:LYS:HB3	36:f:73:PRO:HD3	1.87	0.56
40:j:464:TRP:HB3	47:q:168:TRP:CH2	2.41	0.56
42:l:156:LEU:CD1	44:n:288:LEU:CD1	2.81	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:q:176:MET:O	47:q:177:ARG:HD2	2.06	0.56
48:r:93:ARG:HH21	52:v:23:GLY:H	1.54	0.56
56:z:721:LEU:HD22	56:z:736:TRP:CZ3	2.41	0.56
56:z:764:PRO:O	56:z:766:LYS:N	2.39	0.56
2:1:1198:GLN:NE2	3:2:720:GLU:O	2.39	0.56
5:A:1218:ARG:NH2	5:A:1255:LEU:HA	2.21	0.56
5:A:1622:TYR:CD2	5:A:1622:TYR:C	2.84	0.56
5:A:1622:TYR:HD2	38:h:107:ASP:OD1	1.84	0.56
8:D:78:GLU:C	38:h:51:LEU:HD22	2.30	0.56
17:M:25:VAL:HA	17:M:28:ILE:HD13	1.86	0.56
19:O:37:CYS:SG	19:O:39:LEU:HD23	2.45	0.56
27:W:77:TRP:HB3	30:Z:338:PHE:CD2	2.41	0.56
28:X:310:LEU:CD2	28:X:409:THR:OG1	2.54	0.56
29:Y:470:GLU:OE2	29:Y:474:HIS:NE2	2.38	0.56
39:i:87:ARG:HD3	40:j:296:GLU:OE2	2.06	0.56
40:j:464:TRP:HB3	47:q:168:TRP:HH2	1.69	0.56
44:n:208:PHE:CE1	44:n:259:PRO:HG3	2.40	0.56
48:r:747:LEU:HD22	48:r:806:ARG:HH21	1.70	0.56
52:v:19:ILE:O	52:v:22:LEU:N	2.39	0.56
52:v:124:TYR:CD1	52:v:127:ILE:HD12	2.40	0.56
55:y:99:GLU:OE2	55:y:99:GLU:HA	2.03	0.56
3:2:135:THR:HG23	3:2:157:GLN:HE22	1.71	0.56
3:2:909:SER:HA	3:2:952:VAL:HG11	1.88	0.56
5:A:927:GLU:OE1	5:A:931:ARG:NH1	2.39	0.56
5:A:979:LEU:HD13	5:A:1041:PHE:HD1	1.70	0.56
6:B:274:ARG:NH2	6:B:281:ASP:OD1	2.39	0.56
6:B:508:MET:HB3	6:B:621:ILE:HG21	1.88	0.56
7:C:73:LEU:HD23	7:C:128:ILE:HG21	1.87	0.56
18:N:62:LEU:HA	18:N:76:LEU:HA	1.87	0.56
22:R:117:GLN:O	22:R:121:THR:OG1	2.18	0.56
23:S:49:ARG:HG3	23:S:98:TRP:CE2	2.41	0.56
24:T:105:SER:OG	24:T:106:LEU:N	2.38	0.56
28:X:39:VAL:HG22	28:X:456:ILE:HB	1.88	0.56
29:Y:407:ILE:HG21	32:b:19:PRO:CB	2.36	0.56
38:h:141:GLN:HB3	38:h:145:LYS:HZ1	1.71	0.56
38:h:142:SER:O	38:h:146:MET:HG2	2.06	0.56
40:j:409:GLY:O	42:l:86:ILE:HG21	2.06	0.56
40:j:469:ASP:OD1	44:n:231:TRP:CD1	2.59	0.56
43:m:123:ILE:CG1	47:q:163:LEU:CD1	2.66	0.56
48:r:91:ARG:HH22	53:w:126:SER:CB	2.19	0.56
48:r:247:LEU:HD11	48:r:275:HIS:NE2	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:528:HIS:HD2	48:r:609:ARG:HH21	1.53	0.56
48:r:552:VAL:HG13	48:r:553:GLU:H	1.71	0.56
48:r:822:ILE:HG12	48:r:833:ILE:HG22	1.88	0.56
50:t:75:LYS:NZ	54:x:81:SER:HB3	2.21	0.56
52:v:70:TYR:HH	52:v:80:TYR:N	1.82	0.56
53:w:146:GLY:O	53:w:149:LEU:N	2.37	0.56
55:y:23:GLU:O	55:y:24:PHE:C	2.49	0.56
55:y:31:PRO:O	55:y:34:LEU:HB2	2.06	0.56
2:1:141:ILE:O	2:1:145:ILE:HG13	2.06	0.56
3:2:19:SER:OG	3:2:20:ASP:OD1	2.24	0.56
3:2:745:CYS:SG	3:2:779:VAL:HG13	2.46	0.56
5:A:1481:LYS:HZ1	48:r:331:ALA:HB1	1.70	0.56
19:O:244:LEU:HD21	19:O:295:ARG:HH11	1.71	0.56
20:P:197:PHE:CE1	26:V:77:DT:H5"	2.39	0.56
27:W:640:LEU:CD2	27:W:685:TYR:CZ	2.89	0.56
29:Y:506:CYS:SG	29:Y:529:LEU:HD11	2.46	0.56
40:j:140:ASN:O	40:j:144:LEU:HG	2.06	0.56
41:k:43:CYS:HA	41:k:138:LYS:HB3	1.88	0.56
48:r:234:LEU:C	48:r:246:ARG:O	2.48	0.56
48:r:520:LEU:O	48:r:525:TYR:OH	2.24	0.56
49:s:42:ARG:O	49:s:46:GLU:HG2	2.06	0.56
49:s:147:GLU:HG2	49:s:148:ILE:N	2.21	0.56
52:v:124:TYR:CD1	52:v:127:ILE:HB	2.40	0.56
55:y:13:GLY:O	55:y:17:ARG:HG2	2.06	0.56
2:1:325:GLY:O	2:1:326:THR:HG22	2.06	0.56
3:2:719:LEU:O	3:2:763:ARG:NH1	2.39	0.56
6:B:371:ARG:NH2	6:B:609:GLU:OE1	2.31	0.56
22:R:155:LEU:HD21	22:R:204:ASN:H	1.71	0.56
27:W:371:VAL:CG1	27:W:407:ILE:HG22	2.35	0.56
27:W:469:THR:CB	27:W:634:ARG:HB3	2.36	0.56
30:Z:440:LEU:HD12	33:c:38:ILE:HG22	1.83	0.56
36:f:198:ILE:HD11	36:f:255:MET:SD	2.45	0.56
39:i:115:LEU:HD13	45:o:129:VAL:CG1	2.33	0.56
50:t:160:VAL:HA	50:t:163:MET:HG2	1.87	0.56
52:v:95:VAL:HG13	52:v:96:LYS:HG2	1.87	0.56
55:y:81:TYR:N	55:y:85:ARG:HH22	2.02	0.56
55:y:86:LYS:HB2	55:y:87:GLU:OE2	2.07	0.56
2:1:762:GLU:HA	2:1:765:ARG:HE	1.71	0.55
3:2:124:LEU:HD22	3:2:174:ASN:HD22	1.71	0.55
5:A:853:LYS:HA	5:A:856:GLU:HG3	1.87	0.55
5:A:1162:GLU:H	5:A:1304:ILE:HD11	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:125:PRO:HG3	38:h:168:PRO:CD	2.22	0.55
21:Q:160:GLU:OE2	21:Q:162:GLU:N	2.38	0.55
24:T:38:GLY:O	24:T:39:GLU:HG2	2.05	0.55
24:T:86:GLN:NE2	24:T:115:GLU:HB2	2.20	0.55
33:c:8:VAL:HG11	33:c:50:VAL:HG21	1.88	0.55
37:g:86:ARG:HH21	37:g:90:ALA:H	1.51	0.55
40:j:198:LYS:NZ	40:j:203:ILE:CD1	2.69	0.55
40:j:198:LYS:CG	43:m:88:LEU:HD22	2.36	0.55
48:r:127:ILE:O	48:r:128:LEU:C	2.49	0.55
48:r:129:PHE:CE2	54:x:27:GLN:HA	2.40	0.55
50:t:32:PRO:HB2	55:y:18:PHE:CE1	2.41	0.55
52:v:2:ALA:HA	52:v:5:PHE:HB2	1.88	0.55
52:v:67:VAL:CG2	52:v:70:TYR:HD2	2.19	0.55
52:v:92:ASN:HA	52:v:95:VAL:HG12	1.87	0.55
53:w:129:SER:O	53:w:133:LYS:N	2.36	0.55
54:x:15:LEU:O	54:x:19:PHE:CG	2.59	0.55
55:y:75:MET:O	55:y:76:LEU:C	2.48	0.55
1:0:263:LEU:HD13	1:0:339:TRP:HB2	1.88	0.55
2:1:1071:LEU:HG	2:1:1108:THR:HG23	1.87	0.55
3:2:374:SER:O	3:2:377:SER:OG	2.21	0.55
5:A:1218:ARG:HH21	5:A:1255:LEU:HA	1.71	0.55
6:B:892:CYS:HB2	19:O:53:ARG:HH11	1.71	0.55
28:X:238:ASN:HB3	28:X:241:ASN:HB2	1.88	0.55
29:Y:475:PHE:O	29:Y:479:PHE:HB2	2.06	0.55
30:Z:408:LEU:CD1	33:c:44:PHE:CZ	2.55	0.55
42:l:156:LEU:CD1	44:n:288:LEU:CG	2.67	0.55
44:n:60:LEU:HD22	56:z:618:CYS:SG	2.46	0.55
48:r:247:LEU:HD12	48:r:247:LEU:O	2.06	0.55
48:r:529:PRO:HD2	48:r:609:ARG:NH1	2.21	0.55
49:s:191:ASN:O	49:s:194:SER:N	2.39	0.55
50:t:74:HIS:HA	50:t:77:GLU:CD	2.31	0.55
50:t:75:LYS:HZ2	54:x:79:GLU:C	2.14	0.55
55:y:32:ASN:OD1	55:y:33:TYR:N	2.34	0.55
55:y:71:GLN:OE1	55:y:71:GLN:N	2.38	0.55
1:0:87:LEU:HD22	1:0:96:LEU:HD11	1.88	0.55
1:0:142:LYS:HE3	1:0:162:VAL:HB	1.87	0.55
1:0:835:ARG:HH11	1:0:835:ARG:CG	2.20	0.55
5:A:1227:THR:HB	5:A:1229:GLU:HG2	1.88	0.55
5:A:1313:GLN:HE22	5:A:1333:GLU:H	1.53	0.55
8:D:60:VAL:HG13	11:G:103:PRO:HB3	1.89	0.55
13:I:91:HIS:ND1	13:I:92:LYS:O	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:345:SER:OG	17:M:346:LYS:N	2.39	0.55
30:Z:255:SER:H	30:Z:258:LEU:HD12	1.71	0.55
37:g:85:GLN:OE1	37:g:95:LEU:N	2.35	0.55
43:m:30:MET:O	43:m:34:THR:HG23	2.07	0.55
48:r:69:LEU:HA	48:r:72:LEU:HB2	1.87	0.55
48:r:566:TYR:HB3	48:r:568:TYR:CE1	2.41	0.55
48:r:572:SER:HB3	48:r:610:THR:OG1	2.06	0.55
50:t:17:TYR:CE2	55:y:17:ARG:HD2	2.40	0.55
52:v:104:LYS:HA	52:v:107:SER:HB2	1.89	0.55
3:2:957:LYS:HD3	3:2:967:VAL:HG11	1.88	0.55
5:A:1624:PRO:HB2	5:A:1627:PRO:HG2	1.89	0.55
8:D:41:LEU:HG	8:D:61:PHE:HE1	1.70	0.55
21:Q:107:LEU:HD11	21:Q:111:ARG:HH22	1.69	0.55
28:X:316:GLN:CG	28:X:373:ARG:CZ	2.84	0.55
28:X:325:THR:HB	28:X:328:HIS:HD2	1.71	0.55
39:i:87:ARG:NH2	40:j:299:GLN:CD	2.62	0.55
40:j:195:LYS:HD2	40:j:195:LYS:C	2.31	0.55
40:j:365:GLU:O	40:j:369:TYR:N	2.40	0.55
40:j:469:ASP:HB2	44:n:231:TRP:CD1	2.41	0.55
48:r:486:MET:HA	48:r:488:ARG:H	1.71	0.55
48:r:1189:SER:OG	48:r:1190:PRO:HD2	2.06	0.55
49:s:110:LEU:O	49:s:114:LEU:HG	2.06	0.55
49:s:123:THR:HA	49:s:126:TYR:CE2	2.41	0.55
50:t:142:GLN:O	50:t:146:ARG:HG3	2.06	0.55
52:v:80:TYR:O	52:v:83:GLU:N	2.37	0.55
55:y:45:ASP:H	55:y:48:PHE:HD2	1.54	0.55
55:y:55:LEU:HA	55:y:58:TRP:HD1	1.71	0.55
1:0:116:ASN:HB2	1:0:834:TRP:CE2	2.42	0.55
2:1:627:LEU:HD21	2:1:648:THR:OG1	2.06	0.55
3:2:477:TYR:CZ	3:2:479:SER:HB2	2.41	0.55
3:2:529:MET:SD	3:2:533:MET:HG2	2.47	0.55
3:2:915:ARG:NH1	56:z:702:GLY:N	2.55	0.55
5:A:908:THR:HG22	5:A:963:ARG:HG3	1.87	0.55
6:B:665:ILE:HD11	6:B:695:HIS:CD2	2.41	0.55
9:E:19:GLN:OE1	9:E:138:ASN:ND2	2.40	0.55
21:Q:30:HIS:CD2	21:Q:62:VAL:HG13	2.41	0.55
27:W:109:ARG:NH1	27:W:492:ASN:HB2	2.19	0.55
28:X:237:HIS:CE1	28:X:460:THR:HB	2.42	0.55
28:X:396:PRO:O	28:X:399:LEU:HB3	2.06	0.55
39:i:79:HIS:HB3	43:m:91:PHE:HE1	1.72	0.55
44:n:55:HIS:O	44:n:59:ASN:ND2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:886:PRO:O	48:r:904:PHE:HB2	2.06	0.55
50:t:126:TYR:HA	50:t:129:HIS:CE1	2.41	0.55
50:t:135:LEU:O	50:t:136:ARG:C	2.47	0.55
54:x:115:LEU:O	54:x:118:ILE:HG12	2.06	0.55
55:y:40:ARG:HD3	55:y:42:TYR:CE2	2.42	0.55
55:y:74:HIS:O	55:y:78:LEU:HG	2.07	0.55
5:A:264:VAL:HB	5:A:266:MET:HE3	1.89	0.55
15:K:65:HIS:CE1	15:K:67:LEU:HD23	2.42	0.55
19:O:260:MET:HG3	19:O:313:LEU:HD21	1.88	0.55
27:W:170:LEU:HD11	27:W:175:TYR:CE2	2.42	0.55
30:Z:400:ARG:CD	33:c:16:MET:CG	2.85	0.55
40:j:414:ASP:HB3	40:j:419:ASN:HB2	1.89	0.55
40:j:469:ASP:CB	44:n:231:TRP:NE1	2.69	0.55
40:j:489:LYS:O	40:j:489:LYS:HG3	2.07	0.55
41:k:147:LYS:HD3	41:k:149:PHE:HE1	1.71	0.55
45:o:60:VAL:O	46:p:175:HIS:NE2	2.39	0.55
48:r:51:LEU:N	48:r:54:LEU:HD13	2.22	0.55
49:s:127:GLN:HB3	49:s:131:LYS:NZ	2.21	0.55
1:0:812:ARG:HH21	46:p:90:ASN:CG	2.15	0.55
5:A:338:SER:O	5:A:340:LYS:N	2.39	0.55
5:A:1192:TRP:O	5:A:1195:VAL:HG22	2.07	0.55
6:B:748:ALA:HB3	6:B:811:TYR:HB2	1.89	0.55
11:G:113:ILE:HB	11:G:114:PRO:HD3	1.89	0.55
12:H:125:LEU:HD22	12:H:132:LEU:HD21	1.89	0.55
20:P:212:LEU:HD11	26:V:78:DT:O4'	2.07	0.55
23:S:37:VAL:HG12	24:T:91:GLN:HG2	1.89	0.55
27:W:167:LYS:HG2	27:W:294:GLU:HG2	1.86	0.55
29:Y:374:LEU:HD13	32:b:270:VAL:HG11	1.83	0.55
40:j:190:LEU:HD12	40:j:291:TRP:CG	2.42	0.55
40:j:371:LEU:HD11	40:j:435:ALA:HA	1.89	0.55
41:k:43:CYS:SG	41:k:137:ARG:N	2.79	0.55
42:l:148:VAL:HG21	44:n:196:LYS:HB3	1.88	0.55
45:o:86:ASP:HA	45:o:89:ARG:HG3	1.89	0.55
48:r:126:ALA:O	48:r:130:VAL:HG22	2.07	0.55
48:r:168:ARG:NH2	55:y:73:LEU:HD21	2.21	0.55
49:s:104:ASP:C	49:s:108:GLN:HE22	2.15	0.55
52:v:101:THR:OG1	52:v:102:MET:N	2.37	0.55
54:x:94:GLU:O	54:x:98:HIS:CE1	2.59	0.55
56:z:678:LEU:HD22	56:z:725:VAL:HG21	1.88	0.55
1:0:313:LYS:HZ3	1:0:336:ILE:N	2.04	0.55
2:1:568:SER:HA	2:1:612:MET:HE1	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:125:PHE:CZ	4:3:140:ARG:HB3	2.42	0.55
12:H:48:TYR:OH	12:H:147:LYS:HB2	2.07	0.55
18:N:68:CYS:HB3	18:N:71:VAL:HG22	1.89	0.55
19:O:311:ASP:OD1	19:O:312:LYS:N	2.40	0.55
22:R:170:ASP:HA	22:R:173:GLU:HG2	1.89	0.55
24:T:20:LEU:H	24:T:110:VAL:HG13	1.72	0.55
40:j:582:VAL:HA	40:j:592:ILE:HG12	1.87	0.55
44:n:283:ARG:HD3	44:n:309:CYS:HB3	1.87	0.55
48:r:145:VAL:HG23	48:r:146:HIS:CE1	2.42	0.55
48:r:156:TYR:N	48:r:156:TYR:CD1	2.72	0.55
48:r:797:PHE:CE2	48:r:873:PHE:HA	2.41	0.55
48:r:959:LEU:HG	48:r:963:LEU:HD23	1.89	0.55
52:v:98:LYS:O	52:v:102:MET:HG2	2.07	0.55
54:x:115:LEU:HB2	54:x:119:GLN:NE2	2.22	0.55
55:y:71:GLN:O	55:y:75:MET:HG2	2.07	0.55
56:z:708:CYS:SG	56:z:773:LEU:HD11	2.47	0.55
1:0:741:ARG:HE	1:0:759:PRO:HA	1.72	0.55
2:1:550:LEU:HD23	2:1:559:LEU:HD23	1.88	0.55
2:1:927:LYS:HG2	2:1:928:TYR:CE2	2.42	0.55
4:3:45:GLU:OE1	4:3:51:PRO:CD	2.54	0.55
5:A:893:GLU:OE1	9:E:197:SER:OG	2.13	0.55
5:A:1623:SER:HG	55:y:92:GLN:HG2	1.69	0.55
7:C:38:PHE:HE1	7:C:245:VAL:HA	1.72	0.55
8:D:73:ARG:HD3	8:D:140:PHE:HZ	1.72	0.55
24:T:223:GLN:HA	24:T:233:TRP:HA	1.88	0.55
27:W:520:ARG:C	33:c:22:TYR:HE1	2.09	0.55
30:Z:46:ARG:NH1	32:b:53:ARG:CD	2.64	0.55
31:a:254:PHE:HE2	32:b:274:ILE:HG21	1.70	0.55
40:j:410:PRO:O	42:l:86:ILE:CG1	2.55	0.55
40:j:464:TRP:CE3	40:j:475:VAL:HB	2.42	0.55
41:k:198:HIS:NE2	41:k:200:GLU:CD	2.58	0.55
44:n:53:ILE:CD1	56:z:629:ILE:HD13	2.19	0.55
48:r:114:LYS:O	48:r:117:MET:HE3	2.07	0.55
48:r:179:PRO:HG3	55:y:84:PHE:CZ	2.42	0.55
48:r:536:ASN:HD22	48:r:554:MET:HG3	1.71	0.55
50:t:109:LEU:O	50:t:112:LEU:HG	2.06	0.55
52:v:13:GLU:OE1	52:v:14:LYS:N	2.39	0.55
52:v:81:THR:O	52:v:85:LEU:HB2	2.07	0.55
55:y:110:ARG:HH11	55:y:110:ARG:HB2	1.71	0.55
56:z:626:LEU:HD23	56:z:629:ILE:HD11	1.89	0.55
1:0:114:LEU:HD11	1:0:807:LEU:HD11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:247:SER:O	1:0:249:VAL:N	2.40	0.55
1:0:742:LEU:O	1:0:743:GLN:HG2	2.07	0.55
2:1:708:GLN:OE1	2:1:708:GLN:N	2.36	0.55
2:1:1183:TRP:CE2	3:2:339:GLU:HG2	2.42	0.55
6:B:302:LYS:HG3	13:I:23:MET:HE1	1.88	0.55
7:C:78:ILE:HG13	7:C:127:VAL:HG22	1.89	0.55
24:T:31:TRP:NE1	24:T:62:LEU:O	2.40	0.55
27:W:124:TYR:OH	27:W:291:LEU:C	2.49	0.55
27:W:365:GLY:HA2	27:W:441:ASP:HB2	1.89	0.55
30:Z:384:PRO:HG2	30:Z:387:ILE:HD12	1.88	0.55
30:Z:400:ARG:CB	33:c:16:MET:SD	2.94	0.55
35:e:267:ASP:OD2	35:e:297:ASN:ND2	2.31	0.55
40:j:393:PRO:HG2	41:k:137:ARG:HH22	1.64	0.55
42:l:156:LEU:CD1	44:n:288:LEU:HD11	2.33	0.55
48:r:126:ALA:O	48:r:129:PHE:HB3	2.07	0.55
48:r:520:LEU:HD11	48:r:549:TYR:CE2	2.42	0.55
48:r:685:LEU:HD21	56:z:681:GLU:OE2	2.07	0.55
56:z:681:GLU:O	56:z:685:LEU:HG	2.07	0.55
1:0:17:TYR:CD1	1:0:17:TYR:C	2.86	0.54
1:0:786:HIS:H	56:z:636:HIS:HD2	1.55	0.54
2:1:488:PHE:HA	2:1:491:PRO:HD2	1.89	0.54
2:1:775:ASP:OD1	2:1:775:ASP:N	2.39	0.54
4:3:45:GLU:OE2	4:3:51:PRO:CD	2.55	0.54
5:A:710:LYS:HG2	5:A:817:PRO:HG3	1.88	0.54
5:A:1215:GLU:HG2	5:A:1255:LEU:O	2.06	0.54
5:A:1483:GLY:HA3	10:F:80:MET:SD	2.47	0.54
7:C:148:ILE:HG22	14:J:15:GLY:HA3	1.88	0.54
11:G:14:HIS:HD2	11:G:16:ARG:H	1.53	0.54
20:P:216:SER:OG	25:U:18:DG:H3'	2.07	0.54
20:P:304:ILE:HA	20:P:310:VAL:HG22	1.89	0.54
22:R:147:ASP:HB3	22:R:150:ALA:H	1.71	0.54
27:W:112:HIS:CD2	30:Z:310:GLU:CD	2.80	0.54
27:W:274:GLN:HB2	27:W:459:GLN:NE2	2.01	0.54
35:e:78:LEU:N	35:e:90:VAL:O	2.40	0.54
40:j:374:ASN:HD21	40:j:434:GLN:HE22	1.51	0.54
44:n:289:GLN:OE1	44:n:306:HIS:NE2	2.40	0.54
48:r:154:ILE:O	48:r:157:ALA:HB3	2.08	0.54
49:s:127:GLN:O	49:s:130:GLU:HB2	2.08	0.54
49:s:183:ARG:C	49:s:185:GLY:N	2.65	0.54
50:t:141:VAL:HA	50:t:144:ARG:HB2	1.88	0.54
52:v:70:TYR:HH	52:v:77:PRO:C	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:101:THR:HA	52:v:104:LYS:HE2	1.89	0.54
54:x:98:HIS:O	54:x:101:ALA:HB3	2.07	0.54
3:2:624:LEU:HB3	3:2:643:ILE:HD11	1.89	0.54
5:A:316:THR:HA	5:A:319:ASP:O	2.06	0.54
5:A:1657:TYR:CE2	35:e:58:THR:OG1	2.60	0.54
6:B:331:THR:H	6:B:334:LYS:HE2	1.73	0.54
17:M:342:ILE:HD13	18:N:74:PHE:HZ	1.72	0.54
19:O:169:ARG:HH21	19:O:209:ILE:HG23	1.72	0.54
27:W:480:LEU:HD22	27:W:483:LEU:HD22	1.89	0.54
28:X:166:ARG:HH22	28:X:301:THR:HG21	1.71	0.54
29:Y:403:SER:HB2	32:b:20:ILE:HA	1.89	0.54
29:Y:544:LEU:CA	29:Y:547:LYS:HE3	2.26	0.54
30:Z:122:LEU:O	32:b:100:LYS:CD	2.55	0.54
39:i:22:GLY:HA2	40:j:167:LEU:HD23	1.88	0.54
40:j:500:GLU:HG2	40:j:500:GLU:O	2.06	0.54
43:m:133:GLU:CD	45:o:125:LYS:HE2	2.29	0.54
44:n:109:GLN:NE2	45:o:65:VAL:H	2.05	0.54
49:s:126:TYR:HB2	49:s:127:GLN:OE1	2.07	0.54
50:t:91:ASP:HA	50:t:94:ASP:CG	2.32	0.54
55:y:46:LYS:HA	55:y:49:VAL:HG23	1.88	0.54
56:z:686:ASP:OD1	56:z:687:PRO:HD2	2.07	0.54
1:0:794:GLU:OE1	1:0:835:ARG:NH2	2.40	0.54
3:2:96:ALA:O	3:2:100:ILE:HG12	2.07	0.54
5:A:313:HIS:HA	5:A:316:THR:HG22	1.88	0.54
5:A:1049:LEU:HG	5:A:1054:MET:HE3	1.88	0.54
6:B:755:GLN:HE21	6:B:777:ASN:HD22	1.55	0.54
16:L:21:GLU:HB2	16:L:41:TYR:HD2	1.71	0.54
21:Q:148:MET:HE2	41:k:200:GLU:HA	1.88	0.54
38:h:68:THR:O	38:h:70:LEU:HD22	2.08	0.54
43:m:123:ILE:HD13	47:q:163:LEU:HD11	1.60	0.54
44:n:310:ARG:HD3	48:r:715:ARG:NH2	2.21	0.54
48:r:202:ARG:O	48:r:206:THR:OG1	2.20	0.54
52:v:120:ASP:N	52:v:124:TYR:CZ	2.75	0.54
54:x:128:SER:HA	54:x:131:LYS:HG3	1.87	0.54
55:y:56:LEU:O	55:y:59:LYS:HG2	2.07	0.54
2:1:118:THR:O	2:1:122:VAL:HG23	2.07	0.54
2:1:634:ALA:O	2:1:636:THR:OG1	2.22	0.54
3:2:915:ARG:NH2	56:z:701:ASN:CB	2.69	0.54
5:A:18:ILE:HG22	5:A:1462:GLN:NE2	2.22	0.54
5:A:481:THR:HG22	6:B:1055:VAL:HG21	1.88	0.54
6:B:1066:PRO:HG3	6:B:1077:GLY:HA3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:10:THR:O	24:T:106:LEU:N	2.34	0.54
27:W:276:MET:O	27:W:280:LEU:N	2.32	0.54
27:W:689:VAL:C	30:Z:393:LEU:HD11	2.33	0.54
29:Y:431:ILE:HD11	30:Z:62:LEU:HA	1.90	0.54
40:j:112:LEU:O	40:j:116:LEU:HG	2.07	0.54
40:j:259:VAL:HB	40:j:368:LEU:HD12	1.89	0.54
40:j:464:TRP:CG	40:j:475:VAL:HG23	2.43	0.54
48:r:245:TRP:O	48:r:282:LEU:CD1	2.50	0.54
50:t:78:LEU:HB2	50:t:122:LEU:HD11	1.88	0.54
54:x:66:ALA:O	54:x:68:ASP:N	2.40	0.54
55:y:94:ALA:O	55:y:98:ASP:HB2	2.08	0.54
1:0:166:PRO:HD2	1:0:169:THR:HG22	1.89	0.54
2:1:227:LEU:HD23	2:1:1147:ASN:HB2	1.89	0.54
5:A:702:ILE:HG23	5:A:752:THR:HG23	1.89	0.54
21:Q:32:LEU:O	21:Q:36:ILE:HG12	2.08	0.54
21:Q:76:MET:HG2	21:Q:88:ARG:HB3	1.89	0.54
22:R:170:ASP:OD1	22:R:171:ILE:N	2.40	0.54
27:W:516:PRO:HG3	33:c:18:GLN:CG	2.38	0.54
31:a:80:ARG:NH2	31:a:202:SER:OG	2.41	0.54
40:j:38:GLN:N	40:j:38:GLN:HE21	2.05	0.54
41:k:43:CYS:SG	41:k:136:PHE:HB3	2.47	0.54
50:t:15:MET:HB3	50:t:18:ILE:HG23	1.90	0.54
51:u:122:ARG:O	51:u:123:GLU:C	2.50	0.54
52:v:32:SER:HA	52:v:34:GLN:HE21	1.72	0.54
54:x:85:LEU:O	54:x:88:ALA:N	2.40	0.54
54:x:109:TYR:O	54:x:112:ASP:HB2	2.07	0.54
2:1:623:LEU:HD22	2:1:652:LEU:HD11	1.89	0.54
5:A:979:LEU:HD11	5:A:1044:HIS:CD2	2.43	0.54
6:B:499:ARG:NH1	6:B:518:HIS:O	2.28	0.54
7:C:68:LEU:HD12	7:C:71:ILE:HD12	1.90	0.54
19:O:304:PHE:HB3	19:O:306:PHE:HE1	1.72	0.54
29:Y:383:TYR:O	32:b:174:TYR:HB3	2.07	0.54
35:e:144:LEU:HG	35:e:154:ALA:HB2	1.88	0.54
44:n:60:LEU:CD1	56:z:618:CYS:HB3	2.35	0.54
48:r:150:PRO:HB2	50:t:127:ARG:NH2	2.22	0.54
48:r:871:VAL:O	48:r:875:THR:OG1	2.26	0.54
51:u:120:SER:O	51:u:124:GLN:HG2	2.08	0.54
52:v:75:ARG:HH12	53:w:105:LEU:N	2.00	0.54
54:x:3:ASP:O	54:x:5:LEU:N	2.40	0.54
55:y:53:LYS:O	55:y:56:LEU:HB2	2.07	0.54
55:y:69:TYR:O	55:y:71:GLN:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:73:LEU:O	55:y:76:LEU:N	2.40	0.54
1:0:17:TYR:CE2	1:0:738:LEU:HD23	2.42	0.54
1:0:124:SER:OG	1:0:125:LEU:N	2.40	0.54
1:0:505:GLU:O	1:0:509:GLU:HG3	2.08	0.54
2:1:806:ILE:O	2:1:810:VAL:HG23	2.08	0.54
2:1:810:VAL:O	2:1:814:ILE:HG12	2.07	0.54
5:A:1372:GLU:OE1	9:E:195:ARG:NH2	2.40	0.54
11:G:125:PRO:CG	38:h:168:PRO:HD2	2.23	0.54
19:O:111:ASP:HA	19:O:114:MET:HE3	1.89	0.54
20:P:214:PHE:HB2	20:P:218:LYS:O	2.07	0.54
28:X:722:ARG:HB3	31:a:223:LEU:HD23	1.89	0.54
40:j:482:GLN:CG	43:m:137:SER:HB2	2.37	0.54
52:v:40:LYS:O	52:v:43:PHE:HB2	2.08	0.54
54:x:66:ALA:O	54:x:67:LYS:C	2.50	0.54
54:x:83:ALA:O	54:x:86:GLN:HG2	2.08	0.54
55:y:15:ARG:HA	55:y:18:PHE:CD2	2.42	0.54
1:0:168:LEU:O	1:0:170:LEU:N	2.39	0.54
2:1:633:VAL:C	2:1:635:GLN:H	2.14	0.54
2:1:844:ASN:O	2:1:848:GLU:HG2	2.07	0.54
2:1:1135:PRO:O	2:1:1136:LEU:HB3	2.08	0.54
3:2:481:GLU:OE1	3:2:481:GLU:N	2.39	0.54
6:B:728:MET:HE2	6:B:942:LYS:HE3	1.90	0.54
7:C:72:PRO:HB2	7:C:131:THR:HG21	1.90	0.54
23:S:134:ALA:HB1	24:T:40:VAL:HG21	1.90	0.54
26:V:31:DG:C8	26:V:32:DC:C5	2.95	0.54
28:X:311:PRO:CD	28:X:314:VAL:HB	2.37	0.54
29:Y:381:ARG:HB3	32:b:256:PHE:HB3	1.90	0.54
30:Z:58:ARG:NE	32:b:241:LEU:CD2	2.57	0.54
32:b:255:CYS:SG	32:b:258:HIS:N	2.70	0.54
34:d:307:GLN:CD	36:f:247:GLN:HE21	2.16	0.54
37:g:75:GLU:HA	37:g:79:PHE:HE1	1.72	0.54
39:i:87:ARG:CD	40:j:296:GLU:OE2	2.56	0.54
48:r:135:ARG:NH2	50:t:109:LEU:HB3	2.23	0.54
48:r:534:SER:OG	48:r:535:LYS:N	2.39	0.54
50:t:16:GLN:HG3	50:t:17:TYR:H	1.72	0.54
50:t:90:LEU:O	50:t:91:ASP:C	2.51	0.54
52:v:7:HIS:O	52:v:11:HIS:HD2	1.89	0.54
56:z:731:ALA:CA	56:z:766:LYS:HZ3	2.21	0.54
1:0:13:MET:HB2	1:0:456:ARG:O	2.03	0.54
3:2:194:HIS:HA	3:2:197:LEU:HG	1.90	0.54
5:A:1623:SER:CB	55:y:92:GLN:NE2	2.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:173:HIS:CD2	7:C:174:ALA:H	2.25	0.54
17:M:331:THR:HG23	17:M:333:ASN:OD1	2.08	0.54
20:P:167:ASN:CB	26:V:80:DT:O2	2.55	0.54
26:V:81:DA:H2''	26:V:82:DT:H5'	1.90	0.54
27:W:666:ASP:O	33:c:64:ASN:HB3	2.08	0.54
28:X:531:VAL:O	31:a:174:LEU:HD13	2.08	0.54
40:j:617:HIS:ND1	48:r:741:PRO:HB2	2.22	0.54
48:r:812:TYR:CD2	48:r:818:SER:HB2	2.43	0.54
49:s:65:VAL:O	49:s:69:LEU:HB2	2.07	0.54
50:t:92:LEU:HD23	50:t:108:LYS:HD2	1.89	0.54
55:y:71:GLN:HB3	55:y:75:MET:HE3	1.89	0.54
11:G:34:VAL:HG21	11:G:72:TYR:OH	2.08	0.54
19:O:145:VAL:HG22	19:O:151:LEU:HD11	1.90	0.54
29:Y:422:LEU:HD12	32:b:224:LEU:HD23	1.87	0.54
29:Y:470:GLU:OE1	29:Y:473:ARG:NH1	2.41	0.54
29:Y:504:LYS:C	29:Y:507:PRO:CG	2.81	0.54
42:l:157:LEU:O	42:l:161:LEU:HG	2.07	0.54
42:l:179:ARG:NE	42:l:179:ARG:O	2.41	0.54
48:r:777:TYR:HA	48:r:780:VAL:HG12	1.89	0.54
48:r:802:VAL:HG12	48:r:809:ILE:HB	1.90	0.54
50:t:78:LEU:O	50:t:79:ARG:C	2.51	0.54
54:x:54:TYR:HD1	54:x:57:LEU:HD12	1.73	0.54
55:y:71:GLN:O	55:y:72:CYS:C	2.48	0.54
56:z:715:LEU:CG	56:z:716:PRO:CD	2.81	0.54
2:1:93:PRO:HG2	2:1:96:LEU:HB2	1.89	0.53
2:1:854:VAL:HG23	2:1:860:VAL:O	2.08	0.53
3:2:339:GLU:OE2	3:2:384:LYS:NZ	2.30	0.53
5:A:47:THR:OG1	5:A:51:ARG:O	2.24	0.53
5:A:780:ASN:ND2	6:B:976:MET:SD	2.79	0.53
5:A:1345:ARG:HD2	9:E:133:GLN:NE2	2.23	0.53
12:H:32:SER:OG	12:H:33:GLU:N	2.41	0.53
23:S:45:ALA:HB3	23:S:103:ASN:H	1.73	0.53
27:W:510:VAL:HG22	27:W:690:ILE:HB	1.91	0.53
30:Z:442:VAL:HG11	33:c:9:LEU:CB	2.38	0.53
31:a:256:GLN:NE2	32:b:261:LEU:HD21	2.18	0.53
34:d:255:THR:HG22	36:f:3:HIS:CE1	2.44	0.53
40:j:49:PHE:CD1	40:j:49:PHE:C	2.84	0.53
40:j:367:HIS:NE2	40:j:438:ILE:HG21	2.20	0.53
44:n:175:GLU:HG2	44:n:175:GLU:O	2.08	0.53
47:q:58:MET:SD	47:q:74:ARG:HB3	2.47	0.53
48:r:797:PHE:HB2	48:r:813:GLY:HA3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:1274:LYS:HB2	48:r:1277:GLU:OE1	2.09	0.53
50:t:125:GLU:O	50:t:126:TYR:C	2.51	0.53
50:t:143:LYS:HE3	54:x:100:ALA:HB2	1.89	0.53
56:z:718:VAL:CG2	56:z:719:PRO:HD2	2.38	0.53
2:1:1127:LEU:HB3	2:1:1131:LEU:HD12	1.90	0.53
5:A:18:ILE:N	5:A:1462:GLN:HE22	2.02	0.53
5:A:924:TYR:OH	5:A:952:LEU:HB2	2.08	0.53
5:A:1226:LEU:HD21	5:A:1298:LEU:HD13	1.90	0.53
5:A:1433:GLU:HG2	5:A:1434:GLU:N	2.23	0.53
7:C:189:ASP:HB3	7:C:218:ALA:HB2	1.89	0.53
11:G:60:GLN:HG3	11:G:63:ARG:HH21	1.72	0.53
12:H:37:MET:HE1	12:H:128:ASP:H	1.73	0.53
13:I:40:ARG:HD3	23:S:172:ASN:N	2.23	0.53
17:M:336:VAL:HB	18:N:5:LEU:HD21	1.91	0.53
24:T:130:LEU:HA	24:T:133:GLU:HG2	1.90	0.53
29:Y:381:ARG:HB3	32:b:256:PHE:CB	2.38	0.53
29:Y:414:TYR:CD2	32:b:112:VAL:HG13	2.43	0.53
40:j:415:LYS:HZ3	42:l:123:LEU:HD12	1.55	0.53
43:m:16:GLN:O	43:m:20:LYS:HG3	2.08	0.53
48:r:155:PRO:HG2	48:r:156:TYR:H	1.73	0.53
52:v:90:ALA:C	52:v:93:GLU:HG2	2.32	0.53
54:x:5:LEU:O	54:x:7:GLN:N	2.41	0.53
55:y:81:TYR:O	55:y:83:HIS:N	2.41	0.53
1:0:310:SER:HB3	1:0:342:LEU:HD12	1.91	0.53
1:0:566:PRO:HD3	1:0:576:PRO:HG2	1.91	0.53
2:1:1200:TYR:HD2	3:2:291:VAL:HG22	1.74	0.53
3:2:967:VAL:HA	3:2:970:ILE:HD12	1.89	0.53
5:A:140:ARG:O	5:A:144:VAL:HG23	2.08	0.53
5:A:859:TYR:CE2	5:A:1125:LYS:HE3	2.43	0.53
7:C:103:LEU:HB3	7:C:161:LEU:HG	1.88	0.53
22:R:175:LEU:HB2	22:R:180:LYS:HE2	1.91	0.53
27:W:278:GLU:HG2	27:W:483:LEU:HD21	1.90	0.53
28:X:56:ILE:HG21	28:X:70:LEU:HD13	1.89	0.53
40:j:191:ARG:HH22	40:j:196:LEU:HB3	1.73	0.53
40:j:193:HIS:O	43:m:101:ARG:NH2	2.42	0.53
48:r:433:THR:O	48:r:435:LEU:N	2.41	0.53
51:u:68:LEU:O	51:u:72:ILE:HG12	2.09	0.53
52:v:48:LEU:HA	52:v:51:ILE:HD12	1.88	0.53
55:y:82:GLU:CD	55:y:83:HIS:N	2.66	0.53
1:0:15:LEU:CD1	1:0:455:LEU:HD21	2.37	0.53
1:0:166:PRO:HB2	1:0:169:THR:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:11:GLU:OE2	2:1:36:LYS:NZ	2.38	0.53
2:1:252:LEU:HD11	2:1:262:LEU:HB3	1.88	0.53
5:A:1624:PRO:HD2	38:h:107:ASP:OD2	2.09	0.53
9:E:112:PRO:HA	9:E:115:LYS:HG2	1.89	0.53
11:G:30:LEU:O	11:G:34:VAL:HG12	2.09	0.53
17:M:47:GLU:HA	17:M:50:LEU:HB3	1.91	0.53
17:M:345:SER:HB3	17:M:348:LYS:HB2	1.90	0.53
28:X:292:LEU:CD1	28:X:317:GLU:O	2.57	0.53
29:Y:376:LEU:HD23	32:b:285:CYS:HB3	1.89	0.53
30:Z:424:HIS:HD2	30:Z:451:VAL:HG22	1.73	0.53
37:g:86:ARG:HH21	37:g:89:PRO:HA	1.74	0.53
39:i:53:THR:O	39:i:57:GLN:HG2	2.07	0.53
40:j:191:ARG:NH1	40:j:203:ILE:CD1	2.65	0.53
40:j:398:ALA:HA	41:k:107:ASP:OD2	2.07	0.53
40:j:410:PRO:HA	42:l:86:ILE:CB	2.38	0.53
44:n:32:PHE:HB3	56:z:646:MET:HE1	1.90	0.53
45:o:138:HIS:O	45:o:142:VAL:HG23	2.08	0.53
47:q:87:VAL:HA	47:q:90:ARG:HH21	1.73	0.53
48:r:92:THR:O	48:r:95:LEU:N	2.41	0.53
48:r:477:ASP:O	48:r:480:LYS:HG3	2.09	0.53
50:t:145:GLN:O	50:t:146:ARG:C	2.50	0.53
56:z:715:LEU:CD1	56:z:716:PRO:CD	2.66	0.53
1:0:469:LEU:HD12	1:0:472:ARG:HE	1.73	0.53
2:1:757:LYS:HD3	2:1:832:TYR:CE1	2.44	0.53
3:2:267:LEU:HB3	3:2:281:PHE:HZ	1.73	0.53
3:2:504:ALA:HB1	3:2:529:MET:HE1	1.89	0.53
30:Z:400:ARG:HG2	33:c:16:MET:CG	2.36	0.53
38:h:22:LEU:HD22	40:j:109:MET:HG2	1.89	0.53
39:i:107:VAL:CG1	47:q:162:GLN:HB3	2.39	0.53
40:j:627:TRP:CE3	40:j:627:TRP:HA	2.42	0.53
42:l:146:PRO:HG3	44:n:236:TYR:HB3	1.91	0.53
46:p:60:TYR:HE1	46:p:116:LEU:HD21	1.74	0.53
46:p:86:THR:HG21	56:z:628:ASN:HD21	1.67	0.53
48:r:174:ARG:O	48:r:177:ILE:HG22	2.09	0.53
48:r:398:GLU:OE1	48:r:398:GLU:N	2.38	0.53
49:s:145:SER:OG	49:s:146:GLU:N	2.40	0.53
50:t:143:LYS:HG2	50:t:146:ARG:HH21	1.73	0.53
51:u:125:VAL:HG13	51:u:126:ARG:N	2.23	0.53
54:x:121:ALA:HA	54:x:124:ASP:OD2	2.09	0.53
55:y:33:TYR:HA	55:y:36:PHE:CD2	2.44	0.53
55:y:55:LEU:HA	55:y:58:TRP:CD1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:17:TYR:CD2	1:0:738:LEU:CD2	2.90	0.53
1:0:132:VAL:HG12	1:0:216:ALA:HB3	1.90	0.53
1:0:216:ALA:HA	1:0:283:LEU:HD11	1.90	0.53
1:0:538:PRO:HA	1:0:541:VAL:HG23	1.91	0.53
3:2:48:GLU:HA	3:2:51:MET:HG3	1.90	0.53
4:3:45:GLU:OE2	4:3:51:PRO:HD2	2.07	0.53
4:3:45:GLU:CD	4:3:51:PRO:HD2	2.33	0.53
5:A:632:ASN:HB2	5:A:992:LYS:HZ1	1.73	0.53
6:B:1124:ILE:HG22	6:B:1126:ALA:H	1.73	0.53
9:E:16:THR:HG21	9:E:135:LEU:HB3	1.90	0.53
24:T:4:ARG:HH21	24:T:7:LEU:HA	1.73	0.53
27:W:124:TYR:OH	27:W:292:LEU:N	2.37	0.53
27:W:471:VAL:CB	27:W:634:ARG:NE	2.42	0.53
28:X:288:LEU:HD21	28:X:293:ARG:NE	2.20	0.53
28:X:590:ASN:OD1	31:a:183:TYR:CE2	2.62	0.53
29:Y:536:LEU:O	29:Y:540:GLN:HG3	2.08	0.53
32:b:192:ASP:OD2	32:b:238:ARG:NH2	2.42	0.53
36:f:64:LEU:HB2	36:f:105:MET:HG3	1.89	0.53
40:j:479:ILE:HD13	40:j:529:MET:SD	2.40	0.53
44:n:281:CYS:SG	44:n:306:HIS:HE1	2.32	0.53
48:r:492:TRP:O	48:r:496:LEU:HG	2.08	0.53
49:s:89:ILE:O	49:s:92:GLU:HB3	2.08	0.53
52:v:32:SER:O	52:v:35:ALA:N	2.25	0.53
55:y:21:GLU:HB3	55:y:58:TRP:HE1	1.73	0.53
55:y:64:ALA:C	55:y:66:TYR:N	2.64	0.53
1:0:247:SER:HB3	1:0:254:ARG:HB3	1.90	0.53
2:1:142:LEU:HB3	2:1:190:LEU:HD23	1.90	0.53
2:1:525:MET:HE1	2:1:1093:ARG:HH12	1.74	0.53
2:1:642:HIS:HA	2:1:645:VAL:HG12	1.91	0.53
2:1:787:PRO:HB2	2:1:822:HIS:HA	1.91	0.53
2:1:1200:TYR:HB2	3:2:347:LEU:HD12	1.90	0.53
2:1:1321:LEU:HD23	2:1:1325:LEU:HB3	1.90	0.53
3:2:949:PHE:C	3:2:951:THR:H	2.16	0.53
5:A:330:GLN:HG3	5:A:332:SER:H	1.74	0.53
5:A:433:PRO:HD3	19:O:36:GLU:HA	1.90	0.53
28:X:307:ASN:OD1	28:X:380:ARG:NH2	2.41	0.53
29:Y:436:PRO:HA	29:Y:441:MET:HG2	1.90	0.53
29:Y:544:LEU:HA	29:Y:547:LYS:CE	2.36	0.53
32:b:101:TYR:HD2	32:b:104:LEU:HG	1.74	0.53
34:d:113:VAL:O	34:d:117:ASN:ND2	2.42	0.53
40:j:191:ARG:CZ	43:m:88:LEU:HG	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:544:MET:HG2	44:n:133:LEU:HG	1.90	0.53
40:j:569:ILE:HG23	40:j:582:VAL:C	2.33	0.53
48:r:64:SER:HA	48:r:67:MET:HE3	1.91	0.53
48:r:88:PHE:O	48:r:92:THR:CB	2.56	0.53
48:r:141:ARG:O	48:r:145:VAL:HG22	2.08	0.53
48:r:854:GLN:OE1	48:r:910:SER:HA	2.09	0.53
49:s:180:LEU:O	49:s:183:ARG:C	2.52	0.53
50:t:78:LEU:HB2	50:t:122:LEU:HD21	1.89	0.53
50:t:132:ARG:HH21	54:x:86:GLN:HG2	1.74	0.53
52:v:56:GLN:HE22	52:v:57:GLN:HG3	1.74	0.53
3:2:585:ILE:HG13	3:2:620:ALA:HB1	1.91	0.53
5:A:1629:TYR:HB2	37:g:14:SER:HB3	1.90	0.53
6:B:869:LYS:HB2	6:B:892:CYS:O	2.09	0.53
8:D:81:ALA:O	8:D:85:SER:OG	2.15	0.53
9:E:153:LYS:O	9:E:157:THR:HG23	2.09	0.53
11:G:30:LEU:HD23	11:G:51:ILE:HD12	1.90	0.53
13:I:12:VAL:HG21	13:I:15:ARG:NE	2.24	0.53
19:O:143:LYS:HA	19:O:146:TYR:CE1	2.42	0.53
27:W:640:LEU:HD21	27:W:685:TYR:OH	2.09	0.53
28:X:61:ARG:NH2	28:X:98:GLU:OE2	2.42	0.53
31:a:100:PRO:HG3	31:a:320:ARG:HD2	1.90	0.53
31:a:159:MET:HB2	31:a:165:ARG:HD3	1.91	0.53
31:a:169:ILE:HG22	31:a:171:PHE:HB2	1.91	0.53
38:h:8:LEU:O	38:h:12:LEU:HG	2.07	0.53
40:j:387:LEU:HD21	41:k:46:MET:N	2.23	0.53
40:j:396:ALA:O	41:k:73:ARG:HD2	2.09	0.53
45:o:113:GLU:O	45:o:117:GLU:HG2	2.08	0.53
48:r:94:GLN:O	48:r:95:LEU:C	2.50	0.53
48:r:94:GLN:OE1	48:r:95:LEU:N	2.42	0.53
48:r:1222:ARG:HH22	48:r:1226:GLN:HG3	1.73	0.53
49:s:114:LEU:O	49:s:115:LYS:C	2.51	0.53
52:v:1:MET:HG3	52:v:4:LYS:HB3	1.90	0.53
52:v:67:VAL:HG23	52:v:70:TYR:CD2	2.43	0.53
54:x:87:ALA:O	54:x:90:LEU:HB3	2.09	0.53
54:x:103:CYS:O	54:x:107:VAL:HG23	2.09	0.53
54:x:115:LEU:O	54:x:116:GLU:C	2.50	0.53
2:1:318:GLU:O	2:1:320:LYS:N	2.42	0.53
3:2:251:GLU:HG2	3:2:263:LEU:HD13	1.91	0.53
3:2:491:LEU:HB2	3:2:662:ARG:NH2	2.24	0.53
4:3:222:LEU:HD12	4:3:222:LEU:O	2.09	0.53
5:A:119:VAL:HG11	5:A:126:ILE:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:290:LEU:HD13	5:A:306:ASP:HB2	1.90	0.53
5:A:565:MET:HE1	15:K:74:ARG:HB2	1.90	0.53
5:A:1343:LEU:HD23	5:A:1368:VAL:HG11	1.91	0.53
5:A:1651:SER:HB2	53:w:133:LYS:HD2	1.90	0.53
6:B:47:PHE:O	6:B:51:ILE:HG12	2.09	0.53
6:B:653:TRP:CH2	6:B:662:VAL:HG11	2.44	0.53
27:W:121:TYR:HE2	27:W:487:LYS:N	2.00	0.53
28:X:35:LYS:HG2	28:X:452:GLN:HE21	1.73	0.53
28:X:690:ARG:O	28:X:698:GLN:NE2	2.41	0.53
29:Y:544:LEU:HA	29:Y:547:LYS:CG	2.34	0.53
30:Z:41:CYS:HB3	30:Z:118:LEU:CG	2.39	0.53
30:Z:313:TYR:CE2	30:Z:390:GLN:HG2	2.30	0.53
32:b:257:CYS:SG	32:b:258:HIS:ND1	2.81	0.53
33:c:18:GLN:HG2	33:c:21:LEU:HD12	1.90	0.53
39:i:87:ARG:HH21	40:j:299:GLN:CD	2.16	0.53
40:j:103:ARG:O	40:j:107:THR:HG23	2.09	0.53
40:j:507:ARG:HH21	40:j:507:ARG:HG2	1.73	0.53
40:j:627:TRP:HZ3	40:j:638:LYS:HB3	1.73	0.53
44:n:138:ASN:OD1	44:n:139:GLN:N	2.41	0.53
48:r:277:LEU:O	48:r:280:SER:OG	2.25	0.53
48:r:669:GLN:CD	56:z:770:THR:CG2	2.70	0.53
48:r:868:LEU:HA	48:r:871:VAL:HG12	1.89	0.53
50:t:87:ILE:O	50:t:90:LEU:HB3	2.09	0.53
1:0:154:SER:OG	1:0:155:PHE:N	2.42	0.53
3:2:202:ILE:HA	3:2:205:ASN:HD21	1.74	0.53
5:A:752:THR:HG22	5:A:786:ALA:HB1	1.91	0.53
6:B:897:ARG:HG2	6:B:899:SER:H	1.72	0.53
8:D:78:GLU:HB2	38:h:51:LEU:CD2	2.38	0.53
12:H:121:LEU:H	12:H:121:LEU:HD12	1.73	0.53
13:I:109:ARG:HH21	13:I:124:THR:HG21	1.73	0.53
17:M:344:ARG:NH1	20:P:203:ARG:HH11	2.07	0.53
19:O:29:ALA:HB1	19:O:44:ARG:HG2	1.89	0.53
21:Q:184:ILE:HG23	21:Q:187:ILE:HB	1.91	0.53
22:R:156:ASP:O	22:R:160:GLN:HG2	2.08	0.53
23:S:42:TRP:NE1	23:S:102:VAL:HG22	2.24	0.53
28:X:458:SER:HB2	28:X:461:LEU:HG	1.90	0.53
29:Y:513:ARG:C	29:Y:516:TYR:CE2	2.87	0.53
30:Z:294:VAL:HG12	30:Z:296:GLY:H	1.73	0.53
41:k:27:VAL:O	41:k:166:SER:OG	2.27	0.53
47:q:139:ARG:HA	47:q:142:ILE:HD13	1.90	0.53
52:v:42:ASN:O	52:v:46:THR:HG22	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:128:ARG:O	52:v:131:ASP:N	2.24	0.53
1:0:171:PHE:CZ	4:3:87:PRO:HG3	2.43	0.52
2:1:295:GLN:HG2	2:1:346:PHE:HD1	1.74	0.52
2:1:485:SER:HA	2:1:488:PHE:CE1	2.43	0.52
2:1:531:LEU:HB3	2:1:535:ALA:HB3	1.91	0.52
9:E:4:GLU:HA	9:E:7:THR:HG22	1.90	0.52
19:O:151:LEU:HD13	19:O:159:ILE:HD12	1.91	0.52
29:Y:513:ARG:CA	29:Y:516:TYR:CE2	2.83	0.52
35:e:108:VAL:HA	37:g:53:GLN:HE22	1.72	0.52
38:h:152:GLU:O	38:h:155:SER:OG	2.24	0.52
39:i:26:GLN:O	39:i:30:THR:HG23	2.09	0.52
40:j:478:LEU:HD12	40:j:492:GLN:HG2	1.90	0.52
42:l:122:PHE:CD2	42:l:144:TYR:HD1	2.27	0.52
42:l:156:LEU:HD11	44:n:288:LEU:HD21	1.90	0.52
43:m:134:TYR:CD1	47:q:153:ASN:OD1	2.62	0.52
48:r:154:ILE:HA	48:r:157:ALA:HB3	1.91	0.52
48:r:646:ALA:O	48:r:649:ASP:N	2.36	0.52
51:u:130:GLU:O	51:u:134:LYS:HG2	2.08	0.52
52:v:118:PRO:HD2	52:v:119:GLU:OE2	2.09	0.52
55:y:35:ASN:HB3	55:y:39:GLN:OE1	2.09	0.52
55:y:122:GLN:O	55:y:125:GLN:HB2	2.09	0.52
1:0:40:SER:HB2	1:0:89:TRP:CE2	2.44	0.52
3:2:527:THR:O	3:2:531:THR:HG23	2.08	0.52
3:2:903:ASN:HA	3:2:906:LEU:HD12	1.90	0.52
5:A:68:THR:HB	19:O:12:ARG:HH11	1.75	0.52
6:B:281:ASP:HB2	13:I:22:ASN:HA	1.91	0.52
13:I:59:THR:OG1	13:I:60:HIS:N	2.41	0.52
29:Y:411:MET:HG3	32:b:119:MET:HB3	1.89	0.52
30:Z:379:GLN:HB3	30:Z:381:PRO:HD2	1.92	0.52
41:k:85:LEU:HB2	41:k:108:ILE:HB	1.91	0.52
48:r:200:ARG:NH2	54:x:127:GLN:HE21	2.07	0.52
48:r:328:ARG:HG2	48:r:334:CYS:O	2.09	0.52
52:v:41:LEU:O	52:v:44:ILE:N	2.43	0.52
54:x:113:MET:O	54:x:114:LEU:C	2.52	0.52
56:z:703:THR:HG22	56:z:727:ALA:H	1.74	0.52
3:2:39:ILE:HG13	3:2:40:LEU:H	1.75	0.52
3:2:190:THR:O	3:2:194:HIS:ND1	2.43	0.52
4:3:112:SER:HB3	4:3:148:SER:OG	2.09	0.52
6:B:16:GLU:O	6:B:636:LYS:HE3	2.10	0.52
6:B:59:VAL:HG21	6:B:91:ILE:HD11	1.90	0.52
6:B:988:LYS:HG3	14:J:43:TYR:CE1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:147:ASP:O	7:C:148:ILE:HG23	2.09	0.52
8:D:126:GLU:O	8:D:130:ILE:HG12	2.09	0.52
8:D:139:SER:HB2	43:m:64:ARG:NH1	2.25	0.52
18:N:61:SER:O	18:N:77:ASN:N	2.43	0.52
20:P:305:PHE:CD2	26:V:83:DA:H5'	2.44	0.52
29:Y:514:ARG:NE	29:Y:522:VAL:HG21	1.95	0.52
30:Z:400:ARG:CD	33:c:16:MET:HG3	2.39	0.52
33:c:6:LYS:N	33:c:6:LYS:CD	2.73	0.52
40:j:393:PRO:CA	40:j:406:ARG:NH2	2.73	0.52
48:r:55:ILE:HG23	48:r:58:LEU:HD13	1.91	0.52
48:r:174:ARG:HG2	48:r:178:ILE:CG2	2.39	0.52
48:r:542:LEU:HD23	48:r:542:LEU:H	1.74	0.52
50:t:26:ILE:C	50:t:29:GLY:H	2.18	0.52
52:v:51:ILE:O	52:v:54:CYS:CA	2.57	0.52
55:y:80:GLN:C	55:y:85:ARG:NH2	2.63	0.52
1:0:658:LEU:HA	1:0:661:VAL:HG12	1.91	0.52
4:3:119:SER:HB2	4:3:169:LEU:HD11	1.92	0.52
4:3:182:ILE:HD12	4:3:191:LEU:HB3	1.90	0.52
5:A:350:VAL:HG22	6:B:1158:LEU:HD11	1.92	0.52
15:K:51:LEU:HD13	15:K:59:ALA:HB3	1.91	0.52
27:W:295:TYR:O	27:W:332:ARG:CD	2.27	0.52
27:W:297:PHE:CD1	27:W:297:PHE:C	2.86	0.52
28:X:343:ARG:HG2	28:X:357:PHE:HE1	1.75	0.52
30:Z:313:TYR:CE2	30:Z:394:TRP:CH2	2.91	0.52
39:i:115:LEU:CD1	45:o:129:VAL:CG1	2.85	0.52
40:j:255:ALA:HB1	40:j:304:CYS:HB2	1.91	0.52
41:k:153:VAL:HG13	41:k:156:ASN:HB3	1.90	0.52
44:n:306:HIS:CE1	44:n:309:CYS:HG	2.21	0.52
48:r:128:LEU:HD11	50:t:105:ARG:HH21	1.73	0.52
48:r:739:GLN:OE1	48:r:739:GLN:N	2.41	0.52
48:r:747:LEU:HD22	48:r:806:ARG:NH2	2.23	0.52
48:r:929:ARG:HG2	48:r:930:SER:H	1.74	0.52
49:s:140:LYS:O	49:s:142:ALA:N	2.38	0.52
49:s:141:GLY:CA	49:s:144:SER:HB3	2.32	0.52
50:t:111:ASP:O	50:t:115:LEU:HG	2.10	0.52
50:t:143:LYS:HA	50:t:146:ARG:NE	2.24	0.52
52:v:113:LEU:CA	52:v:116:VAL:HG22	2.38	0.52
54:x:68:ASP:O	54:x:71:VAL:N	2.42	0.52
55:y:118:ALA:O	55:y:121:GLU:HB2	2.10	0.52
1:0:515:THR:CG2	1:0:518:LEU:H	2.23	0.52
1:0:524:THR:HG23	1:0:551:LEU:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:537:SER:OG	1:0:540:THR:OG1	2.26	0.52
2:1:509:LEU:HD23	2:1:514:CYS:SG	2.49	0.52
2:1:1282:ASP:HA	2:1:1288:LEU:HD21	1.92	0.52
3:2:302:GLU:HG3	3:2:354:ARG:HH22	1.74	0.52
5:A:1287:CYS:SG	6:B:249:LYS:HA	2.50	0.52
6:B:60:GLU:OE2	24:T:140:ARG:NE	2.39	0.52
6:B:286:GLU:CD	6:B:558:PRO:HB2	2.35	0.52
6:B:565:THR:OG1	6:B:580:PRO:HG3	2.09	0.52
6:B:841:ARG:NH1	19:O:51:GLU:O	2.42	0.52
17:M:21:VAL:O	17:M:25:VAL:HG23	2.09	0.52
19:O:293:TYR:HE1	19:O:313:LEU:HB3	1.73	0.52
20:P:205:ARG:HB2	20:P:208:ARG:CZ	2.40	0.52
21:Q:183:GLN:NE2	22:R:211:SER:O	2.43	0.52
29:Y:480:PRO:CD	29:Y:481:VAL:N	2.71	0.52
29:Y:524:HIS:CB	31:a:269:PRO:O	2.57	0.52
36:f:275:GLN:O	36:f:278:GLU:HG3	2.10	0.52
40:j:544:MET:HB3	45:o:89:ARG:CD	2.40	0.52
40:j:569:ILE:HG23	40:j:583:ARG:HA	1.92	0.52
43:m:115:LYS:HE3	45:o:146:ILE:HG13	1.92	0.52
45:o:122:LEU:HD22	47:q:149:LEU:HD13	1.92	0.52
46:p:71:LEU:HD22	56:z:617:LEU:HD11	1.82	0.52
48:r:1296:ALA:C	48:r:1298:THR:H	2.16	0.52
49:s:123:THR:O	49:s:124:ALA:C	2.52	0.52
52:v:99:ILE:CB	52:v:103:LYS:HZ1	2.21	0.52
54:x:86:GLN:C	54:x:89:SER:HG	2.16	0.52
1:0:74:HIS:CG	1:0:116:ASN:OD1	2.61	0.52
3:2:155:GLU:HB2	3:2:158:LEU:HD12	1.90	0.52
3:2:556:SER:O	3:2:560:LEU:HG	2.09	0.52
7:C:3:TYR:O	15:K:49:GLN:NE2	2.43	0.52
17:M:369:LYS:H	18:N:55:ARG:HB3	1.75	0.52
20:P:222:THR:HG23	26:V:79:DT:O4'	2.09	0.52
30:Z:400:ARG:NE	33:c:61:MET:HE1	2.25	0.52
30:Z:433:PHE:HB3	30:Z:442:VAL:HB	1.90	0.52
30:Z:442:VAL:HG22	33:c:44:PHE:CE1	2.45	0.52
31:a:257:HIS:CG	32:b:248:HIS:CE1	2.86	0.52
40:j:464:TRP:CH2	40:j:497:ILE:HD11	2.45	0.52
45:o:69:ASP:O	45:o:71:GLU:N	2.43	0.52
48:r:78:ASP:O	48:r:82:LYS:HG2	2.10	0.52
48:r:184:THR:HG23	48:r:188:LYS:HE3	1.92	0.52
48:r:374:HIS:CD2	48:r:377:PRO:HG3	2.45	0.52
48:r:803:TYR:O	48:r:803:TYR:CG	2.61	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:128:ARG:HA	52:v:131:ASP:OD2	2.10	0.52
54:x:96:GLU:HA	54:x:99:GLU:HG3	1.90	0.52
55:y:118:ALA:O	55:y:119:LEU:C	2.52	0.52
1:0:807:LEU:CD1	1:0:835:ARG:HH12	2.23	0.52
3:2:911:ILE:HG23	3:2:920:HIS:HD2	1.74	0.52
3:2:957:LYS:HE2	3:2:989:LEU:HB3	1.92	0.52
5:A:1484:MET:HE1	11:G:20:PRO:HB3	1.92	0.52
6:B:760:THR:OG1	6:B:764:MET:SD	2.68	0.52
28:X:658:ARG:O	28:X:662:GLN:HB2	2.10	0.52
30:Z:440:LEU:HD11	33:c:36:GLN:OE1	2.09	0.52
37:g:18:SER:HB2	37:g:21:ILE:HB	1.92	0.52
40:j:259:VAL:HG22	40:j:372:GLU:HB2	1.91	0.52
44:n:29:SER:OG	46:p:110:TYR:OH	2.11	0.52
44:n:202:VAL:HG13	44:n:209:ILE:HG23	1.91	0.52
48:r:96:PHE:HB3	52:v:16:VAL:HG12	1.91	0.52
48:r:552:VAL:HG22	48:r:553:GLU:O	2.09	0.52
50:t:89:PHE:O	50:t:93:LEU:HG	2.09	0.52
52:v:15:PHE:HD2	52:v:51:ILE:HD11	1.74	0.52
52:v:83:GLU:HA	52:v:86:GLU:OE2	2.10	0.52
1:0:511:TYR:OH	1:0:523:SER:OG	2.28	0.52
1:0:597:ILE:HD13	1:0:660:VAL:HG13	1.90	0.52
2:1:664:GLN:HE22	2:1:667:ARG:HE	1.56	0.52
2:1:759:ASN:HB3	2:1:788:LEU:HD11	1.92	0.52
3:2:491:LEU:HB3	3:2:656:LEU:HD13	1.92	0.52
4:3:18:VAL:HG12	4:3:141:VAL:HB	1.91	0.52
5:A:232:GLU:HA	5:A:235:VAL:HG12	1.91	0.52
5:A:906:LEU:HG	5:A:966:LEU:HD21	1.92	0.52
7:C:37:VAL:HG23	7:C:248:ALA:HB1	1.91	0.52
24:T:132:ILE:C	24:T:134:GLU:O	2.53	0.52
27:W:566:PHE:HZ	27:W:715:LYS:HG2	1.74	0.52
28:X:609:ASP:OD1	28:X:666:ARG:NH1	2.42	0.52
29:Y:512:ILE:O	29:Y:516:TYR:OH	2.24	0.52
39:i:114:MET:HE2	47:q:159:ILE:HD11	1.75	0.52
40:j:38:GLN:CA	40:j:38:GLN:NE2	2.73	0.52
40:j:484:TYR:HD1	44:n:135:ARG:O	1.91	0.52
40:j:571:VAL:HG22	40:j:581:SER:CB	2.39	0.52
42:l:76:PHE:CD1	42:l:86:ILE:HG12	2.45	0.52
44:n:293:PRO:O	44:n:295:THR:HG23	2.09	0.52
45:o:101:GLN:NE2	47:q:108:PRO:HD2	2.21	0.52
48:r:56:GLU:HB3	52:v:55:ARG:CD	2.39	0.52
52:v:29:PHE:CE2	52:v:31:PRO:HA	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:73:LEU:O	55:y:76:LEU:HG	2.10	0.52
55:y:116:GLN:NE2	55:y:119:LEU:CD1	2.71	0.52
2:1:320:LYS:NZ	2:1:325:GLY:HA2	2.25	0.52
2:1:1239:VAL:HG11	2:1:1277:MET:HE2	1.92	0.52
3:2:78:VAL:O	3:2:82:ILE:HG12	2.10	0.52
3:2:757:ARG:O	3:2:761:THR:HG23	2.10	0.52
9:E:17:ILE:HG21	9:E:74:VAL:HG11	1.91	0.52
15:K:65:HIS:HE1	15:K:67:LEU:HD23	1.75	0.52
22:R:75:PHE:HB3	24:T:188:PHE:CE1	2.45	0.52
24:T:29:GLN:HG2	24:T:33:LYS:HZ1	1.75	0.52
24:T:209:PRO:CB	25:U:21:DG:OP1	2.58	0.52
27:W:163:TYR:N	27:W:163:TYR:CD1	2.76	0.52
39:i:101:ARG:HD3	45:o:144:GLU:HB2	1.91	0.52
40:j:248:PRO:O	40:j:250:ASP:N	2.43	0.52
40:j:449:ASP:HB2	47:q:157:LYS:HZ3	1.65	0.52
42:l:116:ARG:HG2	42:l:123:LEU:HD21	1.92	0.52
44:n:49:GLU:OE2	56:z:629:ILE:HG22	2.09	0.52
44:n:273:TYR:CD1	44:n:276:LEU:HD13	2.45	0.52
48:r:570:PHE:HB2	48:r:615:LYS:NZ	2.23	0.52
48:r:794:LEU:N	48:r:794:LEU:CD2	2.73	0.52
49:s:101:GLU:O	49:s:104:ASP:HB3	2.10	0.52
52:v:25:ILE:HG21	52:v:40:LYS:NZ	2.25	0.52
52:v:100:ASP:HA	52:v:103:LYS:CD	2.39	0.52
56:z:726:PRO:O	56:z:729:TYR:N	2.25	0.52
1:0:121:SER:OG	1:0:122:VAL:N	2.40	0.52
1:0:184:VAL:O	1:0:185:SER:OG	2.24	0.52
1:0:382:LEU:HB3	1:0:394:VAL:HB	1.92	0.52
3:2:475:THR:HG21	3:2:493:PHE:HA	1.92	0.52
5:A:1095:LEU:HD13	5:A:1401:LEU:HD23	1.91	0.52
14:J:40:LEU:HD12	14:J:45:CYS:HB2	1.90	0.52
20:P:270:LEU:HD13	20:P:306:VAL:HG12	1.91	0.52
23:S:31:PHE:CD1	24:T:91:GLN:HG3	2.45	0.52
25:U:12:DA:H5'	25:U:12:DA:H8	1.75	0.52
27:W:278:GLU:CG	27:W:483:LEU:HD11	2.34	0.52
27:W:530:ARG:HA	27:W:533:LEU:HD12	1.91	0.52
31:a:269:PRO:O	31:a:269:PRO:HD2	2.10	0.52
38:h:66:GLU:O	38:h:67:LYS:HB2	2.10	0.52
40:j:225:ILE:HD11	40:j:246:GLN:HE22	1.74	0.52
40:j:396:ALA:O	41:k:73:ARG:NH2	2.42	0.52
48:r:127:ILE:O	48:r:129:PHE:N	2.43	0.52
50:t:77:GLU:O	50:t:78:LEU:C	2.48	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:159:ARG:O	50:t:163:MET:HG2	2.10	0.52
52:v:47:GLY:O	52:v:48:LEU:C	2.53	0.52
54:x:54:TYR:O	54:x:57:LEU:N	2.43	0.52
55:y:83:HIS:ND1	55:y:87:GLU:OE2	2.43	0.52
1:0:828:LEU:HD22	1:0:828:LEU:H	1.75	0.51
2:1:584:PHE:HD1	2:1:588:LEU:HD23	1.74	0.51
3:2:174:ASN:O	3:2:178:LEU:HB2	2.11	0.51
5:A:1622:TYR:CE2	5:A:1624:PRO:HD3	2.45	0.51
6:B:623:ARG:HH12	6:B:697:GLU:CD	2.18	0.51
6:B:623:ARG:NH1	6:B:697:GLU:OE2	2.41	0.51
10:F:82:GLU:O	10:F:95:LYS:NZ	2.40	0.51
20:P:296:ILE:O	20:P:299:ARG:NH2	2.43	0.51
21:Q:128:LYS:O	21:Q:162:GLU:HB3	2.10	0.51
22:R:179:GLN:O	22:R:183:LYS:HB2	2.10	0.51
24:T:191:PHE:HE2	24:T:235:LEU:HD22	1.74	0.51
27:W:471:VAL:HG23	27:W:634:ARG:NH2	2.24	0.51
29:Y:414:TYR:HD2	32:b:112:VAL:HG13	1.74	0.51
30:Z:433:PHE:CD2	33:c:38:ILE:HD12	2.40	0.51
35:e:207:LEU:HD11	35:e:268:LEU:HD21	1.92	0.51
35:e:268:LEU:O	35:e:272:ILE:HG12	2.10	0.51
40:j:47:ILE:N	40:j:47:ILE:CD1	2.72	0.51
48:r:64:SER:O	48:r:65:GLU:C	2.52	0.51
48:r:138:SER:OG	48:r:139:LEU:N	2.44	0.51
49:s:127:GLN:O	49:s:131:LYS:NZ	2.36	0.51
50:t:82:ASN:O	50:t:83:MET:C	2.49	0.51
50:t:162:GLU:O	50:t:166:ASN:ND2	2.43	0.51
52:v:83:GLU:CD	52:v:84:CYS:N	2.66	0.51
52:v:107:SER:O	52:v:111:GLN:HG2	2.10	0.51
53:w:90:GLU:C	53:w:93:TYR:H	2.18	0.51
56:z:674:ILE:HB	56:z:679:GLN:HE21	1.75	0.51
1:0:90:ASP:OD1	1:0:91:GLN:N	2.43	0.51
1:0:439:THR:HB	1:0:477:LEU:HD22	1.92	0.51
3:2:25:ILE:HG13	3:2:29:LYS:NZ	2.25	0.51
3:2:342:LEU:HD22	3:2:385:ARG:HD3	1.91	0.51
3:2:610:LYS:HD2	3:2:646:LEU:HA	1.91	0.51
3:2:949:PHE:CE1	3:2:952:VAL:HB	2.45	0.51
5:A:73:THR:C	5:A:75:ALA:H	2.18	0.51
5:A:1348:SER:HB2	9:E:136:LEU:HB2	1.91	0.51
6:B:101:ARG:HG2	19:O:131:PRO:HG2	1.92	0.51
6:B:541:ILE:HG12	6:B:596:ILE:HG22	1.91	0.51
8:D:78:GLU:C	38:h:51:LEU:CD2	2.83	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:142:TYR:HH	43:m:20:LYS:C	2.18	0.51
9:E:185:ILE:HD11	9:E:189:GLN:HB3	1.92	0.51
12:H:35:PHE:HB2	12:H:37:MET:HE3	1.92	0.51
13:I:22:ASN:ND2	13:I:41:ASN:HD22	2.09	0.51
29:Y:377:LYS:HD2	32:b:286:GLU:CG	2.40	0.51
29:Y:383:TYR:HA	32:b:175:MET:HB2	1.91	0.51
29:Y:471:LEU:CD1	29:Y:502:VAL:CG1	2.83	0.51
30:Z:41:CYS:CB	30:Z:118:LEU:HG	2.40	0.51
36:f:7:GLN:HG3	36:f:89:ARG:NH2	2.25	0.51
37:g:118:ARG:NH1	40:j:111:VAL:HG11	2.25	0.51
39:i:101:ARG:CD	45:o:144:GLU:HB2	2.40	0.51
40:j:49:PHE:C	40:j:49:PHE:HD1	2.18	0.51
41:k:74:ARG:HD3	41:k:83:TRP:CZ2	2.45	0.51
42:l:122:PHE:HD2	42:l:144:TYR:HD1	1.58	0.51
43:m:115:LYS:HG3	45:o:146:ILE:HD11	1.91	0.51
44:n:43:GLU:O	44:n:44:THR:HG23	2.11	0.51
48:r:232:ALA:HA	48:r:250:LEU:CG	2.19	0.51
49:s:65:VAL:O	49:s:69:LEU:CB	2.58	0.51
49:s:191:ASN:C	49:s:194:SER:H	2.18	0.51
50:t:76:LYS:HG2	50:t:77:GLU:OE1	2.10	0.51
54:x:89:SER:O	54:x:90:LEU:C	2.54	0.51
1:0:487:ASP:CG	1:0:800:ARG:HH22	2.18	0.51
1:0:700:CYS:SG	1:0:708:GLU:HG3	2.50	0.51
2:1:644:CYS:O	2:1:648:THR:HG23	2.11	0.51
3:2:109:SER:OG	3:2:111:HIS:ND1	2.42	0.51
3:2:172:THR:HA	3:2:176:ALA:HB3	1.92	0.51
3:2:591:ALA:HB1	3:2:597:LEU:HD23	1.92	0.51
3:2:814:VAL:HG21	3:2:930:GLU:HB3	1.92	0.51
5:A:1095:LEU:HD21	5:A:1124:LEU:HD11	1.93	0.51
5:A:1245:CYS:SG	5:A:1246:ILE:N	2.84	0.51
6:B:271:ILE:HG21	6:B:320:PHE:CD2	2.46	0.51
6:B:759:VAL:HG13	6:B:986:GLN:HG2	1.92	0.51
18:N:34:LEU:O	18:N:38:LEU:HG	2.10	0.51
19:O:204:THR:HG22	19:O:205:SER:H	1.75	0.51
27:W:173:ASN:OD1	27:W:460:ALA:HA	2.10	0.51
30:Z:380:THR:N	30:Z:381:PRO:CD	2.72	0.51
30:Z:401:LEU:CD1	33:c:57:VAL:HB	2.40	0.51
35:e:213:LEU:HA	35:e:224:ARG:HD2	1.91	0.51
40:j:373:HIS:ND1	47:q:173:MET:SD	2.84	0.51
40:j:463:HIS:HA	43:m:131:GLU:CD	2.35	0.51
40:j:612:ASP:OD1	40:j:614:LYS:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:529:PRO:HD2	48:r:609:ARG:CZ	2.40	0.51
49:s:63:ASN:O	49:s:67:GLU:HG2	2.11	0.51
50:t:14:PRO:HG3	55:y:37:LEU:HD11	1.90	0.51
50:t:112:LEU:O	50:t:113:LYS:C	2.52	0.51
52:v:73:GLN:C	52:v:75:ARG:H	2.18	0.51
1:0:835:ARG:NH1	1:0:835:ARG:CG	2.72	0.51
5:A:500:GLU:OE1	6:B:1058:LYS:HD3	2.11	0.51
5:A:909:LEU:O	5:A:967:ARG:NH1	2.44	0.51
5:A:1263:ASN:C	5:A:1265:ASP:H	2.17	0.51
5:A:1338:THR:HG22	5:A:1340:GLY:H	1.74	0.51
6:B:635:LEU:HD21	6:B:640:ILE:HD11	1.91	0.51
7:C:44:ILE:HD11	7:C:239:LEU:HD22	1.93	0.51
13:I:60:HIS:HD2	13:I:103:ARG:HE	1.57	0.51
17:M:369:LYS:HB2	18:N:55:ARG:HD2	1.91	0.51
22:R:97:LEU:HG	22:R:101:GLU:CD	2.35	0.51
22:R:213:ASP:O	22:R:217:GLN:N	2.39	0.51
24:T:15:ASN:HB3	24:T:109:ILE:HG23	1.92	0.51
28:X:280:ARG:NH2	28:X:387:GLU:OE1	2.29	0.51
29:Y:377:LYS:N	32:b:284:THR:O	2.43	0.51
30:Z:41:CYS:SG	30:Z:118:LEU:HG	2.50	0.51
30:Z:41:CYS:HA	30:Z:114:PHE:HE1	1.75	0.51
40:j:393:PRO:CA	40:j:406:ARG:HH22	2.21	0.51
48:r:52:SER:OG	52:v:60:ASP:N	2.44	0.51
48:r:93:ARG:CZ	52:v:20:ARG:HA	2.40	0.51
48:r:169:LEU:HD23	48:r:175:ASP:HB2	1.92	0.51
48:r:1275:PRO:O	48:r:1279:GLN:NE2	2.43	0.51
49:s:107:ILE:CG2	54:x:125:ILE:HD13	2.41	0.51
49:s:187:LEU:O	49:s:188:GLY:C	2.52	0.51
54:x:16:ALA:O	54:x:17:ASP:C	2.51	0.51
54:x:23:ILE:HA	54:x:26:LEU:HD13	1.91	0.51
54:x:108:VAL:O	54:x:112:ASP:OD1	2.28	0.51
1:0:46:ALA:HB2	1:0:89:TRP:HZ3	1.75	0.51
1:0:115:ALA:HB3	1:0:834:TRP:CZ3	2.46	0.51
1:0:656:ARG:HH11	1:0:694:THR:HG22	1.75	0.51
2:1:122:VAL:O	2:1:126:ILE:HB	2.11	0.51
5:A:965:VAL:O	5:A:969:ILE:HG12	2.11	0.51
5:A:1364:GLU:O	5:A:1368:VAL:HG12	2.11	0.51
6:B:286:GLU:HG2	6:B:292:PHE:HZ	1.76	0.51
6:B:504:THR:HG22	6:B:667:THR:HG21	1.92	0.51
20:P:323:GLU:HG2	20:P:327:ASN:HD21	1.75	0.51
27:W:379:LYS:HE2	27:W:386:ASP:CB	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:348:ARG:HG3	30:Z:394:TRP:HB3	1.93	0.51
40:j:507:ARG:HG2	40:j:507:ARG:NH2	2.26	0.51
41:k:70:LEU:HD13	41:k:87:TYR:HB2	1.92	0.51
45:o:86:ASP:O	45:o:89:ARG:HB2	2.09	0.51
48:r:68:VAL:C	48:r:70:THR:H	2.17	0.51
48:r:232:ALA:HB2	48:r:250:LEU:CG	2.40	0.51
48:r:397:ILE:HD12	48:r:400:LEU:HD12	1.93	0.51
49:s:109:GLN:HA	49:s:112:LYS:CE	2.41	0.51
52:v:61:ILE:HD12	52:v:61:ILE:H	1.74	0.51
52:v:100:ASP:O	52:v:101:THR:C	2.53	0.51
52:v:114:SER:HA	52:v:118:PRO:CB	2.40	0.51
55:y:110:ARG:CB	55:y:110:ARG:NH1	2.73	0.51
3:2:199:LEU:O	3:2:203:LEU:HB2	2.11	0.51
3:2:538:LYS:HB3	3:2:540:LEU:CD2	2.41	0.51
5:A:367:ILE:HD13	5:A:501:MET:HE1	1.93	0.51
7:C:124:SER:HB2	7:C:127:VAL:HB	1.91	0.51
9:E:54:ARG:HB2	9:E:78:GLU:CD	2.35	0.51
18:N:66:ARG:HH22	20:P:185:LEU:C	2.15	0.51
20:P:305:PHE:HD2	26:V:83:DA:H5'	1.75	0.51
21:Q:74:CYS:HA	21:Q:91:TYR:O	2.11	0.51
21:Q:164:ASP:HB2	21:Q:167:ALA:HA	1.93	0.51
24:T:129:ARG:HA	24:T:132:ILE:HD12	1.92	0.51
43:m:115:LYS:CD	45:o:146:ILE:CD1	2.76	0.51
48:r:89:ALA:O	48:r:92:THR:HB	2.10	0.51
48:r:132:THR:HG22	48:r:135:ARG:NH2	2.26	0.51
48:r:1170:ALA:O	48:r:1173:ILE:HG12	2.11	0.51
49:s:34:LEU:HB3	51:u:98:ARG:NE	2.23	0.51
52:v:118:PRO:C	52:v:124:TYR:CE2	2.88	0.51
54:x:125:ILE:O	54:x:126:ALA:C	2.54	0.51
55:y:26:GLN:OE1	55:y:68:LYS:HG2	2.11	0.51
56:z:715:LEU:N	56:z:715:LEU:CD2	2.73	0.51
1:0:17:TYR:OH	1:0:70:PRO:HG3	2.11	0.51
1:0:22:GLU:OE2	1:0:754:ARG:CZ	2.58	0.51
3:2:171:SER:O	3:2:174:ASN:N	2.44	0.51
3:2:948:PRO:O	3:2:951:THR:OG1	2.27	0.51
3:2:956:VAL:O	3:2:960:ALA:HA	2.11	0.51
5:A:458:PHE:HE2	5:A:484:LEU:HD13	1.76	0.51
11:G:99:THR:OG1	11:G:106:CYS:HB3	2.11	0.51
14:J:65:LEU:HA	16:L:23:HIS:HD2	1.76	0.51
17:M:40:MET:HA	17:M:43:LYS:HB3	1.93	0.51
23:S:35:ASP:OD1	23:S:36:LYS:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:476:TRP:CH2	31:a:294:CYS:HA	2.45	0.51
30:Z:46:ARG:CZ	32:b:53:ARG:CD	2.87	0.51
35:e:209:ARG:HH12	37:g:53:GLN:HE22	1.59	0.51
40:j:104:SER:O	40:j:108:GLU:HG3	2.10	0.51
40:j:319:LYS:HD3	48:r:464:GLN:HE22	1.76	0.51
43:m:140:SER:C	47:q:150:LYS:HG2	2.36	0.51
48:r:93:ARG:NH2	52:v:23:GLY:H	2.09	0.51
48:r:520:LEU:HB2	48:r:539:PHE:HE2	1.74	0.51
48:r:1247:LEU:HD11	48:r:1314:ARG:NH2	2.26	0.51
50:t:21:TYR:HD2	50:t:26:ILE:HB	1.76	0.51
50:t:21:TYR:HA	50:t:25:ASN:HB3	1.92	0.51
55:y:91:ALA:O	55:y:94:ALA:CA	2.59	0.51
1:0:191:SER:HA	1:0:201:THR:HA	1.93	0.51
1:0:263:LEU:HD21	1:0:309:TRP:CD2	2.45	0.51
1:0:299:SER:OG	1:0:300:SER:N	2.43	0.51
1:0:733:PRO:C	1:0:735:SER:H	2.18	0.51
3:2:189:TRP:O	3:2:193:GLU:HG2	2.11	0.51
3:2:920:HIS:O	3:2:924:VAL:HG23	2.10	0.51
4:3:25:THR:HG23	4:3:73:THR:HG23	1.92	0.51
19:O:133:ASN:ND2	19:O:171:GLU:OE1	2.44	0.51
20:P:294:ARG:HH12	25:U:14:DA:P	2.33	0.51
21:Q:69:ASP:OD1	21:Q:69:ASP:N	2.39	0.51
27:W:167:LYS:HB3	27:W:294:GLU:HB2	1.92	0.51
28:X:293:ARG:CZ	28:X:378:ARG:HA	2.40	0.51
28:X:310:LEU:CD1	28:X:409:THR:OG1	2.56	0.51
30:Z:245:LEU:HD11	30:Z:285:ARG:HD3	1.92	0.51
33:c:6:LYS:H	33:c:6:LYS:CD	2.23	0.51
35:e:174:VAL:O	35:e:179:ARG:NH2	2.31	0.51
40:j:325:ILE:HD12	48:r:458:LEU:HD12	1.93	0.51
43:m:115:LYS:CE	45:o:142:VAL:O	2.44	0.51
45:o:107:PRO:HA	45:o:110:VAL:HG12	1.93	0.51
46:p:85:ASN:CG	56:z:640:ARG:NH1	2.67	0.51
48:r:304:GLN:HA	48:r:307:VAL:HG12	1.93	0.51
50:t:147:LEU:HD12	50:t:148:GLU:N	2.26	0.51
54:x:18:GLN:C	54:x:20:CYS:N	2.68	0.51
54:x:63:ALA:O	54:x:66:ALA:HB3	2.11	0.51
55:y:110:ARG:NH1	55:y:110:ARG:HB3	2.24	0.51
1:0:306:VAL:HG23	1:0:399:LEU:HD23	1.93	0.51
5:A:733:LEU:HD23	13:I:107:ALA:HA	1.93	0.51
7:C:35:ARG:HG3	7:C:182:VAL:HG11	1.92	0.51
24:T:232:THR:OG1	24:T:233:TRP:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:293:ARG:NH2	28:X:378:ARG:CD	2.73	0.51
28:X:618:VAL:HG11	28:X:664:VAL:HA	1.91	0.51
28:X:726:GLN:NE2	31:a:223:LEU:CG	2.74	0.51
30:Z:97:HIS:CE1	30:Z:112:PRO:CD	2.94	0.51
31:a:172:SER:HA	31:a:201:LEU:HB2	1.92	0.51
40:j:183:PHE:HD1	40:j:228:THR:HG1	1.58	0.51
42:l:16:SER:H	42:l:19:GLN:HE21	1.57	0.51
44:n:49:GLU:OE2	56:z:629:ILE:CG2	2.59	0.51
44:n:117:LEU:HD11	47:q:55:LEU:HD23	1.92	0.51
48:r:61:ARG:HH12	48:r:65:GLU:HG3	1.74	0.51
48:r:95:LEU:O	48:r:99:LEU:HG	2.11	0.51
48:r:200:ARG:O	48:r:204:VAL:HG23	2.11	0.51
48:r:683:ARG:NH1	48:r:707:ASP:HB2	2.26	0.51
48:r:1310:THR:HA	48:r:1313:LEU:HD12	1.93	0.51
49:s:99:GLU:HB3	49:s:103:ARG:HH22	1.76	0.51
50:t:16:GLN:C	50:t:18:ILE:N	2.69	0.51
52:v:11:HIS:CD2	52:v:12:LEU:H	2.28	0.51
3:2:185:GLU:HG3	3:2:188:SER:HB2	1.93	0.51
4:3:182:ILE:O	4:3:182:ILE:HG13	2.10	0.51
6:B:69:ALA:HB3	6:B:81:PRO:HB2	1.92	0.51
6:B:497:LYS:HD3	6:B:500:GLN:HG3	1.93	0.51
23:S:151:ARG:CZ	23:S:155:LEU:HB2	2.41	0.51
24:T:24:PRO:HB2	24:T:27:LEU:HB2	1.91	0.51
25:U:57:DC:N4	26:V:37:DG:H1	2.05	0.51
27:W:76:LEU:HB2	27:W:144:SER:HA	1.92	0.51
27:W:105:GLU:HG2	27:W:487:LYS:HE2	1.87	0.51
31:a:254:PHE:HE2	32:b:274:ILE:HG23	1.74	0.51
36:f:85:MET:O	36:f:89:ARG:HG3	2.10	0.51
36:f:181:LEU:HD13	36:f:226:ILE:HG21	1.92	0.51
40:j:147:ILE:HG13	40:j:148:SER:N	2.25	0.51
40:j:248:PRO:HD2	40:j:251:LEU:HD21	1.91	0.51
44:n:276:LEU:HA	44:n:297:ARG:HH21	1.76	0.51
48:r:72:LEU:HB2	48:r:76:LYS:HZ1	1.75	0.51
48:r:160:VAL:HA	48:r:164:GLY:N	2.14	0.51
48:r:615:LYS:HD3	48:r:644:PHE:CD1	2.45	0.51
48:r:1439:VAL:HA	48:r:1442:LEU:HG	1.93	0.51
50:t:124:ASN:OD1	50:t:124:ASN:N	2.39	0.51
53:w:128:ARG:NH1	53:w:131:ILE:HB	2.25	0.51
54:x:112:ASP:O	54:x:115:LEU:HG	2.11	0.51
55:y:96:PHE:O	55:y:99:GLU:HB2	2.11	0.51
6:B:608:ARG:HH22	13:I:68:ILE:HG22	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:78:GLU:CB	38:h:51:LEU:CD2	2.89	0.50
9:E:55:ARG:HH12	9:E:75:PHE:HA	1.75	0.50
17:M:13:LEU:HG	17:M:366:ILE:HD11	1.92	0.50
17:M:45:LEU:HA	17:M:48:ASN:HD22	1.75	0.50
17:M:331:THR:HG22	18:N:92:LYS:HB2	1.92	0.50
27:W:128:SER:CB	27:W:334:ARG:CZ	2.89	0.50
27:W:159:CYS:HB3	27:W:163:TYR:CE2	2.35	0.50
27:W:170:LEU:CB	27:W:461:HIS:HA	2.41	0.50
27:W:516:PRO:HG3	33:c:18:GLN:OE1	2.10	0.50
28:X:311:PRO:HD2	28:X:314:VAL:HB	1.92	0.50
29:Y:407:ILE:HD13	32:b:19:PRO:CB	2.41	0.50
42:l:30:MET:HE3	48:r:521:GLN:CD	2.32	0.50
42:l:34:GLU:OE1	42:l:36:GLN:NE2	2.44	0.50
48:r:60:HIS:O	48:r:63:TYR:HB3	2.11	0.50
49:s:89:ILE:O	49:s:93:MET:HG2	2.11	0.50
50:t:108:LYS:HA	50:t:111:ASP:OD2	2.11	0.50
50:t:120:HIS:O	50:t:123:ILE:N	2.44	0.50
50:t:125:GLU:O	50:t:128:PRO:HD2	2.11	0.50
50:t:154:GLN:CG	50:t:155:LYS:N	2.74	0.50
50:t:160:VAL:O	50:t:164:ILE:HG12	2.11	0.50
1:0:583:ILE:HD12	1:0:587:ILE:HD12	1.93	0.50
2:1:510:PRO:HG3	2:1:921:HIS:HE1	1.75	0.50
2:1:753:ARG:NH2	2:1:832:TYR:HB2	2.26	0.50
2:1:1197:HIS:HB2	2:1:1202:GLU:OE2	2.11	0.50
3:2:895:ASP:HB3	3:2:898:ASN:OD1	2.11	0.50
4:3:22:ILE:HD13	4:3:32:PHE:HE2	1.76	0.50
5:A:391:ALA:HB1	5:A:445:LYS:HD3	1.92	0.50
5:A:420:ILE:HB	5:A:445:LYS:HB2	1.93	0.50
5:A:1130:ILE:HG22	5:A:1413:ALA:HB2	1.93	0.50
11:G:138:GLN:HG3	11:G:141:ASP:OD2	2.10	0.50
21:Q:48:MET:O	21:Q:52:LEU:N	2.42	0.50
24:T:91:GLN:HE22	24:T:94:THR:HG23	1.76	0.50
27:W:128:SER:CA	27:W:334:ARG:NH2	2.73	0.50
27:W:167:LYS:HE2	27:W:294:GLU:HG3	1.92	0.50
27:W:388:GLN:HB3	27:W:404:SER:HB3	1.93	0.50
27:W:516:PRO:HD3	33:c:18:GLN:OE1	2.11	0.50
28:X:695:ARG:HH12	28:X:758:GLN:HB2	1.76	0.50
29:Y:510:GLU:OE2	29:Y:526:GLU:HG3	2.11	0.50
33:c:5:LEU:N	33:c:5:LEU:CD1	2.73	0.50
35:e:167:ARG:HG2	35:e:167:ARG:HH21	1.74	0.50
38:h:15:LEU:O	38:h:19:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:198:LYS:CG	40:j:202:LYS:O	2.58	0.50
40:j:214:SER:HA	40:j:383:HIS:CD2	2.45	0.50
43:m:123:ILE:HG12	47:q:163:LEU:HD11	1.84	0.50
48:r:112:VAL:HA	48:r:115:CYS:SG	2.51	0.50
49:s:122:ALA:C	49:s:126:TYR:CE2	2.90	0.50
50:t:154:GLN:O	50:t:157:LEU:N	2.44	0.50
52:v:49:GLN:O	52:v:50:ASP:C	2.54	0.50
52:v:104:LYS:O	52:v:105:PHE:C	2.53	0.50
56:z:701:ASN:N	56:z:701:ASN:ND2	2.59	0.50
1:0:60:ARG:NH2	1:0:60:ARG:CG	2.73	0.50
1:0:89:TRP:CE3	1:0:96:LEU:HD13	2.47	0.50
1:0:515:THR:HG23	1:0:518:LEU:H	1.76	0.50
1:0:640:ARG:CB	1:0:641:PRO:CD	2.67	0.50
1:0:656:ARG:NH1	1:0:694:THR:HG22	2.26	0.50
1:0:741:ARG:HH21	1:0:759:PRO:HA	1.76	0.50
2:1:730:HIS:CD2	2:1:977:LEU:HD13	2.45	0.50
2:1:809:ARG:O	2:1:813:ARG:HD3	2.11	0.50
5:A:1474:LEU:HD11	10:F:107:ARG:CZ	2.41	0.50
6:B:305:LEU:HD13	13:I:23:MET:SD	2.51	0.50
6:B:311:ILE:HG23	6:B:316:VAL:HG12	1.92	0.50
6:B:711:ILE:HD11	6:B:717:ASN:ND2	2.25	0.50
8:D:107:THR:HG23	8:D:110:GLU:H	1.76	0.50
19:O:282:ASP:OD1	19:O:286:ARG:NE	2.43	0.50
24:T:81:HIS:O	24:T:83:PHE:N	2.44	0.50
27:W:85:PHE:HE2	30:Z:336:TYR:HB3	1.71	0.50
27:W:112:HIS:CG	30:Z:310:GLU:CG	2.81	0.50
27:W:172:HIS:C	27:W:434:GLU:CG	2.82	0.50
27:W:363:VAL:HB	27:W:407:ILE:HG12	1.93	0.50
33:c:6:LYS:CA	33:c:6:LYS:NZ	2.73	0.50
37:g:114:VAL:HG23	38:h:111:THR:HG22	1.92	0.50
40:j:619:ARG:NH2	48:r:744:HIS:CE1	2.77	0.50
41:k:173:VAL:HG23	41:k:186:MET:HE2	1.93	0.50
42:l:3:VAL:N	42:l:143:GLU:OE2	2.45	0.50
48:r:119:SER:OG	48:r:120:SER:N	2.45	0.50
50:t:123:ILE:HG13	50:t:124:ASN:N	2.26	0.50
52:v:41:LEU:O	52:v:44:ILE:HB	2.12	0.50
52:v:124:TYR:HD1	52:v:127:ILE:CB	2.25	0.50
53:w:92:ALA:HB1	53:w:96:PHE:HD2	1.76	0.50
55:y:34:LEU:O	55:y:35:ASN:C	2.53	0.50
55:y:74:HIS:NE2	55:y:78:LEU:HD21	2.27	0.50
55:y:78:LEU:HD22	55:y:84:PHE:CE2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:85:ARG:HD3	55:y:85:ARG:H	1.77	0.50
56:z:699:SER:HB2	56:z:704:VAL:HG23	1.88	0.50
2:1:863:ASP:OD2	2:1:962:ARG:NH1	2.44	0.50
2:1:1005:LEU:HD11	2:1:1030:ILE:HB	1.93	0.50
2:1:1090:CYS:SG	2:1:1091:ASP:N	2.85	0.50
3:2:266:GLN:NE2	3:2:773:CYS:SG	2.84	0.50
4:3:73:THR:HG22	4:3:112:SER:HB2	1.94	0.50
5:A:1419:VAL:HA	5:A:1422:GLN:HG2	1.92	0.50
6:B:1119:CYS:HB2	6:B:1127:ILE:HD11	1.94	0.50
18:N:37:LEU:HA	18:N:40:PHE:HB3	1.92	0.50
21:Q:110:MET:O	21:Q:114:ILE:HG12	2.11	0.50
23:S:48:GLU:HB3	23:S:99:LEU:O	2.12	0.50
28:X:417:ILE:HG23	28:X:434:HIS:HB2	1.94	0.50
29:Y:389:ILE:CG1	32:b:259:ARG:HE	2.24	0.50
30:Z:35:TYR:HB3	30:Z:114:PHE:CD1	2.39	0.50
32:b:151:VAL:HG13	32:b:155:GLN:HG3	1.91	0.50
33:c:6:LYS:HD2	33:c:6:LYS:N	2.26	0.50
35:e:75:ILE:HA	35:e:152:LYS:HD3	1.92	0.50
40:j:336:PHE:HE1	40:j:500:GLU:CG	2.22	0.50
43:m:49:SER:HB2	43:m:52:THR:HG23	1.92	0.50
47:q:72:GLN:N	47:q:74:ARG:HH21	2.04	0.50
47:q:86:SER:O	47:q:90:ARG:NE	2.44	0.50
48:r:334:CYS:HB2	48:r:360:LYS:HD2	1.94	0.50
48:r:905:SER:OG	48:r:917:ALA:HB3	2.11	0.50
50:t:80:LYS:O	50:t:81:LEU:C	2.53	0.50
56:z:689:PHE:CD1	56:z:773:LEU:HD12	2.46	0.50
56:z:743:TYR:HB3	56:z:749:LEU:HB3	1.93	0.50
1:0:113:HIS:NE2	4:3:104:MET:HE2	2.26	0.50
1:0:803:CYS:SG	1:0:804:VAL:N	2.84	0.50
2:1:72:SER:O	2:1:76:ILE:HG12	2.11	0.50
3:2:716:ALA:O	3:2:720:GLU:HG2	2.12	0.50
6:B:230:ARG:HA	6:B:230:ARG:HH11	1.77	0.50
10:F:45:PRO:HG3	10:F:115:TYR:OH	2.12	0.50
16:L:33:PRO:O	16:L:35:ARG:N	2.45	0.50
17:M:376:TRP:CZ3	20:P:205:ARG:HB3	2.46	0.50
24:T:198:ASN:HA	24:T:232:THR:OG1	2.10	0.50
34:d:258:PRO:HG2	34:d:301:PHE:CG	2.46	0.50
35:e:20:GLU:HG3	35:e:25:THR:HG22	1.93	0.50
39:i:107:VAL:HG12	47:q:162:GLN:OE1	2.11	0.50
40:j:416:ASN:O	40:j:420:SER:OG	2.19	0.50
44:n:284:CYS:O	44:n:286:LYS:N	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:q:29:ASN:O	47:q:33:LEU:HG	2.12	0.50
48:r:185:LYS:C	48:r:185:LYS:CD	2.84	0.50
48:r:661:LEU:HD22	48:r:668:HIS:HB3	1.94	0.50
49:s:122:ALA:O	49:s:125:VAL:HG22	2.11	0.50
49:s:150:LYS:O	49:s:153:HIS:HB3	2.11	0.50
1:0:812:ARG:NH1	46:p:92:GLN:NE2	2.60	0.50
2:1:316:GLU:HG2	2:1:367:LYS:HD2	1.92	0.50
2:1:1239:VAL:HG11	2:1:1277:MET:HG3	1.92	0.50
5:A:579:ILE:HG21	12:H:47:ILE:HD11	1.93	0.50
5:A:1161:LEU:HB3	5:A:1304:ILE:CD1	2.42	0.50
8:D:47:GLN:O	8:D:50:SER:OG	2.29	0.50
14:J:3:ILE:HD12	14:J:4:PRO:HD2	1.93	0.50
17:M:357:ILE:HD13	18:N:6:TYR:HE1	1.77	0.50
22:R:87:THR:O	22:R:91:ARG:HG2	2.11	0.50
27:W:85:PHE:HE1	30:Z:336:TYR:CE2	2.16	0.50
28:X:314:VAL:HG11	28:X:409:THR:CG2	2.41	0.50
29:Y:411:MET:C	32:b:120:THR:HG22	2.36	0.50
36:f:59:TYR:CZ	36:f:63:ARG:HD2	2.46	0.50
48:r:77:SER:HB3	48:r:80:GLU:OE1	2.11	0.50
48:r:759:GLY:O	48:r:762:VAL:HG12	2.11	0.50
48:r:932:GLY:O	48:r:1179:HIS:HB2	2.10	0.50
50:t:143:LYS:HD3	54:x:97:ASN:HA	1.92	0.50
52:v:98:LYS:CE	52:v:101:THR:HG21	2.39	0.50
52:v:98:LYS:HA	52:v:101:THR:CG2	2.41	0.50
52:v:120:ASP:N	52:v:124:TYR:CE2	2.80	0.50
55:y:52:LEU:O	55:y:56:LEU:HG	2.11	0.50
55:y:122:GLN:HA	55:y:125:GLN:CD	2.37	0.50
1:0:103:GLY:HA2	1:0:130:PRO:HD3	1.93	0.50
1:0:170:LEU:HD21	4:3:84:CYS:SG	2.51	0.50
2:1:1228:PRO:HG2	2:1:1266:CYS:HB2	1.93	0.50
3:2:64:LEU:O	3:2:68:ILE:HG12	2.12	0.50
3:2:547:PHE:O	3:2:582:SER:OG	2.28	0.50
4:3:84:CYS:SG	4:3:85:HIS:N	2.83	0.50
5:A:70:ARG:HD3	5:A:75:ALA:HB1	1.94	0.50
5:A:72:GLN:O	5:A:75:ALA:N	2.45	0.50
6:B:563:ASP:OD2	6:B:578:LYS:HE2	2.11	0.50
6:B:1033:THR:HG23	6:B:1035:ARG:H	1.76	0.50
10:F:84:GLU:HG2	10:F:95:LYS:HZ2	1.76	0.50
16:L:21:GLU:HB2	16:L:41:TYR:CD2	2.46	0.50
21:Q:30:HIS:CE1	21:Q:62:VAL:HG22	2.47	0.50
22:R:227:SER:O	22:R:231:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:17:ILE:HB	28:X:21:GLN:HG2	1.94	0.50
29:Y:136:VAL:CB	29:Y:505:LEU:HD11	2.42	0.50
30:Z:181:GLN:NE2	30:Z:222:THR:OG1	2.45	0.50
40:j:38:GLN:N	40:j:38:GLN:NE2	2.59	0.50
40:j:611:GLN:N	40:j:611:GLN:OE1	2.45	0.50
44:n:116:LYS:HE2	48:r:844:CYS:SG	2.52	0.50
47:q:73:ASP:O	47:q:76:THR:OG1	2.26	0.50
48:r:478:MET:HG3	48:r:492:TRP:CG	2.46	0.50
48:r:1413:MET:SD	48:r:1413:MET:N	2.84	0.50
50:t:160:VAL:HA	50:t:163:MET:CG	2.40	0.50
52:v:103:LYS:O	52:v:107:SER:CB	2.59	0.50
54:x:3:ASP:O	54:x:6:THR:N	2.44	0.50
54:x:73:ILE:C	54:x:76:LEU:HB2	2.37	0.50
55:y:116:GLN:OE1	55:y:119:LEU:HD12	2.11	0.50
1:0:170:LEU:HB3	1:0:173:GLY:N	2.20	0.50
1:0:170:LEU:HB2	1:0:174:LYS:O	2.11	0.50
1:0:456:ARG:HG2	1:0:494:HIS:CE1	2.46	0.50
1:0:671:SER:OG	46:p:88:ILE:CG1	2.53	0.50
1:0:796:LYS:HB2	1:0:833:TRP:CE3	2.47	0.50
2:1:99:GLU:O	2:1:103:ASN:CB	2.47	0.50
2:1:509:LEU:HD22	2:1:516:ALA:HB2	1.93	0.50
3:2:43:ALA:O	3:2:47:LEU:HD23	2.12	0.50
5:A:154:CYS:SG	5:A:155:GLU:N	2.84	0.50
5:A:904:GLN:OE1	5:A:1044:HIS:NE2	2.44	0.50
24:T:121:SER:OG	24:T:122:GLU:N	2.45	0.50
27:W:366:ASN:ND2	27:W:442:GLU:OE1	2.44	0.50
29:Y:382:TYR:CE1	32:b:273:SER:HB3	2.47	0.50
29:Y:417:LYS:HZ2	32:b:42:MET:HE3	1.76	0.50
30:Z:412:PHE:CE2	30:Z:441:MET:CE	2.94	0.50
40:j:191:ARG:CZ	43:m:88:LEU:CD2	2.90	0.50
40:j:290:HIS:HB3	40:j:294:LYS:NZ	2.27	0.50
48:r:142:ASP:OD1	48:r:142:ASP:N	2.44	0.50
49:s:112:LYS:O	49:s:115:LYS:HB2	2.12	0.50
50:t:75:LYS:HD2	54:x:79:GLU:HB3	1.94	0.50
50:t:131:ALA:O	50:t:132:ARG:C	2.54	0.50
51:u:90:LEU:HG	51:u:93:LYS:HE3	1.94	0.50
54:x:112:ASP:O	54:x:113:MET:C	2.53	0.50
56:z:746:ASN:HD22	56:z:746:ASN:N	2.09	0.50
2:1:1186:TYR:CD1	2:1:1187:PRO:HD2	2.46	0.50
2:1:1314:VAL:O	2:1:1318:ILE:HG13	2.12	0.50
3:2:980:GLN:O	3:2:984:LYS:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:805:ARG:HD2	5:A:810:PHE:O	2.11	0.50
7:C:100:GLU:HG3	7:C:164:TYR:HE1	1.77	0.50
9:E:64:HIS:CG	9:E:65:ASN:H	2.30	0.50
24:T:234:GLU:HG3	24:T:235:LEU:H	1.77	0.50
27:W:523:VAL:HG21	33:c:22:TYR:HE2	1.71	0.50
30:Z:35:TYR:CD1	30:Z:114:PHE:CD1	3.00	0.50
30:Z:368:LEU:HB3	30:Z:383:LEU:HD11	1.86	0.50
31:a:270:SER:OG	31:a:297:LYS:HG2	2.12	0.50
40:j:319:LYS:HD3	48:r:464:GLN:NE2	2.27	0.50
40:j:417:GLU:HG2	40:j:418:ILE:N	2.27	0.50
41:k:83:TRP:N	41:k:83:TRP:CD1	2.80	0.50
41:k:193:LEU:HD13	41:k:197:VAL:HG13	1.94	0.50
48:r:70:THR:HG22	53:w:151:GLY:HA3	1.94	0.50
48:r:192:LEU:HD11	48:r:219:ASN:CB	2.41	0.50
49:s:117:ALA:O	49:s:121:LEU:HD13	2.12	0.50
54:x:5:LEU:O	54:x:8:LEU:N	2.45	0.50
55:y:29:ALA:HA	55:y:75:MET:HG3	1.92	0.50
55:y:38:ALA:C	55:y:40:ARG:N	2.67	0.50
1:0:236:ALA:H	1:0:266:ARG:HH12	1.59	0.49
1:0:482:MET:HE3	1:0:522:LEU:HD13	1.94	0.49
2:1:349:PHE:O	2:1:353:VAL:HG23	2.12	0.49
2:1:770:MET:HE2	2:1:772:ASN:ND2	2.26	0.49
2:1:793:LEU:HA	2:1:796:MET:HG2	1.93	0.49
2:1:854:VAL:O	2:1:858:ASN:ND2	2.44	0.49
2:1:1186:TYR:CD1	3:2:238:LYS:HG2	2.46	0.49
3:2:128:LEU:O	3:2:132:LEU:HG	2.11	0.49
3:2:168:THR:HA	3:2:171:SER:OG	2.12	0.49
3:2:509:SER:O	3:2:510:GLU:HG2	2.12	0.49
3:2:678:LEU:HD13	3:2:685:ILE:HG12	1.94	0.49
5:A:566:PHE:CE1	15:K:62:LYS:HG3	2.46	0.49
5:A:1626:SER:CA	55:y:39:GLN:HG2	2.42	0.49
9:E:153:LYS:O	9:E:156:VAL:HG12	2.11	0.49
24:T:204:ASP:OD1	24:T:204:ASP:N	2.45	0.49
27:W:110:PRO:O	27:W:494:MET:CE	2.56	0.49
27:W:158:LEU:O	27:W:163:TYR:CE1	2.63	0.49
30:Z:35:TYR:CG	30:Z:114:PHE:HD1	2.29	0.49
30:Z:266:ARG:HE	30:Z:273:GLN:HB2	1.77	0.49
30:Z:309:VAL:H	30:Z:376:MET:HE3	1.77	0.49
34:d:120:LYS:HE3	34:d:124:ILE:HD11	1.94	0.49
38:h:36:GLU:HG2	40:j:93:TRP:CH2	2.47	0.49
40:j:198:LYS:CG	40:j:203:ILE:CD1	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:75:CYS:SG	42:l:91:PHE:HB3	2.51	0.49
44:n:32:PHE:CB	56:z:646:MET:HE1	2.42	0.49
47:q:110:PRO:O	47:q:113:GLN:HB2	2.12	0.49
48:r:65:GLU:OE2	48:r:66:LEU:HG	2.12	0.49
48:r:944:PHE:CD1	48:r:944:PHE:N	2.76	0.49
48:r:1180:SER:O	48:r:1184:ILE:HG12	2.11	0.49
49:s:75:GLU:O	49:s:79:LEU:HB2	2.12	0.49
51:u:121:LEU:O	51:u:122:ARG:C	2.55	0.49
52:v:86:GLU:HB2	52:v:87:ARG:NH1	2.27	0.49
1:0:710:ASP:OD1	1:0:710:ASP:N	2.44	0.49
2:1:805:GLN:HA	2:1:941:VAL:HG21	1.94	0.49
3:2:25:ILE:HG13	3:2:29:LYS:HZ2	1.76	0.49
3:2:47:LEU:HG	3:2:81:ALA:HB1	1.93	0.49
3:2:477:TYR:CE2	3:2:479:SER:HB2	2.46	0.49
5:A:330:GLN:HE21	5:A:332:SER:H	1.60	0.49
5:A:1161:LEU:HB2	5:A:1307:VAL:HG11	1.94	0.49
6:B:60:GLU:CD	24:T:140:ARG:HE	2.20	0.49
6:B:474:THR:OG1	6:B:732:ALA:O	2.30	0.49
6:B:900:GLU:N	6:B:900:GLU:OE2	2.44	0.49
17:M:361:ASN:OD1	18:N:90:VAL:HA	2.12	0.49
19:O:108:SER:HB3	19:O:111:ASP:HB2	1.94	0.49
27:W:295:TYR:HD2	27:W:333:ALA:O	1.94	0.49
27:W:351:VAL:CG1	27:W:378:PHE:CD1	2.92	0.49
27:W:472:ARG:HH21	27:W:480:LEU:HB2	1.77	0.49
30:Z:100:LEU:HD23	30:Z:106:GLN:HA	1.94	0.49
30:Z:352:GLN:OE1	30:Z:398:ARG:CB	2.60	0.49
40:j:468:ASN:H	47:q:171:ASN:ND2	2.11	0.49
44:n:195:GLY:O	44:n:197:VAL:N	2.45	0.49
48:r:488:ARG:O	48:r:491:PRO:HD2	2.12	0.49
48:r:661:LEU:HD11	48:r:684:LEU:HD21	1.94	0.49
49:s:187:LEU:HD12	55:y:20:LEU:HA	1.94	0.49
50:t:15:MET:HE3	50:t:16:GLN:HG2	1.93	0.49
52:v:7:HIS:O	52:v:11:HIS:CD2	2.65	0.49
54:x:67:LYS:O	54:x:71:VAL:HG23	2.12	0.49
1:0:47:PHE:CD2	1:0:49:MET:HB2	2.47	0.49
1:0:291:SER:OG	1:0:292:GLU:N	2.42	0.49
2:1:403:TYR:OH	2:1:425:MET:HG3	2.12	0.49
2:1:456:GLU:O	2:1:460:GLN:HG3	2.11	0.49
2:1:633:VAL:HG13	2:1:634:ALA:N	2.27	0.49
3:2:158:LEU:O	3:2:162:LEU:HG	2.13	0.49
5:A:545:VAL:HG12	5:A:676:ILE:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1095:LEU:HD12	5:A:1398:LEU:HD23	1.93	0.49
6:B:1081:ASP:OD1	6:B:1083:GLY:N	2.45	0.49
8:D:41:LEU:HG	8:D:61:PHE:CE1	2.46	0.49
8:D:78:GLU:O	38:h:51:LEU:HD21	2.12	0.49
20:P:212:LEU:HD11	26:V:78:DT:C4'	2.42	0.49
22:R:113:LEU:HA	22:R:116:LYS:HE2	1.94	0.49
22:R:234:GLU:HB3	22:R:238:LYS:HZ3	1.77	0.49
27:W:688:LYS:HE3	27:W:690:ILE:HD11	1.94	0.49
28:X:220:LEU:HD12	28:X:221:VAL:HG23	1.94	0.49
29:Y:421:VAL:HG22	32:b:39:ASP:CB	2.42	0.49
36:f:195:LEU:HA	36:f:198:ILE:HG22	1.95	0.49
40:j:387:LEU:CD2	41:k:46:MET:HA	2.40	0.49
40:j:387:LEU:HG	41:k:46:MET:HB2	1.93	0.49
48:r:155:PRO:O	48:r:158:ILE:N	2.45	0.49
48:r:231:GLU:OE1	48:r:251:GLU:CB	2.56	0.49
48:r:254:VAL:HG21	48:r:303:LEU:HD22	1.94	0.49
48:r:1209:ARG:HH22	48:r:1259:GLN:CD	2.21	0.49
52:v:1:MET:CG	52:v:4:LYS:HB3	2.43	0.49
52:v:75:ARG:NH1	53:w:104:LYS:HB2	2.26	0.49
55:y:87:GLU:O	55:y:89:VAL:N	2.45	0.49
55:y:93:CYS:O	55:y:94:ALA:C	2.53	0.49
56:z:704:VAL:O	56:z:725:VAL:HG22	2.11	0.49
1:0:643:HIS:C	1:0:645:PHE:H	2.21	0.49
2:1:151:THR:HG23	3:2:916:THR:HG23	1.95	0.49
2:1:452:ARG:O	2:1:456:GLU:HG2	2.11	0.49
3:2:609:ILE:HD11	3:2:616:LEU:HD23	1.95	0.49
3:2:965:LYS:NZ	3:2:965:LYS:O	2.42	0.49
5:A:641:CYS:O	5:A:645:LEU:HD23	2.11	0.49
8:D:93:HIS:HB3	8:D:96:GLU:OE2	2.11	0.49
9:E:53:PRO:HD2	9:E:57:ASP:HB3	1.94	0.49
11:G:109:SER:OG	11:G:110:ARG:N	2.45	0.49
17:M:335:VAL:HG13	17:M:358:MET:HB3	1.95	0.49
27:W:361:CYS:SG	27:W:362:LEU:N	2.85	0.49
27:W:493:TRP:HE1	27:W:683:GLN:HE21	1.60	0.49
28:X:425:THR:HG23	28:X:428:ILE:HB	1.95	0.49
28:X:592:ARG:HH12	31:a:177:CYS:HA	1.71	0.49
31:a:249:LEU:HB2	32:b:289:PHE:CE1	2.44	0.49
31:a:292:PRO:CB	32:b:264:ILE:CG1	2.79	0.49
32:b:46:ASN:HD22	32:b:104:LEU:HD22	1.77	0.49
37:g:42:ASP:OD1	37:g:68:TYR:OH	2.16	0.49
38:h:77:ILE:HG23	40:j:119:VAL:HG12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:412:ALA:CB	42:l:86:ILE:HD13	2.41	0.49
40:j:565:ASN:ND2	48:r:511:HIS:HB2	2.27	0.49
48:r:156:TYR:O	48:r:160:VAL:HG22	2.12	0.49
48:r:169:LEU:HD23	48:r:175:ASP:CB	2.42	0.49
48:r:276:GLN:HA	48:r:279:GLN:HG3	1.94	0.49
48:r:1279:GLN:OE1	48:r:1279:GLN:N	2.41	0.49
48:r:1438:ALA:O	48:r:1442:LEU:HG	2.12	0.49
49:s:147:GLU:HG2	49:s:148:ILE:H	1.77	0.49
55:y:20:LEU:O	55:y:21:GLU:C	2.55	0.49
55:y:81:TYR:O	55:y:85:ARG:NH1	2.46	0.49
56:z:701:ASN:ND2	56:z:701:ASN:H	2.09	0.49
1:0:235:SER:HA	1:0:266:ARG:HH12	1.78	0.49
1:0:265:MET:HB2	3:2:541:ASN:ND2	2.27	0.49
2:1:108:GLU:HG3	2:1:110:GLU:H	1.76	0.49
2:1:941:VAL:HG22	2:1:942:ASP:H	1.76	0.49
4:3:111:CYS:O	4:3:151:TYR:HD1	1.96	0.49
5:A:155:GLU:HB3	5:A:185:GLY:HA2	1.93	0.49
5:A:769:MET:HE3	6:B:970:HIS:ND1	2.28	0.49
5:A:1132:LYS:HA	5:A:1363:VAL:HG11	1.93	0.49
6:B:489:ILE:CD1	6:B:498:PRO:HG3	2.37	0.49
19:O:14:THR:HG21	19:O:21:ALA:HB3	1.94	0.49
21:Q:177:LEU:CG	34:d:8:ARG:O	2.61	0.49
29:Y:381:ARG:CB	32:b:256:PHE:HB3	2.42	0.49
29:Y:524:HIS:NE2	31:a:270:SER:HB3	2.27	0.49
30:Z:58:ARG:NE	32:b:241:LEU:HD11	2.28	0.49
31:a:322:TYR:HB3	32:b:175:MET:HE1	1.94	0.49
34:d:304:LEU:HD11	36:f:170:PHE:HZ	1.76	0.49
35:e:64:LYS:NZ	36:f:117:GLU:OE2	2.43	0.49
36:f:234:GLU:C	36:f:236:LEU:H	2.20	0.49
40:j:551:PHE:HA	40:j:569:ILE:O	2.12	0.49
41:k:46:MET:O	41:k:47:GLU:HG2	2.11	0.49
41:k:156:ASN:ND2	41:k:158:ASP:HB2	2.26	0.49
48:r:99:LEU:O	48:r:102:LEU:HB3	2.12	0.49
48:r:152:PHE:CE1	49:s:149:ILE:HG22	2.47	0.49
48:r:1191:THR:OG1	48:r:1199:ALA:HB1	2.12	0.49
48:r:1232:ILE:HD12	48:r:1232:ILE:H	1.76	0.49
49:s:186:LEU:HA	49:s:189:GLN:CD	2.38	0.49
52:v:89:LEU:O	52:v:93:GLU:HG2	2.12	0.49
55:y:83:HIS:O	55:y:87:GLU:HG2	2.13	0.49
1:0:265:MET:C	1:0:267:CYS:N	2.68	0.49
2:1:1070:ARG:O	2:1:1074:ARG:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:45:GLU:C	4:3:48:ASN:O	2.54	0.49
5:A:1170:THR:HA	5:A:1216:LEU:HA	1.94	0.49
6:B:289:ILE:HG12	6:B:297:MET:HE2	1.95	0.49
11:G:158:PHE:HD1	21:Q:142:ASN:HD22	1.60	0.49
15:K:8:GLU:HG2	15:K:13:PHE:HE1	1.76	0.49
24:T:20:LEU:O	24:T:113:ARG:HA	2.13	0.49
27:W:275:GLU:HA	27:W:456:THR:CG2	2.36	0.49
28:X:237:HIS:HE1	28:X:460:THR:HB	1.78	0.49
28:X:310:LEU:CD2	28:X:409:THR:HB	2.35	0.49
31:a:258:THR:O	31:a:288:GLY:N	2.44	0.49
40:j:567:SER:CB	40:j:584:ASN:O	2.60	0.49
40:j:593:MET:SD	48:r:676:ASP:HB3	2.52	0.49
47:q:58:MET:HE1	47:q:74:ARG:HB3	1.93	0.49
48:r:168:ARG:HG2	55:y:74:HIS:CG	2.48	0.49
48:r:231:GLU:O	48:r:250:LEU:CA	2.54	0.49
48:r:1255:PRO:C	48:r:1256:LYS:HD3	2.36	0.49
48:r:1434:THR:OG1	48:r:1435:ILE:HD12	2.12	0.49
50:t:89:PHE:CE1	50:t:93:LEU:HD21	2.47	0.49
50:t:158:GLU:O	50:t:159:ARG:C	2.56	0.49
52:v:6:ASP:HA	52:v:9:GLU:HB2	1.95	0.49
55:y:56:LEU:C	55:y:58:TRP:N	2.68	0.49
55:y:88:LEU:C	55:y:90:ASN:N	2.66	0.49
56:z:721:LEU:HD11	56:z:736:TRP:CH2	2.19	0.49
2:1:792:LEU:O	2:1:796:MET:HG2	2.12	0.49
3:2:180:ILE:HD11	3:2:973:LEU:HB2	1.95	0.49
3:2:755:GLU:HB2	3:2:761:THR:HG22	1.94	0.49
5:A:41:ILE:HG12	5:A:88:ILE:HG12	1.94	0.49
5:A:1167:ARG:HH11	13:I:58:ILE:HD11	1.77	0.49
5:A:1353:ASP:OD2	5:A:1356:ARG:NH1	2.45	0.49
6:B:276:LEU:HD21	6:B:347:MET:HE1	1.94	0.49
6:B:365:LEU:O	6:B:369:VAL:HG23	2.12	0.49
6:B:593:GLN:O	6:B:594:MET:HG2	2.13	0.49
19:O:154:ARG:HB2	19:O:159:ILE:HD11	1.95	0.49
19:O:192:GLY:HA3	20:P:287:LEU:HD21	1.93	0.49
21:Q:30:HIS:NE2	21:Q:62:VAL:HA	2.28	0.49
24:T:172:ASP:O	24:T:175:ARG:HG2	2.12	0.49
27:W:77:TRP:CZ3	30:Z:341:MET:HE1	2.48	0.49
33:c:5:LEU:C	33:c:5:LEU:CD1	2.85	0.49
35:e:97:ASP:HA	35:e:144:LEU:HA	1.94	0.49
40:j:484:TYR:CD1	44:n:135:ARG:O	2.65	0.49
44:n:38:GLY:HA3	56:z:638:LEU:CD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:122:LEU:O	48:r:125:GLN:N	2.44	0.49
48:r:212:LEU:HB3	48:r:215:LEU:HD11	1.93	0.49
48:r:314:MET:HA	48:r:317:ARG:NE	2.28	0.49
48:r:735:SER:HB2	48:r:738:GLU:OE1	2.12	0.49
49:s:120:ILE:O	49:s:121:LEU:C	2.52	0.49
50:t:16:GLN:O	50:t:18:ILE:HG13	2.13	0.49
50:t:120:HIS:O	50:t:124:ASN:OD1	2.30	0.49
50:t:129:HIS:O	50:t:132:ARG:N	2.46	0.49
50:t:168:LEU:O	50:t:171:LEU:N	2.35	0.49
52:v:82:LYS:HE2	53:w:96:PHE:CA	2.39	0.49
53:w:93:TYR:CD2	53:w:97:CYS:HB3	2.48	0.49
2:1:6:GLN:O	2:1:10:GLU:HG2	2.13	0.49
2:1:867:LEU:HD13	2:1:966:VAL:HG13	1.93	0.49
3:2:261:GLN:HE21	3:2:265:GLU:HG2	1.77	0.49
4:3:145:ILE:HG23	4:3:183:VAL:HG23	1.95	0.49
5:A:14:PRO:HG2	11:G:12:LEU:HD11	1.95	0.49
5:A:95:PHE:HE1	5:A:221:VAL:HG21	1.78	0.49
5:A:146:ASP:O	5:A:149:LYS:HG2	2.12	0.49
5:A:457:ILE:HD13	6:B:1102:PHE:CE1	2.48	0.49
6:B:235:ILE:HD12	6:B:348:LEU:HG	1.93	0.49
6:B:1037:ILE:HG21	6:B:1041:ILE:HD11	1.93	0.49
12:H:148:LEU:HD23	12:H:150:PHE:N	2.25	0.49
28:X:293:ARG:HD3	28:X:381:SER:OG	2.12	0.49
29:Y:460:GLU:OE1	29:Y:513:ARG:HD3	2.13	0.49
34:d:44:GLY:HA2	34:d:53:LEU:HD22	1.94	0.49
40:j:412:ALA:O	42:l:186:PRO:HG3	2.13	0.49
40:j:534:VAL:CG2	40:j:568:ALA:O	2.58	0.49
43:m:73:GLU:HG3	43:m:76:MET:HE2	1.95	0.49
47:q:139:ARG:HG3	47:q:140:ARG:HD3	1.95	0.49
50:t:135:LEU:O	50:t:138:MET:HB2	2.13	0.49
52:v:81:THR:O	52:v:85:LEU:CB	2.61	0.49
53:w:91:GLN:CB	53:w:95:LYS:HE3	2.43	0.49
55:y:56:LEU:O	55:y:57:TYR:C	2.55	0.49
55:y:82:GLU:N	55:y:85:ARG:NH2	2.60	0.49
2:1:9:PHE:O	2:1:13:VAL:HG23	2.13	0.49
2:1:237:ILE:HB	2:1:285:ASN:HD22	1.76	0.49
2:1:339:ILE:HD11	2:1:378:GLN:HB3	1.94	0.49
2:1:371:HIS:O	2:1:375:VAL:HG23	2.12	0.49
4:3:23:GLU:OE2	4:3:28:LEU:HB3	2.11	0.49
4:3:116:GLU:O	4:3:120:THR:HG23	2.13	0.49
5:A:320:ASN:HB2	5:A:338:SER:CB	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:891:TYR:CE1	5:A:1087:VAL:HG21	2.48	0.49
5:A:1118:THR:O	5:A:1119:LEU:HD23	2.13	0.49
5:A:1382:LEU:HB3	5:A:1398:LEU:HD22	1.95	0.49
5:A:1419:VAL:HG21	5:A:1432:PHE:CZ	2.48	0.49
5:A:1479:LYS:NZ	10:F:121:ASP:OD2	2.29	0.49
6:B:123:PRO:HG3	24:T:147:LYS:HE2	1.95	0.49
6:B:420:GLN:HA	6:B:423:ILE:HG12	1.95	0.49
7:C:169:PHE:O	7:C:176:TRP:HB2	2.12	0.49
11:G:123:SER:OG	11:G:124:ASN:N	2.44	0.49
17:M:342:ILE:HD13	18:N:74:PHE:CZ	2.47	0.49
19:O:142:PHE:HA	19:O:145:VAL:HG12	1.95	0.49
21:Q:44:LYS:HG3	21:Q:89:HIS:CD2	2.48	0.49
23:S:49:ARG:HA	23:S:98:TRP:HA	1.95	0.49
24:T:42:LYS:NZ	24:T:57:THR:O	2.45	0.49
24:T:197:TYR:C	24:T:232:THR:HG1	2.21	0.49
27:W:112:HIS:CG	30:Z:310:GLU:HG2	2.45	0.49
27:W:121:TYR:CE2	27:W:486:PRO:C	2.91	0.49
27:W:125:ALA:CA	27:W:486:PRO:CB	2.90	0.49
30:Z:58:ARG:NE	32:b:241:LEU:CG	2.76	0.49
40:j:290:HIS:O	40:j:294:LYS:HD2	2.13	0.49
40:j:479:ILE:HD12	40:j:529:MET:CE	2.27	0.49
40:j:482:GLN:NE2	40:j:482:GLN:C	2.71	0.49
40:j:615:TRP:CH2	56:z:680:GLY:HA3	2.48	0.49
40:j:631:GLU:O	40:j:638:LYS:HG2	2.12	0.49
43:m:22:LEU:O	43:m:26:ILE:HG12	2.13	0.49
44:n:195:GLY:C	44:n:197:VAL:H	2.20	0.49
48:r:1283:LYS:O	48:r:1287:THR:HG23	2.13	0.49
48:r:1323:GLU:OE2	48:r:1331:GLN:O	2.27	0.49
49:s:148:ILE:HA	49:s:151:TYR:CB	2.42	0.49
49:s:151:TYR:OH	55:y:66:TYR:N	2.46	0.49
50:t:130:GLN:O	50:t:134:THR:HG23	2.12	0.49
52:v:67:VAL:HG23	52:v:70:TYR:HD2	1.77	0.49
52:v:89:LEU:O	52:v:90:ALA:C	2.56	0.49
55:y:76:LEU:O	55:y:77:GLU:C	2.56	0.49
55:y:92:GLN:O	55:y:93:CYS:C	2.54	0.49
56:z:746:ASN:N	56:z:746:ASN:ND2	2.60	0.49
1:0:61:MET:CE	1:0:75:SER:HB3	2.42	0.49
3:2:175:ARG:HD3	3:2:176:ALA:N	2.27	0.49
3:2:310:PHE:CZ	3:2:407:ILE:HD13	2.48	0.49
5:A:1210:TRP:HB3	5:A:1285:LEU:HD12	1.93	0.49
5:A:1311:LEU:HD13	5:A:1337:GLU:HG2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:45:ASP:OD1	6:B:46:SER:N	2.46	0.49
6:B:1127:ILE:HG21	6:B:1146:ILE:HG21	1.95	0.49
19:O:282:ASP:O	19:O:286:ARG:HG2	2.13	0.49
26:V:35:DG:H2"	26:V:36:DA:C8	2.48	0.49
27:W:159:CYS:SG	27:W:163:TYR:CE2	3.06	0.49
27:W:640:LEU:HG	27:W:644:LEU:HD12	1.95	0.49
29:Y:420:GLN:O	32:b:36:LYS:HD3	2.12	0.49
29:Y:499:ARG:NH1	29:Y:536:LEU:HD13	2.28	0.49
30:Z:32:ASP:OD1	30:Z:111:ASN:ND2	2.41	0.49
30:Z:407:VAL:HA	33:c:7:GLY:H	1.77	0.49
32:b:178:MET:HA	32:b:181:ILE:HD12	1.94	0.49
37:g:86:ARG:NH2	37:g:89:PRO:HA	2.28	0.49
40:j:412:ALA:HB3	42:l:186:PRO:HB2	1.94	0.49
40:j:455:ILE:HG22	40:j:457:ASP:H	1.77	0.49
40:j:495:LEU:HD22	40:j:504:VAL:HG22	1.94	0.49
42:l:162:GLN:HA	42:l:166:GLY:HA3	1.94	0.49
44:n:49:GLU:OE2	56:z:630:ARG:HD2	2.13	0.49
44:n:165:VAL:HG11	44:n:207:LEU:HD11	1.95	0.49
44:n:223:THR:HG22	44:n:229:ASP:HB2	1.94	0.49
48:r:125:GLN:O	48:r:128:LEU:HB3	2.13	0.49
51:u:94:PHE:O	51:u:98:ARG:HG3	2.12	0.49
52:v:68:PHE:O	52:v:69:GLU:C	2.52	0.49
52:v:106:LYS:C	52:v:109:LEU:HB3	2.38	0.49
1:0:147:VAL:HG11	1:0:361:ILE:HG23	1.94	0.48
1:0:307:GLU:HG3	1:0:309:TRP:HE1	1.77	0.48
2:1:411:VAL:HG11	2:1:457:PHE:CD2	2.47	0.48
2:1:991:LEU:O	2:1:991:LEU:HD12	2.13	0.48
3:2:131:LEU:HG	3:2:160:MET:HE3	1.94	0.48
3:2:494:ASP:HB2	3:2:613:VAL:HG12	1.95	0.48
3:2:661:GLU:O	3:2:664:VAL:HG12	2.12	0.48
5:A:1343:LEU:HD13	5:A:1359:SER:HB3	1.95	0.48
5:A:1484:MET:O	5:A:1485:GLU:HG3	2.12	0.48
6:B:1028:LEU:HB2	6:B:1041:ILE:HD13	1.95	0.48
7:C:80:ASP:OD1	7:C:81:LYS:HG3	2.13	0.48
8:D:134:ILE:O	8:D:138:ARG:HB2	2.13	0.48
11:G:124:ASN:N	38:h:167:ARG:NH2	2.59	0.48
27:W:129:VAL:HG23	27:W:334:ARG:NH1	2.28	0.48
27:W:282:LYS:HE2	27:W:478:VAL:CG1	2.41	0.48
28:X:461:LEU:HD22	28:X:467:TYR:HE2	1.77	0.48
29:Y:411:MET:HG3	32:b:119:MET:HB2	1.94	0.48
29:Y:422:LEU:HD11	32:b:224:LEU:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:392:ARG:HA	30:Z:395:GLU:HB2	1.94	0.48
34:d:303:GLY:O	36:f:210:SER:HB2	2.13	0.48
36:f:96:VAL:HG13	36:f:101:PRO:CG	2.43	0.48
40:j:332:ILE:HD13	48:r:434:ALA:HB3	1.95	0.48
40:j:433:LYS:HB3	40:j:471:TYR:HE1	1.77	0.48
40:j:649:CYS:C	40:j:651:LEU:H	2.21	0.48
43:m:31:ASP:O	43:m:34:THR:OG1	2.24	0.48
46:p:73:THR:O	46:p:77:VAL:HG23	2.13	0.48
47:q:114:LEU:HG	47:q:116:PRO:HD3	1.95	0.48
48:r:72:LEU:HA	48:r:75:ARG:H	1.78	0.48
48:r:569:TYR:CE2	48:r:614:ARG:HB2	2.48	0.48
49:s:67:GLU:O	49:s:71:HIS:ND1	2.46	0.48
50:t:16:GLN:NE2	50:t:17:TYR:CD1	2.81	0.48
50:t:108:LYS:O	50:t:111:ASP:HB2	2.12	0.48
50:t:142:GLN:O	50:t:143:LYS:C	2.56	0.48
51:u:113:GLN:O	51:u:117:GLN:HB2	2.13	0.48
52:v:6:ASP:HA	52:v:9:GLU:CD	2.38	0.48
52:v:56:GLN:NE2	52:v:57:GLN:HG3	2.28	0.48
53:w:83:LEU:N	53:w:83:LEU:HD12	2.28	0.48
53:w:90:GLU:H	53:w:90:GLU:CD	2.19	0.48
54:x:115:LEU:HB2	54:x:119:GLN:HE21	1.78	0.48
55:y:123:GLN:O	55:y:124:GLN:C	2.56	0.48
1:0:49:MET:SD	1:0:49:MET:C	2.93	0.48
1:0:812:ARG:NH2	46:p:92:GLN:NE2	2.60	0.48
2:1:305:VAL:HG21	2:1:355:SER:OG	2.13	0.48
3:2:86:ASP:O	3:2:88:PHE:N	2.46	0.48
5:A:454:ASP:HA	5:A:512:ARG:HH12	1.78	0.48
5:A:723:ASN:HD22	13:I:109:ARG:HD3	1.77	0.48
6:B:144:HIS:O	6:B:145:GLN:HB2	2.11	0.48
19:O:128:ILE:HG13	19:O:130:LEU:HG	1.94	0.48
22:R:110:ASP:OD1	22:R:114:LYS:HD3	2.12	0.48
23:S:102:VAL:HB	23:S:107:GLY:HA3	1.95	0.48
28:X:235:GLU:OE2	28:X:666:ARG:NH2	2.33	0.48
29:Y:538:THR:HG22	29:Y:542:ARG:NE	2.29	0.48
34:d:22:MET:HA	34:d:59:ARG:O	2.13	0.48
40:j:191:ARG:NE	43:m:88:LEU:HG	2.28	0.48
40:j:479:ILE:HD13	40:j:529:MET:HE1	0.52	0.48
42:l:76:PHE:CZ	42:l:86:ILE:HG12	2.49	0.48
42:l:120:CYS:SG	44:n:291:GLY:CA	2.86	0.48
48:r:1280:VAL:HG11	48:r:1321:LYS:HB2	1.96	0.48
49:s:152:ALA:CA	49:s:155:ILE:HB	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:15:MET:C	50:t:18:ILE:HG12	2.38	0.48
50:t:136:ARG:NH1	54:x:86:GLN:O	2.46	0.48
52:v:117:PHE:HD2	52:v:119:GLU:HB2	1.78	0.48
53:w:90:GLU:O	53:w:93:TYR:N	2.46	0.48
54:x:129:GLN:C	54:x:132:THR:H	2.21	0.48
55:y:55:LEU:CA	55:y:58:TRP:HD1	2.26	0.48
2:1:1072:ILE:O	2:1:1076:VAL:HG23	2.13	0.48
5:A:698:THR:O	5:A:702:ILE:HG12	2.12	0.48
5:A:964:GLU:O	5:A:968:VAL:HG23	2.13	0.48
5:A:1003:ASP:OD1	5:A:1003:ASP:N	2.43	0.48
5:A:1134:PRO:HG2	5:A:1137:PRO:HG3	1.95	0.48
7:C:44:ILE:CG1	7:C:178:PRO:HG3	2.44	0.48
8:D:78:GLU:CD	38:h:51:LEU:CD2	2.86	0.48
11:G:43:GLY:HA2	11:G:157:ILE:HD12	1.95	0.48
26:V:38:DT:H3'	27:W:565:VAL:HG21	1.96	0.48
27:W:172:HIS:C	27:W:434:GLU:OE2	2.55	0.48
27:W:298:ARG:HD2	27:W:298:ARG:HA	1.53	0.48
30:Z:41:CYS:CB	30:Z:118:LEU:CG	2.91	0.48
30:Z:61:PHE:CE1	32:b:228:LEU:CD1	2.83	0.48
31:a:167:VAL:HB	31:a:196:VAL:HG22	1.95	0.48
37:g:56:THR:OG1	37:g:57:LEU:N	2.46	0.48
38:h:23:LYS:HD2	40:j:113:TYR:HB2	1.95	0.48
42:l:197:PHE:HA	42:l:200:ILE:HG22	1.94	0.48
48:r:464:GLN:HA	48:r:479:GLU:OE1	2.13	0.48
50:t:105:ARG:CA	50:t:108:LYS:HG2	2.44	0.48
50:t:111:ASP:O	50:t:112:LEU:C	2.53	0.48
52:v:78:GLN:O	52:v:82:LYS:HG2	2.13	0.48
52:v:104:LYS:HD3	54:x:55:ALA:HB1	1.95	0.48
54:x:57:LEU:O	54:x:60:ALA:HB3	2.13	0.48
1:0:266:ARG:HD3	1:0:280:ILE:HD11	1.96	0.48
1:0:812:ARG:HH12	46:p:92:GLN:NE2	2.11	0.48
2:1:428:ILE:HG13	2:1:429:TRP:N	2.28	0.48
3:2:175:ARG:HG3	3:2:225:ILE:HA	1.94	0.48
3:2:714:ILE:HG13	3:2:731:ILE:HG21	1.95	0.48
3:2:908:ILE:HG12	3:2:924:VAL:HG13	1.95	0.48
5:A:625:ASP:O	5:A:639:ILE:HG22	2.13	0.48
6:B:310:VAL:HG12	23:S:174:PHE:HE2	1.77	0.48
11:G:18:PHE:HA	11:G:22:LEU:HD13	1.95	0.48
18:N:61:SER:C	18:N:76:LEU:HD23	2.37	0.48
24:T:187:LEU:HB2	24:T:191:PHE:CZ	2.48	0.48
29:Y:442:GLN:HE22	32:b:247:VAL:HG22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:445:THR:HG23	32:b:245:PRO:HB3	1.95	0.48
29:Y:485:PHE:O	29:Y:489:LYS:HG3	2.13	0.48
39:i:104:LEU:CD2	45:o:136:LEU:CD2	2.88	0.48
40:j:458:PRO:HD3	40:j:533:GLN:NE2	2.28	0.48
48:r:51:LEU:N	52:v:60:ASP:CG	2.70	0.48
48:r:61:ARG:HH12	48:r:65:GLU:HB2	1.79	0.48
48:r:92:THR:O	48:r:93:ARG:C	2.55	0.48
49:s:38:GLU:HG2	51:u:98:ARG:NH2	2.28	0.48
49:s:143:ILE:C	49:s:146:GLU:OE2	2.56	0.48
55:y:90:ASN:ND2	55:y:93:CYS:SG	2.86	0.48
2:1:874:HIS:O	2:1:879:ALA:HB2	2.14	0.48
4:3:39:TYR:CZ	4:3:221:VAL:HG21	2.48	0.48
6:B:597:ILE:HG13	6:B:599:SER:H	1.79	0.48
6:B:1027:VAL:HG23	7:C:195:THR:HG21	1.95	0.48
9:E:18:MET:HE1	9:E:60:VAL:HG21	1.95	0.48
17:M:49:LYS:HE2	18:N:17:GLU:HB2	1.95	0.48
20:P:259:VAL:HG23	20:P:313:THR:HG22	1.95	0.48
29:Y:505:LEU:C	29:Y:507:PRO:CD	2.87	0.48
30:Z:185:MET:HE2	30:Z:194:PRO:HB2	1.96	0.48
35:e:59:ALA:HB1	35:e:87:ILE:HD11	1.94	0.48
40:j:46:ARG:HB2	40:j:47:ILE:HD13	1.95	0.48
40:j:186:GLU:HG2	40:j:291:TRP:CH2	2.48	0.48
40:j:249:SER:HA	40:j:252:GLU:OE1	2.13	0.48
40:j:491:ILE:HD11	40:j:532:HIS:N	2.22	0.48
42:l:12:ALA:O	42:l:14:GLY:HA3	2.13	0.48
46:p:160:TYR:O	46:p:164:ILE:HG12	2.13	0.48
48:r:611:ASN:OD1	48:r:611:ASN:N	2.44	0.48
48:r:734:THR:HG22	48:r:801:ARG:HA	1.95	0.48
49:s:43:GLU:O	49:s:47:MET:HG2	2.13	0.48
49:s:116:GLU:O	49:s:117:ALA:C	2.54	0.48
52:v:39:GLN:O	52:v:42:ASN:HB3	2.12	0.48
52:v:41:LEU:C	52:v:44:ILE:H	2.20	0.48
54:x:120:SER:O	54:x:121:ALA:C	2.56	0.48
55:y:50:ASN:O	55:y:51:TYR:C	2.57	0.48
1:0:792:THR:HG22	44:n:41:ASN:N	2.28	0.48
3:2:452:LEU:HD21	3:2:499:MET:HE1	1.94	0.48
4:3:41:LEU:O	4:3:45:GLU:HG2	2.13	0.48
4:3:142:CYS:O	4:3:180:PHE:HB2	2.14	0.48
8:D:70:ARG:N	43:m:20:LYS:HZ3	2.10	0.48
9:E:1:MET:HA	9:E:6:GLU:HG2	1.95	0.48
17:M:333:ASN:HB3	17:M:359:ASN:C	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:56:VAL:HG12	18:N:57:ASN:H	1.78	0.48
20:P:186:ARG:HG2	20:P:244:LEU:HD22	1.95	0.48
20:P:241:VAL:HG12	20:P:248:ALA:HB2	1.96	0.48
22:R:234:GLU:HB3	22:R:238:LYS:NZ	2.28	0.48
23:S:28:ILE:HD13	24:T:95:VAL:HG22	1.94	0.48
27:W:105:GLU:CG	27:W:487:LYS:HE2	2.43	0.48
28:X:316:GLN:HG3	28:X:373:ARG:CZ	2.37	0.48
28:X:650:ASP:OD1	28:X:692:LYS:NZ	2.35	0.48
30:Z:442:VAL:HG22	33:c:44:PHE:HE1	1.77	0.48
35:e:142:ASN:ND2	35:e:155:ASP:OD2	2.47	0.48
38:h:74:GLN:C	38:h:76:ILE:H	2.21	0.48
38:h:141:GLN:HB3	38:h:145:LYS:NZ	2.29	0.48
39:i:96:ARG:NH1	43:m:113:ASP:OD1	2.44	0.48
40:j:328:LYS:O	48:r:319:ARG:NH2	2.47	0.48
41:k:29:ASP:O	41:k:32:LEU:HB3	2.14	0.48
48:r:890:MET:HB2	48:r:893:LEU:CD2	2.43	0.48
49:s:103:ARG:O	49:s:106:ASP:N	2.45	0.48
49:s:120:ILE:O	49:s:123:THR:N	2.46	0.48
49:s:146:GLU:N	49:s:146:GLU:CD	2.70	0.48
50:t:88:ASN:O	50:t:89:PHE:C	2.56	0.48
51:u:70:HIS:O	51:u:74:LYS:HG2	2.13	0.48
52:v:77:PRO:O	52:v:78:GLN:C	2.56	0.48
54:x:73:ILE:HA	54:x:76:LEU:HD12	1.94	0.48
55:y:14:ASN:O	55:y:18:PHE:CE2	2.67	0.48
2:1:707:ILE:O	2:1:710:THR:OG1	2.20	0.48
2:1:931:LYS:HB3	2:1:935:GLU:HB2	1.95	0.48
3:2:17:ARG:HG3	3:2:59:LEU:HD22	1.95	0.48
3:2:269:MET:HB3	3:2:269:MET:HE3	1.35	0.48
3:2:347:LEU:HD23	3:2:348:LEU:HD23	1.94	0.48
5:A:767:LYS:HA	5:A:770:VAL:HG22	1.95	0.48
5:A:808:PRO:HB2	6:B:675:LEU:HD13	1.94	0.48
5:A:978:VAL:HG21	5:A:1392:TYR:OH	2.14	0.48
5:A:982:ASN:HD22	5:A:985:ARG:HE	1.61	0.48
6:B:252:ILE:HB	6:B:303:PRO:HB3	1.94	0.48
6:B:472:ARG:HH21	6:B:737:ILE:HD13	1.79	0.48
7:C:118:ARG:HD3	7:C:133:ARG:HH22	1.79	0.48
8:D:83:VAL:HG13	8:D:84:ARG:H	1.79	0.48
27:W:319:TYR:CE1	27:W:501:TYR:CE2	3.02	0.48
27:W:473:GLU:CD	27:W:632:SER:N	2.71	0.48
30:Z:19:LEU:HD23	30:Z:47:GLU:HG3	1.96	0.48
30:Z:152:ALA:HB1	30:Z:286:LEU:HG	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:45:LEU:HD11	35:e:86:ASN:HB3	1.96	0.48
35:e:61:ARG:HD3	35:e:159:ALA:H	1.78	0.48
40:j:505:VAL:HG11	44:n:247:THR:OG1	2.13	0.48
41:k:30:HIS:CD2	41:k:30:HIS:H	2.32	0.48
42:l:137:GLY:O	42:l:138:ILE:HD13	2.13	0.48
44:n:87:HIS:HD1	44:n:88:ASN:H	1.60	0.48
47:q:33:LEU:HD13	47:q:98:LYS:HB3	1.95	0.48
48:r:69:LEU:HA	48:r:72:LEU:HD12	1.96	0.48
48:r:918:PHE:O	48:r:919:ARG:C	2.56	0.48
49:s:99:GLU:O	49:s:102:LYS:HB3	2.13	0.48
50:t:144:ARG:HA	50:t:144:ARG:HD2	1.63	0.48
55:y:58:TRP:O	55:y:63:TYR:HB3	2.13	0.48
56:z:715:LEU:HD13	56:z:715:LEU:HA	1.53	0.48
1:0:348:LEU:HD13	1:0:386:PHE:HZ	1.78	0.48
1:0:511:TYR:CD1	1:0:526:ILE:HG13	2.49	0.48
1:0:719:LEU:HB3	1:0:723:GLN:HE22	1.79	0.48
2:1:4:GLN:O	2:1:8:ILE:HG13	2.14	0.48
2:1:510:PRO:HG3	2:1:921:HIS:CE1	2.48	0.48
6:B:96:PRO:HG2	6:B:162:LEU:HG	1.96	0.48
6:B:110:PRO:HB2	6:B:176:GLU:OE2	2.13	0.48
6:B:787:GLY:O	6:B:790:GLN:HG3	2.14	0.48
17:M:376:TRP:HE1	20:P:189:ASN:HD22	1.59	0.48
21:Q:140:GLU:HB3	21:Q:144:LEU:HD23	1.95	0.48
22:R:176:PRO:O	22:R:178:SER:N	2.46	0.48
24:T:138:PRO:O	24:T:139:VAL:HG23	2.13	0.48
24:T:151:THR:O	24:T:152:ASN:C	2.56	0.48
28:X:191:PRO:HA	28:X:194:LEU:HB3	1.96	0.48
40:j:190:LEU:CD1	40:j:291:TRP:CD1	2.97	0.48
40:j:191:ARG:CZ	43:m:88:LEU:CG	2.91	0.48
40:j:392:MET:HG3	41:k:49:GLU:OE1	2.01	0.48
40:j:461:GLN:HG2	43:m:135:TYR:HB3	1.94	0.48
47:q:81:ASN:HA	47:q:84:GLN:OE1	2.14	0.48
48:r:166:TYR:CZ	48:r:170:PRO:HB3	2.49	0.48
48:r:568:TYR:CE1	48:r:641:LEU:HG	2.47	0.48
48:r:1178:THR:O	48:r:1180:SER:N	2.47	0.48
50:t:11:PRO:C	55:y:40:ARG:HH22	2.21	0.48
50:t:132:ARG:NH1	54:x:87:ALA:HB2	2.29	0.48
50:t:143:LYS:HB3	50:t:143:LYS:HE2	1.63	0.48
52:v:15:PHE:CD2	52:v:51:ILE:HD11	2.48	0.48
54:x:21:ASN:C	54:x:23:ILE:N	2.70	0.48
55:y:74:HIS:O	55:y:75:MET:C	2.55	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:935:GLU:O	2:1:939:GLU:HG2	2.14	0.48
3:2:202:ILE:HD12	3:2:205:ASN:HD21	1.79	0.48
3:2:957:LYS:HE3	3:2:967:VAL:HG21	1.94	0.48
5:A:533:PRO:HD3	5:A:654:HIS:CD2	2.49	0.48
6:B:992:ASN:ND2	14:J:43:TYR:HE1	2.10	0.48
7:C:133:ARG:HE	7:C:133:ARG:HA	1.79	0.48
8:D:66:ASN:OD1	43:m:13:THR:CG2	2.57	0.48
8:D:114:LEU:O	8:D:115:ILE:HD13	2.13	0.48
20:P:277:HIS:O	20:P:281:SER:OG	2.25	0.48
28:X:27:GLU:OE2	28:X:30:ARG:NH1	2.46	0.48
28:X:592:ARG:NH1	31:a:177:CYS:CA	2.67	0.48
30:Z:160:LEU:HA	30:Z:163:MET:HE3	1.94	0.48
40:j:588:SER:O	40:j:588:SER:OG	2.31	0.48
42:l:36:GLN:N	42:l:116:ARG:O	2.37	0.48
44:n:194:LEU:HD21	44:n:198:LEU:HD23	1.95	0.48
44:n:260:ASP:N	44:n:260:ASP:OD1	2.46	0.48
48:r:111:LYS:O	48:r:114:LYS:N	2.47	0.48
48:r:212:LEU:CD2	48:r:224:PHE:CD2	2.96	0.48
48:r:878:PRO:HD3	48:r:1179:HIS:NE2	2.28	0.48
49:s:63:ASN:O	49:s:66:LEU:HG	2.14	0.48
49:s:132:LEU:O	49:s:136:GLU:HG3	2.14	0.48
51:u:118:LEU:HD23	51:u:121:LEU:HD12	1.94	0.48
54:x:5:LEU:O	54:x:6:THR:C	2.56	0.48
54:x:18:GLN:NE2	54:x:65:THR:HA	2.28	0.48
55:y:84:PHE:O	55:y:87:GLU:N	2.47	0.48
1:0:216:ALA:HB1	1:0:230:THR:O	2.14	0.48
2:1:622:GLN:O	2:1:625:SER:OG	2.30	0.48
2:1:787:PRO:HG2	2:1:825:THR:OG1	2.13	0.48
3:2:628:VAL:O	3:2:636:ARG:NH2	2.47	0.48
5:A:68:THR:HB	19:O:12:ARG:NH1	2.29	0.48
5:A:467:MET:SD	5:A:524:MET:HE2	2.54	0.48
5:A:1120:GLY:H	5:A:1385:VAL:HG23	1.78	0.48
8:D:45:LYS:O	8:D:49:GLU:HB2	2.14	0.48
8:D:110:GLU:OE1	11:G:167:TYR:HB2	2.14	0.48
21:Q:14:LEU:HD13	21:Q:197:VAL:HG22	1.96	0.48
24:T:177:ARG:HG3	24:T:212:TYR:CE1	2.49	0.48
29:Y:377:LYS:HD2	32:b:286:GLU:HG3	1.94	0.48
30:Z:61:PHE:O	32:b:225:GLN:OE1	2.32	0.48
34:d:275:VAL:HG21	34:d:293:CYS:HB2	1.95	0.48
37:g:55:LEU:HB3	37:g:59:HIS:CD2	2.49	0.48
39:i:104:LEU:HD11	43:m:119:LEU:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:406:ARG:O	40:j:410:PRO:HD2	2.14	0.48
40:j:415:LYS:CG	40:j:416:ASN:N	2.76	0.48
42:l:148:VAL:HG12	44:n:217:TYR:HB3	1.96	0.48
43:m:29:ILE:HD11	43:m:68:ILE:HG23	1.95	0.48
43:m:111:GLU:OE1	45:o:146:ILE:HD13	2.14	0.48
48:r:51:LEU:HD11	48:r:102:LEU:HD11	1.95	0.48
48:r:95:LEU:HD13	53:w:127:LEU:HD12	1.96	0.48
48:r:963:LEU:O	48:r:967:VAL:HG23	2.13	0.48
49:s:124:ALA:O	49:s:125:VAL:C	2.57	0.48
50:t:84:SER:O	50:t:85:ILE:C	2.54	0.48
50:t:149:THR:O	50:t:152:ARG:HB3	2.13	0.48
51:u:70:HIS:HA	51:u:73:ILE:HG22	1.96	0.48
51:u:114:GLN:OE1	51:u:118:LEU:HG	2.14	0.48
51:u:127:THR:OG1	51:u:128:LYS:N	2.46	0.48
54:x:23:ILE:O	54:x:24:GLY:C	2.57	0.48
54:x:23:ILE:O	54:x:26:LEU:N	2.47	0.48
54:x:98:HIS:ND1	54:x:98:HIS:N	2.62	0.48
55:y:120:ALA:O	55:y:121:GLU:C	2.57	0.48
1:0:377:TYR:CD2	1:0:461:MET:HG2	2.49	0.47
2:1:1039:PRO:HB2	2:1:1088:PRO:HG2	1.95	0.47
2:1:1177:LEU:HD22	2:1:1243:PHE:HB3	1.96	0.47
3:2:210:GLN:CD	3:2:210:GLN:H	2.22	0.47
3:2:939:GLY:HA3	3:2:943:VAL:HB	1.96	0.47
5:A:394:VAL:HG11	5:A:440:LEU:HD13	1.94	0.47
5:A:660:MET:HE3	5:A:664:ILE:HG21	1.96	0.47
5:A:1265:ASP:HB3	5:A:1269:MET:HA	1.96	0.47
6:B:84:TYR:HE1	6:B:132:VAL:HG13	1.79	0.47
17:M:45:LEU:HD23	17:M:49:LYS:NZ	2.29	0.47
23:S:178:GLN:HG3	23:S:179:GLN:H	1.78	0.47
30:Z:123:LEU:HA	32:b:100:LYS:HE2	1.96	0.47
30:Z:400:ARG:CG	33:c:16:MET:CG	2.90	0.47
35:e:61:ARG:HH11	35:e:158:LEU:HA	1.79	0.47
36:f:146:TYR:HD1	36:f:149:LEU:HD23	1.78	0.47
37:g:40:PHE:CD2	37:g:105:ILE:HG12	2.49	0.47
40:j:618:LEU:HD12	56:z:684:ARG:HG2	1.96	0.47
46:p:94:SER:OG	46:p:95:SER:N	2.47	0.47
47:q:71:TYR:HB3	47:q:74:ARG:NE	2.28	0.47
48:r:452:LEU:HD13	48:r:467:LEU:HD22	1.96	0.47
48:r:922:TYR:CE2	48:r:1215:ILE:HG12	2.49	0.47
50:t:18:ILE:O	55:y:47:ALA:HB1	2.14	0.47
50:t:145:GLN:OE1	50:t:148:GLU:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:12:LEU:O	52:v:15:PHE:HB2	2.14	0.47
1:0:447:ASP:OD1	1:0:448:SER:N	2.47	0.47
2:1:47:PHE:O	2:1:51:LEU:N	2.47	0.47
2:1:325:GLY:C	2:1:327:SER:H	2.22	0.47
2:1:804:ASN:OD1	2:1:805:GLN:N	2.46	0.47
6:B:1133:HIS:O	11:G:155:ASN:ND2	2.47	0.47
10:F:57:MET:HE1	10:F:120:VAL:HG23	1.97	0.47
10:F:102:ILE:HG22	10:F:104:ILE:HG12	1.95	0.47
11:G:95:VAL:HG12	21:Q:163:GLU:HG3	1.95	0.47
21:Q:76:MET:HB2	21:Q:90:ASN:OD1	2.14	0.47
21:Q:99:LEU:O	21:Q:103:VAL:HG23	2.13	0.47
28:X:25:MET:HE3	28:X:51:SER:HB2	1.95	0.47
28:X:180:LEU:HD21	28:X:195:ALA:HB2	1.95	0.47
40:j:412:ALA:HB2	42:l:86:ILE:CD1	2.45	0.47
41:k:93:MET:O	41:k:98:ARG:NH1	2.47	0.47
44:n:53:ILE:HG23	56:z:626:LEU:HD21	1.95	0.47
47:q:32:SER:O	47:q:36:ILE:HG12	2.13	0.47
48:r:51:LEU:O	48:r:53:THR:N	2.47	0.47
48:r:327:GLU:O	48:r:336:SER:OG	2.23	0.47
48:r:1216:MET:HE1	48:r:1295:LYS:O	2.14	0.47
52:v:76:ASN:HB3	52:v:77:PRO:HD2	1.96	0.47
53:w:105:LEU:HD12	53:w:106:SER:N	2.28	0.47
55:y:21:GLU:O	55:y:22:LEU:C	2.54	0.47
1:0:95:ARG:HD2	1:0:136:TRP:HH2	1.78	0.47
1:0:812:ARG:HH22	46:p:92:GLN:NE2	2.12	0.47
2:1:440:ASN:HB3	2:1:442:LYS:NZ	2.30	0.47
2:1:1186:TYR:CE1	3:2:238:LYS:HG2	2.49	0.47
3:2:502:HIS:O	3:2:506:THR:HG22	2.14	0.47
4:3:27:ASN:OD1	4:3:147:ASN:HB3	2.13	0.47
4:3:65:GLN:HB3	4:3:128:PHE:HZ	1.78	0.47
5:A:551:ARG:HB3	5:A:625:ASP:OD2	2.13	0.47
5:A:1164:THR:OG1	5:A:1299:GLN:HB3	2.13	0.47
6:B:1125:MET:HB3	6:B:1171:MET:HE1	1.94	0.47
19:O:271:GLN:HE22	19:O:286:ARG:HB3	1.80	0.47
20:P:203:ARG:HG2	20:P:210:THR:HG22	1.95	0.47
22:R:225:VAL:HG13	22:R:226:ASP:OD2	2.14	0.47
27:W:591:GLN:OE1	27:W:595:ASN:ND2	2.47	0.47
29:Y:381:ARG:HG2	32:b:256:PHE:HB3	1.94	0.47
34:d:125:TYR:O	34:d:129:ASN:CB	2.61	0.47
36:f:186:ILE:H	36:f:186:ILE:HD12	1.79	0.47
37:g:38:ASN:OD1	37:g:41:TYR:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:140:ILE:HG13	40:j:146:LEU:HD22	1.96	0.47
39:i:20:GLU:HG2	39:i:58:HIS:CD2	2.48	0.47
40:j:195:LYS:C	40:j:195:LYS:CD	2.87	0.47
43:m:36:ILE:HG13	43:m:61:MET:SD	2.54	0.47
47:q:39:GLU:HA	47:q:42:GLN:OE1	2.14	0.47
48:r:65:GLU:OE2	48:r:66:LEU:N	2.48	0.47
48:r:925:ASP:OD1	48:r:937:ARG:HB3	2.14	0.47
48:r:944:PHE:N	48:r:944:PHE:HD1	2.12	0.47
48:r:1210:PHE:O	48:r:1214:VAL:HG23	2.14	0.47
49:s:109:GLN:HG3	49:s:110:LEU:N	2.28	0.47
50:t:82:ASN:O	50:t:86:LEU:HD12	2.14	0.47
55:y:45:ASP:O	55:y:46:LYS:C	2.57	0.47
1:0:16:ALA:HB3	1:0:454:VAL:O	2.13	0.47
1:0:345:THR:HG21	1:0:348:LEU:HD11	1.96	0.47
1:0:609:ASN:HD21	1:0:814:THR:HB	1.79	0.47
2:1:342:VAL:HA	2:1:347:ALA:HB3	1.96	0.47
2:1:728:ALA:HB2	2:1:873:SER:HB2	1.97	0.47
2:1:1044:LEU:HD13	2:1:1048:TYR:HE2	1.80	0.47
5:A:1620:PRO:HG2	38:h:104:VAL:HG11	1.94	0.47
6:B:104:ALA:HB2	19:O:216:SER:O	2.15	0.47
12:H:148:LEU:C	12:H:150:PHE:H	2.22	0.47
17:M:356:GLY:N	17:M:367:PHE:O	2.42	0.47
28:X:494:ILE:HD12	28:X:706:LEU:HD12	1.96	0.47
29:Y:384:HIS:HD2	32:b:259:ARG:CZ	2.28	0.47
30:Z:41:CYS:HB3	30:Z:118:LEU:CD2	2.42	0.47
40:j:574:PRO:HD3	40:j:578:TYR:O	2.14	0.47
41:k:99:HIS:HB2	41:k:183:SER:OG	2.15	0.47
45:o:89:ARG:HH22	48:r:737:ARG:HH12	1.62	0.47
49:s:179:ASP:CG	49:s:180:LEU:N	2.69	0.47
50:t:81:LEU:HD23	50:t:85:ILE:HD11	1.96	0.47
50:t:121:HIS:HA	50:t:124:ASN:HB2	1.95	0.47
52:v:52:ASP:OD1	52:v:53:LYS:N	2.48	0.47
52:v:52:ASP:O	52:v:56:GLN:HG3	2.14	0.47
52:v:65:LEU:HD12	52:v:65:LEU:H	1.79	0.47
52:v:121:MET:HE2	52:v:124:TYR:HD2	1.79	0.47
52:v:128:ARG:C	52:v:130:GLU:N	2.73	0.47
55:y:16:LEU:O	55:y:17:ARG:C	2.58	0.47
55:y:78:LEU:C	55:y:80:GLN:N	2.71	0.47
1:0:49:MET:HB3	1:0:63:HIS:ND1	2.29	0.47
1:0:170:LEU:HG	1:0:171:PHE:N	2.29	0.47
1:0:812:ARG:HH12	46:p:92:GLN:HE21	1.60	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:385:GLN:NE2	2:1:483:THR:HG22	2.29	0.47
2:1:517:SER:HB2	2:1:560:ALA:HB2	1.95	0.47
5:A:18:ILE:HG23	5:A:1451:MET:HE2	1.96	0.47
5:A:343:LEU:HD23	5:A:349:ARG:HB2	1.95	0.47
5:A:528:PRO:O	5:A:1397:HIS:HE1	1.97	0.47
5:A:1142:PHE:HB3	5:A:1356:ARG:HH21	1.80	0.47
5:A:1338:THR:HG22	5:A:1339:ASP:N	2.29	0.47
6:B:57:ARG:O	6:B:61:ASP:HB2	2.15	0.47
6:B:65:ILE:HG22	6:B:67:LEU:HD11	1.96	0.47
7:C:190:ASN:HD22	7:C:217:GLN:HE21	1.63	0.47
20:P:193:ASN:ND2	20:P:195:LYS:HB2	2.29	0.47
23:S:159:GLU:O	23:S:162:GLU:HG2	2.15	0.47
27:W:472:ARG:HD2	27:W:474:ASP:H	1.79	0.47
28:X:273:ILE:HG21	28:X:386:LEU:HD22	1.96	0.47
29:Y:449:ILE:HG21	29:Y:451:GLN:HG3	1.95	0.47
33:c:5:LEU:HD12	33:c:5:LEU:H	1.76	0.47
40:j:417:GLU:HG2	40:j:418:ILE:HG12	1.97	0.47
42:l:116:ARG:CZ	42:l:123:LEU:HD11	2.45	0.47
48:r:51:LEU:O	48:r:52:SER:C	2.57	0.47
48:r:298:SER:O	48:r:301:LEU:HG	2.14	0.47
48:r:814:THR:N	48:r:815:THR:HA	2.28	0.47
49:s:179:ASP:N	49:s:181:GLU:HB2	2.29	0.47
50:t:22:THR:HG22	50:t:23:ASP:H	1.79	0.47
50:t:74:HIS:CD2	50:t:77:GLU:HG2	2.49	0.47
52:v:90:ALA:HB3	52:v:91:LYS:NZ	2.29	0.47
55:y:32:ASN:O	55:y:33:TYR:C	2.58	0.47
55:y:91:ALA:O	55:y:92:GLN:C	2.54	0.47
3:2:447:SER:O	3:2:451:LEU:HD13	2.15	0.47
5:A:138:LYS:HE2	5:A:1441:GLU:HG3	1.95	0.47
5:A:1042:ASN:HB3	5:A:1046:ARG:NH2	2.30	0.47
5:A:1622:TYR:HE2	38:h:107:ASP:OD1	1.84	0.47
6:B:152:ILE:HD12	6:B:153:PRO:HD2	1.97	0.47
6:B:428:ASP:OD1	6:B:429:PHE:N	2.47	0.47
7:C:38:PHE:CE1	7:C:245:VAL:HA	2.48	0.47
9:E:104:ILE:HG13	9:E:129:GLN:HA	1.95	0.47
11:G:98:PHE:HA	11:G:107:PHE:HA	1.95	0.47
24:T:42:LYS:HZ1	24:T:59:ASN:HA	1.79	0.47
27:W:274:GLN:O	27:W:456:THR:HG23	2.15	0.47
28:X:486:ALA:HB2	28:X:736:LEU:HB2	1.97	0.47
35:e:110:THR:OG1	35:e:113:HIS:ND1	2.33	0.47
38:h:7:GLN:OE1	38:h:7:GLN:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:172:THR:O	41:k:28:LEU:HG	2.14	0.47
40:j:336:PHE:CZ	40:j:500:GLU:HG3	2.47	0.47
43:m:117:ILE:CG1	47:q:174:LEU:HD23	2.44	0.47
46:p:173:ASP:HA	46:p:176:THR:HG22	1.96	0.47
48:r:55:ILE:O	48:r:58:LEU:HD22	2.15	0.47
48:r:122:LEU:O	48:r:124:GLN:N	2.48	0.47
48:r:128:LEU:HD21	50:t:105:ARG:NH2	2.30	0.47
48:r:885:LEU:HD21	48:r:1186:LEU:HD22	1.97	0.47
49:s:188:GLY:HA2	49:s:191:ASN:ND2	2.29	0.47
50:t:16:GLN:HG3	50:t:17:TYR:HD1	1.77	0.47
50:t:137:VAL:O	50:t:138:MET:C	2.55	0.47
52:v:94:GLN:O	52:v:98:LYS:HG2	2.14	0.47
53:w:92:ALA:O	53:w:96:PHE:CA	2.62	0.47
54:x:83:ALA:C	54:x:86:GLN:HE21	2.23	0.47
55:y:14:ASN:O	55:y:18:PHE:CD2	2.67	0.47
1:0:92:SER:HB2	4:3:78:PRO:O	2.14	0.47
1:0:111:ALA:O	1:0:112:ASP:C	2.56	0.47
1:0:132:VAL:CG2	1:0:182:VAL:HB	2.44	0.47
1:0:247:SER:C	1:0:249:VAL:H	2.23	0.47
1:0:264:PHE:HB2	3:2:630:MET:SD	2.55	0.47
1:0:743:GLN:HG3	1:0:746:GLN:HB2	1.96	0.47
2:1:35:THR:O	2:1:38:ILE:HG22	2.14	0.47
2:1:426:THR:O	2:1:430:ILE:HG12	2.15	0.47
2:1:1258:ARG:HE	2:1:1258:ARG:HB3	1.55	0.47
3:2:7:LYS:HE2	3:2:11:LEU:HD21	1.96	0.47
3:2:243:THR:O	3:2:247:VAL:HG23	2.15	0.47
4:3:19:VAL:O	4:3:142:CYS:HA	2.14	0.47
4:3:116:GLU:OE1	4:3:157:GLU:HB3	2.15	0.47
4:3:188:LEU:HD23	4:3:188:LEU:HA	1.74	0.47
5:A:322:LEU:O	5:A:327:ARG:NH2	2.48	0.47
5:A:865:ILE:HD13	6:B:1092:ASP:HB3	1.97	0.47
5:A:959:MET:HE2	5:A:959:MET:HB3	1.81	0.47
5:A:1146:GLN:HE22	5:A:1150:ASP:HB2	1.79	0.47
5:A:1201:ASP:O	5:A:1202:PHE:HB2	2.15	0.47
5:A:1428:MET:HE3	5:A:1432:PHE:CE1	2.50	0.47
5:A:1622:TYR:OH	37:g:118:ARG:CZ	2.53	0.47
6:B:835:GLU:O	6:B:836:THR:OG1	2.30	0.47
9:E:41:LYS:HE3	9:E:47:LYS:HD2	1.96	0.47
9:E:171:PRO:HB2	9:E:207:ARG:HG2	1.96	0.47
11:G:14:HIS:CD2	11:G:16:ARG:H	2.33	0.47
17:M:335:VAL:HG22	17:M:358:MET:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:376:TRP:O	20:P:205:ARG:NE	2.41	0.47
20:P:222:THR:OG1	26:V:79:DT:O2	2.33	0.47
20:P:226:SER:HB3	20:P:229:GLN:HB2	1.96	0.47
21:Q:114:ILE:O	21:Q:174:ARG:NH2	2.47	0.47
21:Q:179:ARG:HA	21:Q:182:GLU:HG2	1.96	0.47
23:S:28:ILE:HG12	23:S:140:VAL:HG21	1.97	0.47
24:T:206:THR:O	24:T:207:LYS:HD2	2.15	0.47
27:W:187:HIS:HD2	27:W:289:TYR:HE2	1.63	0.47
27:W:354:ALA:HB3	27:W:378:PHE:HZ	1.79	0.47
27:W:521:GLU:HG3	27:W:713:LEU:HD11	1.96	0.47
28:X:305:LEU:CD2	28:X:391:LEU:CD1	2.79	0.47
28:X:567:LEU:HA	28:X:595:ILE:HG23	1.96	0.47
29:Y:384:HIS:CD2	32:b:259:ARG:NH1	2.82	0.47
31:a:257:HIS:HB3	32:b:248:HIS:CE1	2.49	0.47
35:e:136:ARG:NH1	35:e:160:LYS:HD3	2.29	0.47
36:f:171:LEU:O	36:f:175:LYS:HG3	2.15	0.47
39:i:78:PRO:CG	40:j:197:ARG:CG	2.93	0.47
40:j:205:GLY:O	40:j:222:PHE:N	2.48	0.47
40:j:260:SER:N	40:j:368:LEU:HG	2.30	0.47
40:j:410:PRO:C	42:l:86:ILE:HG21	2.38	0.47
40:j:440:LEU:C	40:j:440:LEU:CD2	2.88	0.47
40:j:525:LEU:O	40:j:529:MET:HG2	2.15	0.47
41:k:171:LEU:HD21	41:k:189:PHE:HD2	1.78	0.47
44:n:99:ASP:N	44:n:99:ASP:OD1	2.46	0.47
48:r:68:VAL:C	48:r:70:THR:N	2.71	0.47
48:r:77:SER:HB3	48:r:80:GLU:CD	2.40	0.47
48:r:91:ARG:NH2	53:w:127:LEU:HD22	2.27	0.47
48:r:142:ASP:O	48:r:143:ALA:C	2.56	0.47
48:r:158:ILE:O	48:r:161:LEU:HB2	2.15	0.47
48:r:324:VAL:HA	48:r:338:SER:O	2.14	0.47
48:r:685:LEU:CD2	56:z:681:GLU:OE2	2.63	0.47
48:r:1315:ASP:OD1	48:r:1436:PHE:N	2.48	0.47
48:r:1324:LEU:HG	48:r:1325:PHE:CE1	2.49	0.47
49:s:86:GLN:O	49:s:90:HIS:HB3	2.15	0.47
49:s:127:GLN:C	49:s:131:LYS:HZ2	2.20	0.47
49:s:138:ALA:O	49:s:139:ARG:NE	2.47	0.47
49:s:179:ASP:HA	49:s:182:MET:HB2	1.97	0.47
50:t:122:LEU:O	50:t:125:GLU:HB2	2.15	0.47
51:u:122:ARG:O	51:u:126:ARG:HG3	2.14	0.47
54:x:54:TYR:HA	54:x:57:LEU:CD1	2.42	0.47
54:x:114:LEU:O	54:x:115:LEU:C	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:y:15:ARG:O	55:y:18:PHE:HB2	2.15	0.47
55:y:46:LYS:O	55:y:47:ALA:C	2.58	0.47
55:y:94:ALA:O	55:y:98:ASP:OD1	2.31	0.47
55:y:116:GLN:O	55:y:119:LEU:HB2	2.14	0.47
1:0:17:TYR:CZ	1:0:70:PRO:HG3	2.49	0.47
1:0:60:ARG:HH21	1:0:60:ARG:CG	2.19	0.47
1:0:100:ASP:O	1:0:130:PRO:HD2	2.15	0.47
1:0:111:ALA:HB3	1:0:117:SER:O	2.15	0.47
1:0:142:LYS:HD2	1:0:143:LEU:N	2.30	0.47
1:0:730:ASP:OD1	1:0:784:ARG:NH1	2.47	0.47
1:0:832:LEU:CD2	1:0:832:LEU:N	2.72	0.47
2:1:824:ARG:HA	2:1:868:CYS:SG	2.55	0.47
2:1:936:GLY:O	2:1:940:GLN:HG2	2.14	0.47
4:3:27:ASN:O	4:3:30:PRO:HD2	2.15	0.47
4:3:71:PHE:HB3	4:3:82:VAL:HG12	1.97	0.47
5:A:467:MET:SD	5:A:524:MET:HB3	2.54	0.47
5:A:814:ASP:OD2	6:B:689:TYR:OH	2.30	0.47
6:B:954:MET:HE3	6:B:954:MET:HB3	1.82	0.47
7:C:73:LEU:O	7:C:238:SER:OG	2.26	0.47
17:M:22:ILE:HD13	17:M:43:LYS:HE3	1.97	0.47
17:M:311:GLU:OE2	20:P:235:ARG:NH2	2.48	0.47
20:P:166:GLN:HB3	26:V:81:DA:H5''	1.97	0.47
20:P:333:LYS:HE3	20:P:333:LYS:HB3	1.76	0.47
22:R:103:LEU:HA	22:R:106:THR:HG22	1.96	0.47
23:S:118:VAL:HG13	23:S:119:THR:HG23	1.95	0.47
24:T:24:PRO:HD3	24:T:116:CYS:HB2	1.96	0.47
24:T:186:MET:SD	24:T:187:LEU:N	2.88	0.47
26:V:74:DC:H2''	26:V:75:DC:H5'	1.96	0.47
40:j:617:HIS:CE1	48:r:741:PRO:CB	2.98	0.47
43:m:130:LEU:C	47:q:160:MET:HE3	2.11	0.47
44:n:281:CYS:SG	44:n:306:HIS:CE1	3.08	0.47
48:r:154:ILE:O	48:r:155:PRO:C	2.56	0.47
48:r:165:SER:N	48:r:168:ARG:HH12	2.13	0.47
48:r:169:LEU:HD21	48:r:176:LYS:H	1.78	0.47
50:t:75:LYS:N	50:t:77:GLU:OE1	2.48	0.47
52:v:91:LYS:O	52:v:95:VAL:HG12	2.14	0.47
54:x:74:ASP:C	54:x:76:LEU:N	2.70	0.47
55:y:90:ASN:HB2	55:y:92:GLN:OE1	2.14	0.47
55:y:122:GLN:HA	55:y:125:GLN:OE1	2.15	0.47
1:0:60:ARG:HG2	1:0:60:ARG:NH2	2.25	0.47
1:0:70:PRO:O	1:0:71:TRP:CG	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:516:ALA:HA	1:0:519:GLN:CD	2.40	0.47
2:1:568:SER:O	2:1:572:VAL:HG23	2.15	0.47
2:1:712:CYS:O	2:1:716:LEU:HG	2.15	0.47
2:1:835:SER:HA	2:1:881:VAL:HG11	1.97	0.47
5:A:125:LYS:O	5:A:129:ILE:HG12	2.14	0.47
5:A:917:GLU:HG2	5:A:956:PHE:CZ	2.50	0.47
5:A:1369:LEU:HD23	9:E:139:ILE:HG23	1.96	0.47
18:N:68:CYS:SG	18:N:69:ASP:N	2.86	0.47
20:P:239:ARG:HE	20:P:243:LYS:HG3	1.79	0.47
24:T:10:THR:HA	24:T:105:SER:HA	1.96	0.47
24:T:131:GLN:O	24:T:135:SER:HB3	2.15	0.47
27:W:177:VAL:O	27:W:269:SER:HA	2.15	0.47
27:W:292:LEU:HG	27:W:294:GLU:CD	2.38	0.47
28:X:530:VAL:HG21	28:X:714:VAL:HG13	1.96	0.47
28:X:619:ILE:HA	28:X:678:VAL:HG22	1.97	0.47
29:Y:428:SER:HB2	30:Z:64:GLN:HE21	1.79	0.47
34:d:264:GLU:HG2	34:d:265:MET:N	2.30	0.47
37:g:130:PHE:HD1	38:h:49:PHE:HD2	1.61	0.47
40:j:548:VAL:HG23	40:j:572:ALA:HB2	1.97	0.47
48:r:524:ASN:OD1	48:r:528:HIS:ND1	2.48	0.47
48:r:894:THR:OG1	48:r:895:GLN:N	2.48	0.47
48:r:1230:GLN:CD	48:r:1244:THR:HA	2.40	0.47
49:s:187:LEU:HD13	55:y:23:GLU:HB3	1.96	0.47
50:t:85:ILE:O	50:t:86:LEU:C	2.55	0.47
50:t:139:MET:O	50:t:142:GLN:HB2	2.15	0.47
51:u:119:GLN:O	51:u:123:GLU:HG2	2.14	0.47
52:v:25:ILE:HG21	52:v:40:LYS:HZ3	1.80	0.47
52:v:76:ASN:H	53:w:104:LYS:HB3	1.79	0.47
52:v:83:GLU:HB2	52:v:87:ARG:NH2	2.30	0.47
53:w:103:GLU:C	53:w:107:ASN:H	2.20	0.47
53:w:127:LEU:HD23	53:w:128:ARG:H	1.80	0.47
55:y:26:GLN:NE2	55:y:67:LEU:HA	2.30	0.47
55:y:73:LEU:CG	55:y:74:HIS:N	2.78	0.47
55:y:116:GLN:HA	55:y:119:LEU:CD1	2.44	0.47
56:z:691:VAL:HG23	56:z:708:CYS:HB3	1.97	0.47
2:1:51:LEU:HD12	2:1:52:SER:H	1.81	0.47
3:2:909:SER:HB3	3:2:952:VAL:HG21	1.96	0.47
4:3:65:GLN:CB	4:3:128:PHE:CZ	2.98	0.47
5:A:26:LEU:HD21	5:A:34:MET:HE1	1.96	0.47
5:A:36:VAL:HA	6:B:1138:ARG:NH1	2.29	0.47
5:A:618:TYR:OH	12:H:29:HIS:CE1	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1243:LEU:HD11	5:A:1288:ILE:HG21	1.96	0.47
11:G:127:CYS:SG	11:G:129:LYS:HD3	2.55	0.47
15:K:88:THR:O	15:K:91:ILE:HG22	2.15	0.47
20:P:174:LEU:HD13	20:P:241:VAL:HG11	1.96	0.47
20:P:195:LYS:HE3	24:T:172:ASP:H	1.80	0.47
21:Q:140:GLU:OE1	21:Q:140:GLU:N	2.48	0.47
27:W:511:TRP:HH2	30:Z:348:ARG:HH12	1.61	0.47
31:a:76:LEU:HD23	31:a:80:ARG:HG2	1.96	0.47
35:e:62:GLU:OE2	35:e:157:GLY:N	2.48	0.47
37:g:50:VAL:HG21	37:g:60:LEU:HD23	1.96	0.47
40:j:465:SER:OG	40:j:466:ASN:N	2.45	0.47
44:n:298:ASP:HB2	44:n:305:PHE:CZ	2.50	0.47
48:r:274:ILE:O	48:r:278:VAL:HG22	2.14	0.47
48:r:410:HIS:O	48:r:414:GLN:HG2	2.15	0.47
48:r:1226:GLN:OE1	48:r:1227:GLU:HG3	2.15	0.47
50:t:106:GLU:HA	50:t:109:LEU:HD23	1.97	0.47
50:t:126:TYR:N	50:t:126:TYR:CD1	2.82	0.47
50:t:133:GLU:HA	50:t:136:ARG:HG2	1.97	0.47
50:t:143:LYS:N	50:t:146:ARG:NE	2.59	0.47
53:w:103:GLU:O	53:w:104:LYS:C	2.56	0.47
54:x:83:ALA:C	54:x:86:GLN:HG2	2.40	0.47
55:y:25:VAL:C	55:y:27:CYS:N	2.71	0.47
1:0:478:LEU:HD22	1:0:529:MET:HE3	1.97	0.46
2:1:789:PHE:HE2	2:1:811:LEU:HG	1.80	0.46
2:1:1173:SER:O	2:1:1173:SER:OG	2.32	0.46
5:A:487:SER:O	5:A:535:MET:HB2	2.15	0.46
5:A:609:HIS:HD2	5:A:610:PRO:HD2	1.80	0.46
6:B:1066:PRO:HG2	6:B:1075:MET:O	2.14	0.46
7:C:37:VAL:HG11	7:C:252:LEU:HD13	1.97	0.46
16:L:32:ASP:OD1	16:L:32:ASP:N	2.48	0.46
20:P:186:ARG:HH21	20:P:244:LEU:HA	1.80	0.46
20:P:235:ARG:HG3	20:P:250:PHE:CD1	2.50	0.46
25:U:57:DC:H42	26:V:37:DG:H22	1.61	0.46
27:W:438:MET:HE2	27:W:440:LEU:HD21	1.96	0.46
29:Y:421:VAL:CG2	32:b:39:ASP:HB3	2.44	0.46
36:f:178:TYR:CE2	36:f:228:MET:HG2	2.50	0.46
37:g:118:ARG:HH11	40:j:111:VAL:HG11	1.79	0.46
40:j:479:ILE:HD11	40:j:529:MET:CE	2.28	0.46
40:j:569:ILE:HG12	40:j:583:ARG:HA	1.95	0.46
40:j:614:LYS:HE2	40:j:615:TRP:NE1	2.30	0.46
44:n:108:LEU:HD21	46:p:129:GLN:HE22	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:78:ASP:C	48:r:82:LYS:HZ3	2.23	0.46
48:r:82:LYS:O	48:r:85:ILE:HG22	2.15	0.46
48:r:155:PRO:HB2	48:r:156:TYR:CD1	2.50	0.46
48:r:169:LEU:HB2	48:r:172:CYS:C	2.40	0.46
48:r:270:GLN:H	48:r:270:GLN:CD	2.23	0.46
49:s:148:ILE:C	49:s:151:TYR:HB3	2.40	0.46
52:v:6:ASP:O	52:v:9:GLU:HB2	2.15	0.46
52:v:9:GLU:O	52:v:12:LEU:N	2.48	0.46
53:w:83:LEU:O	53:w:86:HIS:N	2.49	0.46
1:0:39:TRP:HD1	1:0:40:SER:O	1.98	0.46
1:0:479:GLU:O	1:0:483:VAL:HG23	2.16	0.46
2:1:1072:ILE:HD11	2:1:1126:LEU:HD13	1.97	0.46
3:2:573:LYS:C	3:2:575:HIS:H	2.23	0.46
4:3:45:GLU:CD	4:3:51:PRO:CD	2.89	0.46
4:3:170:VAL:HA	4:3:173:ILE:HG22	1.97	0.46
5:A:413:TYR:HB3	5:A:414:PRO:HD3	1.95	0.46
5:A:663:ASP:O	5:A:666:ARG:HG3	2.15	0.46
6:B:47:PHE:CE2	6:B:51:ILE:HD13	2.50	0.46
6:B:267:VAL:HG13	6:B:320:PHE:HE2	1.81	0.46
6:B:268:PRO:HB2	6:B:271:ILE:HD12	1.96	0.46
6:B:834:ARG:HG3	6:B:835:GLU:N	2.30	0.46
8:D:142:TYR:OH	43:m:21:ARG:N	2.47	0.46
9:E:25:GLY:HA3	9:E:65:ASN:HD21	1.81	0.46
12:H:39:LEU:HA	12:H:124:ARG:O	2.14	0.46
18:N:78:ASP:HB2	18:N:93:VAL:HG21	1.96	0.46
27:W:167:LYS:HD3	27:W:294:GLU:CG	2.45	0.46
27:W:364:LEU:HD21	27:W:413:LEU:HD22	1.97	0.46
28:X:403:PHE:HE1	28:X:435:PHE:HB2	1.80	0.46
29:Y:504:LYS:C	29:Y:508:PHE:HD2	2.17	0.46
30:Z:56:VAL:HG13	30:Z:110:LEU:HD21	1.96	0.46
30:Z:240:LEU:HD11	30:Z:265:LEU:HD21	1.97	0.46
38:h:114:ASP:O	38:h:118:GLU:N	2.44	0.46
39:i:82:SER:HB3	40:j:211:SER:HB2	1.96	0.46
40:j:209:TYR:HB2	40:j:214:SER:HB3	1.97	0.46
40:j:624:GLU:O	47:q:116:PRO:HB3	2.15	0.46
42:l:76:PHE:CE1	42:l:86:ILE:CG2	2.97	0.46
45:o:45:VAL:HG22	45:o:49:GLU:OE2	2.16	0.46
45:o:112:LYS:O	45:o:115:VAL:HG12	2.15	0.46
48:r:69:LEU:O	48:r:72:LEU:C	2.58	0.46
48:r:93:ARG:HG2	52:v:19:ILE:HB	1.98	0.46
48:r:136:LEU:O	48:r:139:LEU:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:209:PRO:HD3	48:r:290:GLN:NE2	2.29	0.46
49:s:124:ALA:O	49:s:127:GLN:N	2.48	0.46
50:t:17:TYR:OH	55:y:17:ARG:HD2	2.14	0.46
50:t:152:ARG:HD3	50:t:153:PHE:N	2.30	0.46
51:u:66:LEU:N	51:u:67:PRO:HD2	2.30	0.46
52:v:119:GLU:HA	52:v:121:MET:HG2	1.97	0.46
1:0:132:VAL:HG11	1:0:182:VAL:HB	1.96	0.46
2:1:387:ASN:OD1	2:1:388:ALA:N	2.48	0.46
2:1:760:VAL:HG21	2:1:829:PHE:CE1	2.51	0.46
2:1:938:ALA:O	2:1:941:VAL:HG12	2.15	0.46
3:2:183:LEU:HB3	3:2:979:ARG:HH11	1.79	0.46
3:2:186:ALA:O	3:2:190:THR:HG23	2.15	0.46
5:A:1020:LEU:HD13	5:A:1041:PHE:HE2	1.79	0.46
5:A:1623:SER:HA	5:A:1624:PRO:HD2	1.34	0.46
10:F:44:ARG:HB3	10:F:115:TYR:CD2	2.50	0.46
21:Q:112:ARG:O	21:Q:115:GLU:HG2	2.16	0.46
22:R:176:PRO:C	22:R:178:SER:H	2.24	0.46
27:W:109:ARG:CZ	27:W:492:ASN:CB	2.93	0.46
27:W:125:ALA:CB	27:W:487:LYS:O	2.64	0.46
30:Z:159:VAL:HG12	30:Z:163:MET:HE2	1.96	0.46
30:Z:313:TYR:HE2	30:Z:394:TRP:HZ2	1.56	0.46
31:a:256:GLN:NE2	32:b:252:ARG:HH11	2.14	0.46
33:c:6:LYS:N	33:c:6:LYS:CE	2.78	0.46
39:i:14:LEU:O	39:i:17:ILE:HG22	2.16	0.46
42:l:43:CYS:SG	42:l:44:GLU:N	2.88	0.46
48:r:78:ASP:O	48:r:82:LYS:NZ	2.48	0.46
49:s:98:LYS:O	49:s:102:LYS:CB	2.63	0.46
49:s:126:TYR:O	49:s:129:LYS:HG2	2.14	0.46
51:u:125:VAL:O	51:u:126:ARG:C	2.57	0.46
52:v:17:GLU:O	52:v:20:ARG:N	2.48	0.46
52:v:96:LYS:HA	52:v:99:ILE:HG12	1.98	0.46
53:w:93:TYR:O	53:w:94:ASN:C	2.58	0.46
54:x:15:LEU:O	54:x:19:PHE:CE2	2.68	0.46
55:y:19:GLN:O	55:y:22:LEU:HB3	2.16	0.46
1:0:105:ILE:HG21	1:0:179:TRP:CE3	2.51	0.46
1:0:107:CYS:HB3	1:0:122:VAL:O	2.15	0.46
1:0:437:SER:OG	1:0:438:TRP:N	2.48	0.46
2:1:213:ARG:HH11	3:2:757:ARG:HH22	1.64	0.46
2:1:751:GLU:OE1	2:1:755:ASN:HB2	2.16	0.46
3:2:182:LYS:HA	3:2:185:GLU:C	2.40	0.46
3:2:628:VAL:HG21	3:2:640:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:698:TRP:CG	3:2:699:ASN:N	2.84	0.46
3:2:915:ARG:CZ	56:z:702:GLY:H	2.27	0.46
3:2:957:LYS:HD3	3:2:967:VAL:HG21	1.98	0.46
5:A:204:HIS:HB3	5:A:208:ASP:O	2.15	0.46
5:A:479:TRP:CZ3	15:K:67:LEU:HD12	2.50	0.46
5:A:1216:LEU:N	5:A:1255:LEU:HD12	2.31	0.46
7:C:108:ASN:O	7:C:155:LYS:NZ	2.48	0.46
8:D:78:GLU:CD	38:h:48:SER:HA	2.41	0.46
12:H:65:TYR:H	12:H:70:LEU:HD11	1.80	0.46
27:W:77:TRP:CE3	30:Z:341:MET:CE	2.97	0.46
27:W:124:TYR:CE1	27:W:292:LEU:HA	2.47	0.46
28:X:193:PHE:CE2	28:X:302:ASP:CG	2.93	0.46
36:f:255:MET:O	36:f:259:VAL:HG23	2.15	0.46
39:i:12:ARG:NE	39:i:12:ARG:HA	2.31	0.46
39:i:36:SER:HB3	40:j:153:LEU:HD22	1.97	0.46
40:j:409:GLY:O	42:l:86:ILE:CG2	2.63	0.46
40:j:546:TRP:CZ3	40:j:643:MET:HE3	2.50	0.46
42:l:146:PRO:HB2	44:n:239:PHE:HE2	1.80	0.46
48:r:143:ALA:O	48:r:144:LEU:C	2.57	0.46
48:r:185:LYS:O	48:r:185:LYS:HG2	2.16	0.46
48:r:641:LEU:CD1	48:r:644:PHE:HB2	2.36	0.46
49:s:92:GLU:HA	49:s:95:VAL:HG22	1.96	0.46
50:t:145:GLN:O	50:t:145:GLN:OE1	2.33	0.46
51:u:123:GLU:HA	51:u:127:THR:HG23	1.97	0.46
52:v:86:GLU:O	52:v:89:LEU:HB2	2.16	0.46
1:0:61:MET:HE3	1:0:75:SER:CB	2.45	0.46
1:0:521:VAL:HG13	4:3:74:VAL:HG21	1.98	0.46
2:1:297:CYS:O	2:1:301:GLU:HG2	2.15	0.46
2:1:569:ARG:NH2	2:1:911:HIS:O	2.48	0.46
2:1:1044:LEU:HD13	2:1:1048:TYR:CE2	2.51	0.46
3:2:189:TRP:O	3:2:192:ILE:HG12	2.16	0.46
3:2:196:LEU:HA	3:2:199:LEU:HB3	1.97	0.46
5:A:460:ARG:HD2	5:A:492:TYR:O	2.16	0.46
5:A:721:HIS:HE1	13:I:98:GLN:HE21	1.63	0.46
5:A:1236:ASN:O	5:A:1240:GLY:N	2.37	0.46
5:A:1346:VAL:O	5:A:1352:VAL:HG11	2.15	0.46
6:B:764:MET:HE1	6:B:938:ARG:NH1	2.31	0.46
6:B:779:ILE:HG13	14:J:47:ARG:NH1	2.30	0.46
7:C:74:ILE:O	7:C:128:ILE:HG13	2.15	0.46
8:D:27:GLU:OE2	8:D:28:THR:OG1	2.34	0.46
9:E:160:LEU:HD21	9:E:167:GLU:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:36:GLU:O	17:M:40:MET:HG2	2.16	0.46
19:O:29:ALA:O	19:O:31:ASP:N	2.47	0.46
20:P:328:ILE:HA	20:P:331:ILE:HD12	1.98	0.46
23:S:117:GLY:HA2	23:S:120:GLU:OE1	2.15	0.46
27:W:109:ARG:NH1	27:W:492:ASN:CG	2.73	0.46
27:W:469:THR:HB	27:W:634:ARG:CB	2.44	0.46
28:X:292:LEU:CD2	28:X:318:ALA:O	2.63	0.46
28:X:304:HIS:ND1	28:X:380:ARG:NH2	2.64	0.46
28:X:305:LEU:CD2	28:X:391:LEU:HD13	2.43	0.46
30:Z:123:LEU:HD23	32:b:100:LYS:HE2	1.98	0.46
30:Z:171:VAL:HG13	30:Z:175:LEU:HB3	1.98	0.46
30:Z:409:TYR:CD1	33:c:4:VAL:CG1	2.99	0.46
31:a:60:HIS:HD2	31:a:163:THR:HG21	1.80	0.46
32:b:250:ASP:HB2	32:b:252:ARG:HG2	1.97	0.46
38:h:152:GLU:O	38:h:156:LYS:HG3	2.16	0.46
39:i:32:ILE:HG22	40:j:157:ALA:HB2	1.98	0.46
40:j:489:LYS:HZ2	44:n:256:PRO:HD3	1.81	0.46
42:l:146:PRO:HB3	44:n:236:TYR:CG	2.50	0.46
48:r:70:THR:O	48:r:73:LEU:HB3	2.16	0.46
49:s:124:ALA:HB2	50:t:153:PHE:CE2	2.51	0.46
50:t:17:TYR:CD1	50:t:17:TYR:N	2.72	0.46
50:t:132:ARG:O	50:t:133:GLU:C	2.58	0.46
51:u:118:LEU:O	51:u:122:ARG:HD3	2.15	0.46
52:v:67:VAL:CG2	52:v:70:TYR:CD2	2.99	0.46
54:x:60:ALA:O	54:x:62:ILE:C	2.55	0.46
55:y:74:HIS:HA	55:y:77:GLU:HG3	1.96	0.46
1:0:161:ARG:NH2	4:3:156:VAL:O	2.47	0.46
1:0:272:ASN:HB3	1:0:273:ARG:NH2	2.31	0.46
2:1:55:SER:O	2:1:55:SER:OG	2.29	0.46
2:1:631:ALA:HB2	2:1:645:VAL:HG21	1.98	0.46
2:1:764:TYR:CZ	2:1:768:LYS:HD3	2.50	0.46
2:1:794:TRP:CD1	2:1:829:PHE:HE2	2.34	0.46
5:A:100:LEU:HD12	5:A:100:LEU:HA	1.77	0.46
5:A:132:LYS:HD3	5:A:133:SER:N	2.29	0.46
5:A:790:GLN:NE2	5:A:797:ARG:HG2	2.30	0.46
5:A:1316:ASN:OD1	5:A:1317:LYS:N	2.49	0.46
5:A:1471:PHE:CE1	10:F:64:ARG:HD3	2.51	0.46
6:B:217:TYR:CE2	6:B:376:ALA:HA	2.50	0.46
6:B:811:TYR:CE1	6:B:924:ARG:HB2	2.51	0.46
9:E:54:ARG:HA	9:E:58:LEU:HD22	1.96	0.46
19:O:137:ARG:HH21	19:O:170:GLN:HB3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:178:GLN:C	23:S:180:ARG:H	2.23	0.46
24:T:131:GLN:O	24:T:135:SER:CB	2.63	0.46
27:W:121:TYR:CE2	27:W:486:PRO:HA	2.44	0.46
28:X:726:GLN:NE2	31:a:223:LEU:HG	2.30	0.46
36:f:266:ARG:HB2	36:f:269:GLU:HB3	1.98	0.46
42:l:126:VAL:HG22	42:l:140:VAL:HG12	1.98	0.46
47:q:83:ARG:O	47:q:87:VAL:HG23	2.16	0.46
48:r:105:TRP:C	48:r:107:ASN:H	2.23	0.46
48:r:188:LYS:CE	48:r:188:LYS:CA	2.91	0.46
48:r:514:THR:CG2	48:r:540:ILE:HG23	2.44	0.46
50:t:147:LEU:O	50:t:151:GLU:HG3	2.15	0.46
52:v:63:VAL:HG13	52:v:68:PHE:CE2	2.50	0.46
53:w:128:ARG:HD2	53:w:131:ILE:HB	1.97	0.46
54:x:65:THR:OG1	54:x:66:ALA:N	2.48	0.46
54:x:100:ALA:O	54:x:101:ALA:C	2.58	0.46
55:y:96:PHE:CD1	55:y:96:PHE:N	2.82	0.46
1:0:619:GLN:NE2	1:0:675:VAL:H	2.14	0.46
2:1:144:LYS:O	2:1:147:THR:OG1	2.34	0.46
3:2:794:ASP:OD2	3:2:797:LYS:HG2	2.16	0.46
4:3:113:LEU:HA	4:3:151:TYR:HB2	1.97	0.46
5:A:36:VAL:HG12	5:A:61:ARG:HB3	1.97	0.46
5:A:1322:ILE:HG12	5:A:1328:PHE:CE1	2.51	0.46
6:B:59:VAL:HG22	6:B:408:PHE:CZ	2.51	0.46
6:B:235:ILE:HD11	6:B:347:MET:HA	1.98	0.46
6:B:310:VAL:HG23	6:B:311:ILE:HD12	1.96	0.46
6:B:400:LEU:HD22	6:B:444:LEU:HD22	1.98	0.46
6:B:605:ARG:NH2	13:I:74:GLN:OE1	2.47	0.46
6:B:785:TYR:CE1	6:B:955:PRO:HG3	2.50	0.46
6:B:789:ASN:HA	6:B:793:SER:HB3	1.98	0.46
11:G:86:ASP:OD1	11:G:144:ARG:NH1	2.49	0.46
17:M:49:LYS:NZ	18:N:18:SER:HB2	2.25	0.46
20:P:240:VAL:O	20:P:244:LEU:HG	2.16	0.46
23:S:100:LEU:HD23	23:S:101:ARG:N	2.31	0.46
24:T:195:GLN:HG3	24:T:196:TYR:CD2	2.51	0.46
29:Y:411:MET:O	32:b:120:THR:HG21	2.13	0.46
31:a:292:PRO:HB2	32:b:264:ILE:CD1	2.46	0.46
40:j:147:ILE:O	40:j:151:LYS:HG2	2.16	0.46
40:j:464:TRP:CG	40:j:475:VAL:CG2	2.99	0.46
40:j:573:SER:OG	40:j:574:PRO:CD	2.61	0.46
48:r:72:LEU:HA	48:r:75:ARG:HB2	1.97	0.46
48:r:327:GLU:HB2	48:r:336:SER:OG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:128:ALA:O	49:s:131:LYS:CA	2.64	0.46
50:t:120:HIS:O	50:t:121:HIS:C	2.58	0.46
50:t:139:MET:HE3	54:x:97:ASN:ND2	2.30	0.46
50:t:154:GLN:HA	50:t:157:LEU:HD23	1.97	0.46
55:y:39:GLN:NE2	55:y:89:VAL:C	2.74	0.46
55:y:69:TYR:C	55:y:71:GLN:H	2.23	0.46
2:1:423:PHE:HE1	2:1:458:LEU:HD13	1.80	0.46
3:2:168:THR:O	3:2:173:LYS:HB2	2.16	0.46
3:2:176:ALA:HA	3:2:179:HIS:CD2	2.51	0.46
3:2:602:ILE:O	3:2:606:THR:HG23	2.16	0.46
5:A:618:TYR:CE1	12:H:40:ILE:HD13	2.51	0.46
5:A:1345:ARG:HD2	9:E:133:GLN:HE21	1.79	0.46
7:C:107:CYS:HB2	7:C:153:LEU:HD12	1.98	0.46
19:O:105:ARG:HH11	19:O:112:ARG:HG2	1.80	0.46
21:Q:148:MET:HE2	41:k:200:GLU:CB	2.41	0.46
23:S:173:HIS:C	23:S:175:SER:H	2.24	0.46
27:W:83:HIS:CG	30:Z:336:TYR:OH	2.68	0.46
30:Z:35:TYR:CG	30:Z:114:PHE:CD1	3.03	0.46
36:f:11:TRP:CZ3	36:f:89:ARG:HB3	2.50	0.46
36:f:101:PRO:O	36:f:105:MET:HB2	2.14	0.46
38:h:172:THR:OG1	41:k:196:LEU:O	2.19	0.46
40:j:367:HIS:ND1	40:j:368:LEU:HD22	2.31	0.46
41:k:108:ILE:HG12	42:l:90:ASN:O	2.16	0.46
43:m:47:GLN:CG	43:m:48:VAL:H	2.29	0.46
43:m:130:LEU:CD1	47:q:160:MET:HE3	2.46	0.46
43:m:140:SER:CB	47:q:146:ASN:HB3	2.10	0.46
44:n:275:LYS:HG2	44:n:278:GLN:NE2	2.31	0.46
48:r:153:ALA:CA	48:r:155:PRO:HD2	2.46	0.46
48:r:1415:VAL:HA	48:r:1418:ILE:HG22	1.97	0.46
49:s:147:GLU:O	49:s:149:ILE:N	2.49	0.46
50:t:83:MET:O	50:t:84:SER:C	2.59	0.46
52:v:80:TYR:O	52:v:83:GLU:HG3	2.15	0.46
54:x:53:GLU:OE1	54:x:57:LEU:HD21	2.15	0.46
54:x:103:CYS:HA	54:x:106:ASP:OD2	2.15	0.46
1:0:78:SER:HA	1:0:108:TRP:HZ2	1.78	0.46
2:1:1045:SER:O	2:1:1049:LEU:HG	2.16	0.46
3:2:360:THR:OG1	3:2:385:ARG:HG2	2.15	0.46
5:A:556:GLU:O	5:A:560:VAL:HG12	2.16	0.46
6:B:711:ILE:HD13	6:B:722:ASN:OD1	2.16	0.46
7:C:44:ILE:HG12	7:C:178:PRO:HG3	1.97	0.46
8:D:141:GLN:HB3	43:m:67:ASN:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:104:MET:HE2	11:G:104:MET:HB3	1.80	0.46
11:G:145:LEU:HA	11:G:168:LEU:HD21	1.97	0.46
22:R:96:PRO:HB3	22:R:136:LYS:HD2	1.98	0.46
22:R:129:LYS:HA	22:R:129:LYS:HE3	1.97	0.46
23:S:31:PHE:HD1	24:T:91:GLN:HG3	1.80	0.46
27:W:297:PHE:O	27:W:297:PHE:CG	2.68	0.46
29:Y:412:GLU:HA	32:b:120:THR:HG21	1.98	0.46
29:Y:449:ILE:CG2	29:Y:451:GLN:HG3	2.46	0.46
29:Y:480:PRO:CD	29:Y:481:VAL:H	2.26	0.46
30:Z:58:ARG:HH21	32:b:237:GLN:CB	2.27	0.46
30:Z:408:LEU:HB2	33:c:7:GLY:HA3	1.98	0.46
39:i:31:VAL:O	39:i:34:GLU:HG3	2.15	0.46
40:j:394:HIS:N	40:j:406:ARG:HH12	2.13	0.46
43:m:127:LEU:O	43:m:131:GLU:HG3	2.16	0.46
43:m:140:SER:HB3	45:o:118:LEU:HD11	1.98	0.46
44:n:223:THR:HG23	44:n:227:LYS:HB2	1.97	0.46
45:o:144:GLU:O	45:o:148:VAL:HG23	2.16	0.46
48:r:93:ARG:HE	52:v:19:ILE:CG2	2.29	0.46
48:r:110:GLY:O	48:r:114:LYS:HG3	2.15	0.46
48:r:230:PHE:CD1	48:r:296:LEU:HD13	2.50	0.46
48:r:424:ASN:ND2	48:r:561:PRO:HB2	2.31	0.46
48:r:520:LEU:HB2	48:r:539:PHE:CE2	2.51	0.46
48:r:810:LEU:HD12	48:r:820:ILE:HD11	1.98	0.46
48:r:1300:ILE:O	48:r:1303:THR:OG1	2.27	0.46
49:s:104:ASP:O	49:s:105:SER:C	2.59	0.46
49:s:127:GLN:C	49:s:131:LYS:NZ	2.74	0.46
54:x:112:ASP:O	54:x:115:LEU:CD1	2.64	0.46
54:x:120:SER:HG	54:x:121:ALA:H	1.64	0.46
55:y:52:LEU:O	55:y:53:LYS:C	2.58	0.46
1:0:521:VAL:HA	4:3:151:TYR:OH	2.16	0.46
1:0:600:LYS:HZ3	1:0:664:ILE:CD1	2.29	0.46
1:0:679:THR:O	48:r:945:ASP:OD1	2.34	0.46
2:1:509:LEU:HD21	2:1:955:TYR:CE1	2.51	0.46
2:1:978:LEU:HB2	2:1:979:PRO:HD3	1.98	0.46
2:1:1044:LEU:HB3	2:1:1048:TYR:HD2	1.81	0.46
2:1:1189:ARG:HG2	2:1:1196:CYS:SG	2.56	0.46
3:2:4:VAL:O	3:2:8:GLN:N	2.44	0.46
3:2:551:SER:OG	3:2:552:THR:N	2.49	0.46
4:3:164:CYS:SG	4:3:169:LEU:HG	2.56	0.46
5:A:1460:LEU:HD22	6:B:1155:CYS:SG	2.56	0.46
6:B:37:LYS:O	6:B:41:ARG:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:546:GLU:HG3	23:S:121:ASN:HB2	1.97	0.46
11:G:134:ASP:CG	11:G:135:ILE:HD12	2.41	0.46
18:N:67:PHE:HB3	20:P:191:GLU:HA	1.98	0.46
19:O:169:ARG:NH2	20:P:284:GLU:OE1	2.36	0.46
21:Q:49:LEU:O	21:Q:53:LYS:HA	2.15	0.46
21:Q:76:MET:CG	21:Q:88:ARG:HB3	2.46	0.46
28:X:53:LEU:HD11	28:X:83:VAL:HG13	1.97	0.46
29:Y:440:LEU:HD11	32:b:218:PRO:HD3	1.97	0.46
36:f:106:LEU:HB3	36:f:143:ILE:HD11	1.96	0.46
39:i:91:GLN:HG2	39:i:95:LYS:HE3	1.97	0.46
40:j:409:GLY:O	42:l:74:SER:OG	2.33	0.46
43:m:140:SER:HB2	47:q:146:ASN:OD1	1.76	0.46
48:r:109:ALA:O	48:r:110:GLY:C	2.58	0.46
48:r:269:MET:O	48:r:272:SER:OG	2.27	0.46
48:r:539:PHE:CD1	48:r:551:VAL:HG13	2.50	0.46
49:s:111:GLN:C	49:s:111:GLN:CD	2.84	0.46
49:s:145:SER:O	49:s:146:GLU:C	2.58	0.46
50:t:22:THR:O	50:t:23:ASP:C	2.59	0.46
50:t:139:MET:HE1	54:x:94:GLU:HG2	1.98	0.46
55:y:69:TYR:C	55:y:71:GLN:N	2.74	0.46
55:y:116:GLN:HA	55:y:119:LEU:CG	2.46	0.46
56:z:746:ASN:HB3	56:z:747:PRO:HD2	1.97	0.46
2:1:579:LEU:O	2:1:583:GLY:N	2.34	0.45
2:1:772:ASN:HB3	2:1:775:ASP:OD1	2.16	0.45
3:2:500:LEU:HB3	3:2:525:PHE:CE2	2.51	0.45
5:A:44:PRO:HB3	5:A:284:VAL:HG13	1.96	0.45
5:A:184:CYS:C	5:A:186:ARG:H	2.24	0.45
19:O:149:LYS:NZ	19:O:152:LYS:HD3	2.31	0.45
20:P:249:LYS:HB2	20:P:251:LEU:HD12	1.99	0.45
25:U:59:DC:H5"	27:W:629:HIS:CE1	2.51	0.45
27:W:105:GLU:CA	27:W:487:LYS:NZ	2.68	0.45
27:W:128:SER:O	27:W:334:ARG:NH1	2.48	0.45
29:Y:411:MET:CB	32:b:119:MET:HB2	2.46	0.45
29:Y:499:ARG:CZ	29:Y:535:LYS:HE3	2.46	0.45
31:a:80:ARG:HD3	31:a:201:LEU:HD13	1.97	0.45
37:g:46:ASN:O	37:g:50:VAL:HG23	2.16	0.45
40:j:391:MET:HG3	40:j:400:PHE:CD1	2.49	0.45
44:n:36:LYS:HE2	44:n:36:LYS:HB3	1.69	0.45
46:p:81:ASN:HD22	46:p:102:PHE:HB2	1.82	0.45
48:r:107:ASN:OD1	48:r:107:ASN:N	2.49	0.45
48:r:167:PRO:HD2	48:r:168:ARG:CD	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:221:ARG:HD2	48:r:223:LYS:NZ	2.30	0.45
48:r:797:PHE:CD1	48:r:797:PHE:O	2.69	0.45
49:s:96:LEU:HG	51:u:114:GLN:HG2	1.97	0.45
49:s:100:VAL:CG1	49:s:103:ARG:HH21	2.29	0.45
50:t:15:MET:CG	50:t:16:GLN:H	2.29	0.45
51:u:121:LEU:O	51:u:125:VAL:HG12	2.15	0.45
52:v:81:THR:HA	52:v:84:CYS:SG	2.56	0.45
54:x:106:ASP:HB2	54:x:110:ARG:NH2	2.31	0.45
55:y:24:PHE:CE1	55:y:28:LEU:HD21	2.51	0.45
55:y:30:ASN:C	55:y:32:ASN:OD1	2.59	0.45
55:y:76:LEU:HA	55:y:79:LEU:HG	1.97	0.45
1:0:17:TYR:CD1	1:0:17:TYR:O	2.69	0.45
1:0:155:PHE:CZ	1:0:479:GLU:HG2	2.52	0.45
1:0:168:LEU:HD13	1:0:248:VAL:HB	1.97	0.45
1:0:185:SER:HB2	1:0:210:ARG:HD3	1.96	0.45
2:1:846:CYS:O	2:1:849:ILE:HG12	2.16	0.45
5:A:1361:ASP:OD1	5:A:1363:VAL:HG12	2.16	0.45
7:C:66:HIS:HA	16:L:57:ALA:O	2.16	0.45
11:G:160:ILE:HG21	21:Q:139:LEU:HD23	1.98	0.45
19:O:251:ILE:HD12	19:O:251:ILE:H	1.81	0.45
23:S:101:ARG:HG3	23:S:109:LYS:HE3	1.98	0.45
23:S:173:HIS:NE2	23:S:177:MET:HB2	2.31	0.45
26:V:59:DG:H2"	26:V:60:DA:C8	2.50	0.45
27:W:171:LYS:HA	27:W:461:HIS:HD1	1.79	0.45
27:W:278:GLU:CD	27:W:452:ARG:CB	2.88	0.45
29:Y:504:LYS:HA	29:Y:507:PRO:HG3	1.98	0.45
31:a:75:ASP:OD2	31:a:80:ARG:NH2	2.37	0.45
33:c:8:VAL:CG2	33:c:45:VAL:O	2.64	0.45
40:j:534:VAL:CG1	40:j:568:ALA:O	2.62	0.45
48:r:79:VAL:O	48:r:83:ILE:HG12	2.15	0.45
48:r:174:ARG:O	48:r:178:ILE:HG23	2.16	0.45
48:r:920:ASN:O	48:r:953:PHE:HB3	2.16	0.45
49:s:148:ILE:CA	49:s:151:TYR:HB3	2.47	0.45
50:t:116:PHE:CD1	50:t:116:PHE:N	2.83	0.45
1:0:158:LYS:HE3	1:0:479:GLU:OE1	2.16	0.45
2:1:891:LEU:O	2:1:897:ARG:NH2	2.50	0.45
3:2:46:LEU:HD22	3:2:64:LEU:HB2	1.98	0.45
3:2:138:SER:OG	3:2:154:GLY:O	2.19	0.45
5:A:117:LEU:HD12	5:A:117:LEU:HA	1.87	0.45
5:A:255:VAL:HG13	5:A:280:LEU:HD13	1.99	0.45
5:A:769:MET:CE	6:B:973:PRO:HG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1622:TYR:O	5:A:1622:TYR:CG	2.68	0.45
5:A:1657:TYR:HE2	35:e:58:THR:OG1	1.98	0.45
6:B:30:ILE:HD13	6:B:702:MET:HE3	1.98	0.45
12:H:104:THR:OG1	12:H:107:GLU:OE1	2.34	0.45
18:N:56:VAL:HB	18:N:81:PHE:CZ	2.52	0.45
23:S:45:ALA:HB3	23:S:103:ASN:N	2.31	0.45
27:W:413:LEU:HD23	27:W:454:VAL:HG22	1.99	0.45
29:Y:510:GLU:OE2	29:Y:526:GLU:OE2	2.33	0.45
29:Y:524:HIS:NE2	31:a:270:SER:HB2	2.27	0.45
33:c:8:VAL:CB	33:c:45:VAL:O	2.62	0.45
34:d:114:ASP:HA	34:d:117:ASN:HD22	1.81	0.45
36:f:218:LEU:HD11	36:f:232:LEU:HD21	1.98	0.45
38:h:122:LYS:HA	38:h:125:THR:HG22	1.98	0.45
40:j:191:ARG:NE	43:m:88:LEU:CG	2.79	0.45
40:j:449:ASP:OD1	40:j:450:SER:N	2.49	0.45
40:j:582:VAL:HG13	40:j:592:ILE:HD11	1.99	0.45
42:l:68:ASN:HB2	42:l:190:MET:HE2	1.98	0.45
44:n:41:ASN:O	44:n:42:LYS:HG3	2.16	0.45
48:r:174:ARG:O	48:r:178:ILE:HG12	2.17	0.45
48:r:185:LYS:HA	48:r:188:LYS:HG2	1.98	0.45
48:r:812:TYR:O	48:r:816:LYS:HA	2.16	0.45
48:r:1417:ASN:HA	48:r:1420:LYS:HG2	1.98	0.45
50:t:32:PRO:O	55:y:18:PHE:CE1	2.67	0.45
50:t:126:TYR:O	50:t:129:HIS:ND1	2.49	0.45
50:t:132:ARG:HH22	54:x:86:GLN:N	2.14	0.45
52:v:1:MET:SD	52:v:4:LYS:HB3	2.56	0.45
52:v:4:LYS:HZ2	52:v:57:GLN:HB3	1.81	0.45
52:v:19:ILE:O	52:v:20:ARG:C	2.58	0.45
52:v:75:ARG:CZ	53:w:104:LYS:HB2	2.46	0.45
52:v:128:ARG:C	52:v:130:GLU:H	2.24	0.45
54:x:96:GLU:O	54:x:97:ASN:C	2.58	0.45
55:y:116:GLN:CD	55:y:119:LEU:CD1	2.80	0.45
1:0:262:SER:HB3	3:2:630:MET:HA	1.99	0.45
1:0:556:ILE:HG12	1:0:819:TRP:CZ2	2.51	0.45
1:0:703:GLU:C	1:0:705:PRO:HD3	2.41	0.45
2:1:301:GLU:OE2	2:1:347:ALA:HA	2.17	0.45
2:1:662:GLN:HB3	2:1:663:PRO:HD3	1.99	0.45
3:2:10:ILE:H	3:2:10:ILE:HD12	1.82	0.45
3:2:196:LEU:HD21	3:2:222:ILE:HD13	1.98	0.45
3:2:251:GLU:HG2	3:2:263:LEU:HD22	1.98	0.45
3:2:267:LEU:HD23	3:2:267:LEU:HA	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:952:VAL:HA	3:2:955:LEU:HG	1.98	0.45
4:3:180:PHE:CE1	4:3:198:ALA:HB3	2.47	0.45
5:A:218:PRO:HA	5:A:221:VAL:HG22	1.96	0.45
5:A:1657:TYR:OH	35:e:158:LEU:CA	2.64	0.45
6:B:1075:MET:HE2	6:B:1075:MET:HB3	1.84	0.45
11:G:41:LYS:HD3	11:G:41:LYS:HA	1.74	0.45
17:M:22:ILE:O	17:M:26:ARG:HG2	2.17	0.45
17:M:338:GLN:OE1	18:N:5:LEU:HD13	2.16	0.45
24:T:85:LEU:HD12	24:T:86:GLN:H	1.81	0.45
31:a:87:LEU:HD23	31:a:87:LEU:HA	1.78	0.45
38:h:182:VAL:HG21	41:k:202:ILE:HG12	1.99	0.45
40:j:260:SER:CA	40:j:368:LEU:HG	2.47	0.45
40:j:392:MET:CB	41:k:49:GLU:OE1	2.61	0.45
40:j:430:LYS:O	40:j:433:LYS:HB2	2.16	0.45
40:j:467:ILE:HA	47:q:171:ASN:HD21	1.82	0.45
40:j:615:TRP:CZ3	56:z:680:GLY:HA2	2.47	0.45
44:n:43:GLU:HG2	44:n:44:THR:OG1	2.15	0.45
44:n:103:LEU:C	44:n:105:SER:H	2.24	0.45
46:p:163:VAL:O	46:p:167:GLN:HG3	2.17	0.45
48:r:167:PRO:HD2	48:r:168:ARG:CZ	2.47	0.45
48:r:965:MET:HE1	48:r:1258:ASN:H	1.82	0.45
48:r:1417:ASN:HB3	48:r:1421:ARG:HH22	1.81	0.45
49:s:40:LEU:HD21	49:s:72:ARG:CZ	2.47	0.45
50:t:82:ASN:O	50:t:85:ILE:N	2.50	0.45
50:t:114:LEU:O	50:t:117:VAL:HG22	2.17	0.45
50:t:168:LEU:HD22	51:u:129:ASN:ND2	2.31	0.45
51:u:73:ILE:HD12	51:u:76:MET:HB2	1.98	0.45
54:x:98:HIS:HD1	54:x:98:HIS:N	2.13	0.45
54:x:118:ILE:O	54:x:122:LEU:HG	2.16	0.45
55:y:74:HIS:CD2	55:y:78:LEU:HD21	2.52	0.45
56:z:726:PRO:O	56:z:728:ASP:N	2.49	0.45
1:0:143:LEU:HD12	1:0:143:LEU:HA	1.67	0.45
1:0:630:ALA:O	1:0:633:PRO:HD2	2.16	0.45
2:1:433:ASN:ND2	2:1:447:ILE:HD11	2.31	0.45
2:1:866:ILE:HD11	2:1:889:LEU:HD22	1.98	0.45
2:1:1044:LEU:HB3	2:1:1048:TYR:CD2	2.51	0.45
2:1:1187:PRO:HA	2:1:1190:LEU:HD23	1.98	0.45
2:1:1224:LEU:HD22	2:1:1227:ILE:HD11	1.98	0.45
3:2:179:HIS:CE1	3:2:180:ILE:HG12	2.51	0.45
3:2:698:TRP:O	3:2:699:ASN:C	2.59	0.45
3:2:698:TRP:O	3:2:700:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1060:HIS:HB3	6:B:1081:ASP:OD2	2.16	0.45
8:D:84:ARG:HA	8:D:87:LEU:HB2	1.98	0.45
17:M:49:LYS:HD2	18:N:14:SER:HA	1.98	0.45
17:M:308:GLN:NE2	17:M:310:GLU:O	2.49	0.45
17:M:342:ILE:HD12	18:N:72:TRP:CD1	2.52	0.45
19:O:193:ARG:NH1	25:U:13:DT:OP2	2.50	0.45
20:P:173:ASN:HA	20:P:218:LYS:HA	1.98	0.45
21:Q:36:ILE:HG21	21:Q:48:MET:CE	2.45	0.45
21:Q:179:ARG:HH21	21:Q:183:GLN:HG3	1.81	0.45
27:W:295:TYR:CG	27:W:333:ALA:O	2.69	0.45
32:b:18:ASN:HD22	32:b:19:PRO:HD2	1.82	0.45
35:e:34:THR:HG22	35:e:34:THR:O	2.17	0.45
40:j:195:LYS:HG3	40:j:195:LYS:O	2.17	0.45
40:j:197:ARG:HE	40:j:204:LEU:CG	2.22	0.45
41:k:21:TYR:CD2	41:k:102:VAL:HG22	2.51	0.45
43:m:134:TYR:CG	43:m:134:TYR:O	2.70	0.45
48:r:70:THR:O	48:r:74:PRO:HD3	2.16	0.45
48:r:211:GLN:HG2	48:r:293:TYR:CD1	2.52	0.45
48:r:797:PHE:O	48:r:797:PHE:CG	2.70	0.45
48:r:851:ILE:HG22	48:r:854:GLN:HB2	1.97	0.45
50:t:140:GLU:O	50:t:143:LYS:HB2	2.16	0.45
53:w:84:ILE:HG13	53:w:89:LEU:HB3	1.99	0.45
53:w:128:ARG:O	53:w:131:ILE:HB	2.17	0.45
54:x:54:TYR:O	54:x:56:GLN:N	2.49	0.45
54:x:97:ASN:ND2	54:x:97:ASN:H	2.14	0.45
2:1:37:LEU:HD21	2:1:78:PHE:HD2	1.82	0.45
2:1:231:VAL:HB	2:1:1099:ASN:ND2	2.32	0.45
2:1:751:GLU:OE2	2:1:756:LEU:HB2	2.17	0.45
3:2:121:CYS:SG	3:2:177:LEU:HD12	2.57	0.45
3:2:568:LYS:HG3	3:2:569:LEU:N	2.30	0.45
4:3:37:LYS:HA	4:3:41:LEU:HG	1.98	0.45
5:A:417:LYS:HD3	19:O:28:ARG:NH1	2.31	0.45
5:A:488:VAL:C	5:A:491:PRO:HD2	2.42	0.45
5:A:581:LYS:HB3	5:A:581:LYS:HE2	1.73	0.45
6:B:246:GLY:O	6:B:250:SER:HB2	2.16	0.45
6:B:388:TYR:H	6:B:504:THR:HG21	1.82	0.45
6:B:674:MET:HG2	6:B:690:CYS:SG	2.56	0.45
6:B:681:ASP:C	6:B:683:GLN:H	2.25	0.45
6:B:825:GLN:HE22	6:B:874:PRO:HA	1.81	0.45
8:D:70:ARG:HG3	43:m:20:LYS:HZ1	1.68	0.45
11:G:7:LEU:HD12	11:G:72:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:1:MET:O	14:J:56:ILE:HB	2.17	0.45
16:L:37:ARG:C	16:L:39:CYS:H	2.23	0.45
19:O:209:ILE:HG13	19:O:250:PRO:HG2	1.98	0.45
21:Q:112:ARG:HA	21:Q:115:GLU:OE2	2.16	0.45
25:U:16:DA:H2"	25:U:17:DA:C8	2.52	0.45
34:d:70:LYS:NZ	34:d:110:THR:O	2.41	0.45
35:e:134:LEU:HD22	35:e:162:PHE:HB3	1.98	0.45
36:f:256:ARG:O	36:f:260:LYS:HG3	2.17	0.45
40:j:256:TYR:CE2	40:j:258:LYS:HD3	2.51	0.45
40:j:403:LYS:O	40:j:403:LYS:HG2	2.17	0.45
45:o:100:LEU:O	45:o:103:SER:OG	2.29	0.45
46:p:110:TYR:HE2	56:z:649:ILE:HD13	1.74	0.45
48:r:139:LEU:O	48:r:140:ALA:C	2.57	0.45
48:r:668:HIS:O	48:r:668:HIS:ND1	2.50	0.45
48:r:803:TYR:HD1	48:r:808:LEU:HD13	1.81	0.45
48:r:1318:HIS:O	48:r:1322:LEU:HG	2.17	0.45
49:s:151:TYR:CD1	49:s:155:ILE:HD11	2.51	0.45
52:v:121:MET:HA	52:v:124:TYR:CD2	2.51	0.45
1:0:343:SER:OG	1:0:399:LEU:HB2	2.17	0.45
1:0:606:LEU:HG	1:0:665:TRP:CH2	2.50	0.45
2:1:8:ILE:O	2:1:12:VAL:HG13	2.16	0.45
2:1:1267:MET:SD	2:1:1305:PHE:HB3	2.57	0.45
5:A:551:ARG:HH12	12:H:27:ARG:NH2	2.12	0.45
5:A:1255:LEU:HD23	5:A:1255:LEU:H	1.80	0.45
7:C:68:LEU:HB2	7:C:150:ILE:HD11	1.99	0.45
7:C:187:ASP:CG	7:C:191:ALA:H	2.25	0.45
17:M:351:PHE:HB3	17:M:353:LEU:HD13	1.97	0.45
20:P:212:LEU:HB2	20:P:220:VAL:HG22	1.98	0.45
23:S:114:LYS:HA	23:S:144:TYR:CB	2.47	0.45
25:U:57:DC:H2"	25:U:58:DT:C5'	2.45	0.45
28:X:307:ASN:CG	28:X:380:ARG:HH12	2.24	0.45
28:X:500:ASP:HB2	28:X:502:VAL:HG23	1.99	0.45
30:Z:54:ASN:ND2	32:b:237:GLN:HG2	2.31	0.45
30:Z:308:VAL:HB	30:Z:316:TYR:HB2	1.98	0.45
31:a:314:SER:HB3	31:a:317:HIS:HD2	1.81	0.45
35:e:167:ARG:HG2	35:e:167:ARG:NH2	2.30	0.45
36:f:7:GLN:HG3	36:f:89:ARG:HH21	1.81	0.45
38:h:42:TRP:HA	38:h:45:VAL:HG12	1.98	0.45
39:i:63:LEU:O	39:i:67:ILE:HG12	2.17	0.45
40:j:49:PHE:CD1	40:j:49:PHE:O	2.69	0.45
41:k:53:ASP:O	41:k:130:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:16:GLN:NE2	43:m:20:LYS:HE3	2.32	0.45
48:r:93:ARG:O	48:r:97:VAL:N	2.50	0.45
48:r:340:TRP:O	48:r:354:VAL:N	2.49	0.45
48:r:1285:PHE:HA	48:r:1289:VAL:HB	1.99	0.45
50:t:10:LEU:HG	50:t:11:PRO:CD	2.45	0.45
52:v:18:ASN:O	52:v:22:LEU:HD23	2.16	0.45
54:x:68:ASP:O	54:x:72:LEU:HG	2.17	0.45
55:y:72:CYS:SG	55:y:73:LEU:N	2.90	0.45
1:0:16:ALA:N	1:0:454:VAL:O	2.44	0.45
1:0:732:LEU:HD13	1:0:781:HIS:CG	2.51	0.45
2:1:780:PHE:CE2	2:1:810:VAL:HG11	2.51	0.45
3:2:243:THR:HG21	3:2:274:GLN:OE1	2.17	0.45
3:2:538:LYS:NZ	3:2:540:LEU:HD21	2.31	0.45
3:2:950:THR:O	3:2:953:SER:OG	2.35	0.45
3:2:978:GLY:HA2	3:2:981:VAL:HG12	1.99	0.45
5:A:340:LYS:HD3	5:A:1436:VAL:HG21	1.99	0.45
6:B:490:GLY:O	6:B:492:ASP:N	2.50	0.45
7:C:42:VAL:HB	7:C:178:PRO:HG2	1.98	0.45
11:G:107:PHE:CE1	11:G:160:ILE:HG22	2.51	0.45
21:Q:73:LYS:HD3	21:Q:73:LYS:HA	1.70	0.45
21:Q:181:ASN:O	21:Q:185:GLU:HG3	2.17	0.45
22:R:168:LEU:O	22:R:172:GLU:HG2	2.16	0.45
28:X:592:ARG:HH12	31:a:177:CYS:CB	2.30	0.45
29:Y:499:ARG:NH2	29:Y:535:LYS:CE	2.80	0.45
35:e:11:ARG:HH11	35:e:33:ASN:HD22	1.64	0.45
40:j:409:GLY:CA	42:l:74:SER:HG	2.29	0.45
41:k:78:ARG:C	41:k:80:GLY:H	2.25	0.45
41:k:147:LYS:HB2	41:k:167:TYR:CD2	2.51	0.45
42:l:148:VAL:HG21	44:n:196:LYS:CB	2.46	0.45
44:n:215:LYS:CE	44:n:232:SER:HG	2.28	0.45
44:n:281:CYS:SG	44:n:285:GLY:HA2	2.56	0.45
46:p:112:LEU:HD23	46:p:112:LEU:HA	1.86	0.45
48:r:229:GLU:O	48:r:252:ILE:HA	2.17	0.45
48:r:463:PHE:CZ	48:r:486:MET:HE1	2.52	0.45
48:r:797:PHE:HZ	48:r:873:PHE:HA	1.82	0.45
50:t:78:LEU:HD13	50:t:122:LEU:HD22	1.99	0.45
50:t:164:ILE:HG13	51:u:136:LYS:NZ	2.32	0.45
52:v:120:ASP:O	52:v:124:TYR:CG	2.69	0.45
54:x:115:LEU:C	54:x:119:GLN:NE2	2.74	0.45
55:y:55:LEU:O	55:y:57:TYR:N	2.50	0.45
1:0:348:LEU:HD13	1:0:386:PHE:CZ	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:563:LEU:HB3	1:0:606:LEU:HD11	1.98	0.45
2:1:505:MET:HE3	2:1:505:MET:HB3	1.89	0.45
2:1:609:SER:HB3	2:1:648:THR:HG22	1.99	0.45
2:1:1087:PHE:HE2	2:1:1104:ALA:HA	1.82	0.45
5:A:339:LEU:HA	5:A:342:ARG:HD3	1.99	0.45
6:B:608:ARG:NH2	13:I:68:ILE:HG22	2.32	0.45
6:B:746:THR:HG22	6:B:747:LEU:HD12	1.99	0.45
8:D:96:GLU:HA	8:D:99:CYS:SG	2.57	0.45
9:E:51:GLY:O	9:E:53:PRO:HD3	2.17	0.45
15:K:77:THR:CG2	15:K:81:TYR:HB3	2.47	0.45
21:Q:54:PHE:CE1	22:R:195:PRO:HG3	2.52	0.45
27:W:342:CYS:HG	27:W:638:GLN:CA	2.12	0.45
38:h:18:GLN:O	38:h:55:GLN:NE2	2.50	0.45
43:m:117:ILE:HG13	47:q:174:LEU:HD23	1.98	0.45
43:m:133:GLU:HG2	45:o:128:LEU:HD23	1.99	0.45
45:o:112:LYS:HE2	45:o:112:LYS:HB3	1.84	0.45
46:p:85:ASN:HA	46:p:88:ILE:HG22	1.99	0.45
48:r:89:ALA:C	48:r:92:THR:HB	2.42	0.45
48:r:110:GLY:O	48:r:113:GLU:HG3	2.15	0.45
48:r:111:LYS:HD3	48:r:114:LYS:HZ1	1.81	0.45
48:r:894:THR:HG23	48:r:896:ARG:H	1.82	0.45
48:r:1322:LEU:HD21	48:r:1436:PHE:HE1	1.81	0.45
49:s:133:LYS:HG3	49:s:137:LYS:NZ	2.32	0.45
52:v:76:ASN:ND2	52:v:76:ASN:N	2.65	0.45
55:y:114:ARG:HD3	55:y:114:ARG:HA	1.53	0.45
2:1:673:LYS:HE2	2:1:722:PHE:CE2	2.51	0.45
3:2:135:THR:HG23	3:2:157:GLN:NE2	2.31	0.45
5:A:1480:CYS:SG	11:G:19:GLY:N	2.90	0.45
5:A:1650:TYR:HD2	35:e:177:TRP:HZ2	1.65	0.45
6:B:231:PRO:C	6:B:233:SER:H	2.25	0.45
7:C:37:VAL:O	7:C:42:VAL:HG23	2.17	0.45
8:D:110:GLU:OE2	8:D:114:LEU:HD23	2.16	0.45
9:E:13:ILE:HA	9:E:16:THR:HG22	1.98	0.45
11:G:117:MET:HE3	11:G:129:LYS:HA	1.99	0.45
13:I:68:ILE:HG13	13:I:122:ARG:HD2	1.98	0.45
17:M:312:GLU:O	17:M:314:LEU:HD12	2.17	0.45
24:T:192:GLU:OE1	24:T:192:GLU:N	2.46	0.45
24:T:230:LYS:HG2	24:T:231:ASN:H	1.81	0.45
27:W:109:ARG:HD2	27:W:492:ASN:OD1	2.10	0.45
29:Y:414:TYR:HB3	32:b:116:LYS:HE3	1.89	0.45
29:Y:524:HIS:CE1	31:a:270:SER:CB	2.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:96:SER:HB3	32:b:102:GLU:HG2	2.00	0.45
32:b:255:CYS:HB3	32:b:262:ILE:HD11	1.97	0.45
38:h:28:SER:O	38:h:32:LYS:HG3	2.17	0.45
39:i:17:ILE:HD12	39:i:17:ILE:HA	1.85	0.45
40:j:415:LYS:HZ3	42:l:123:LEU:HD13	1.78	0.45
40:j:459:GLN:OE1	43:m:137:SER:N	2.50	0.45
48:r:100:LEU:HD13	48:r:104:LYS:HD2	1.99	0.45
48:r:115:CYS:O	48:r:116:ALA:C	2.57	0.45
48:r:615:LYS:HD3	48:r:644:PHE:CE1	2.52	0.45
48:r:810:LEU:O	48:r:819:SER:HA	2.17	0.45
50:t:76:LYS:HA	50:t:79:ARG:NE	2.31	0.45
52:v:89:LEU:O	52:v:92:ASN:N	2.49	0.45
54:x:67:LYS:HA	54:x:70:ASP:CG	2.42	0.45
55:y:16:LEU:O	55:y:18:PHE:N	2.50	0.45
55:y:26:GLN:CD	55:y:68:LYS:H	2.25	0.45
3:2:145:GLY:O	3:2:149:GLY:N	2.50	0.44
3:2:303:LEU:HD23	3:2:303:LEU:HA	1.56	0.44
4:3:146:CYS:SG	4:3:191:LEU:HD21	2.57	0.44
6:B:93:LEU:HD13	6:B:124:LEU:HD13	1.98	0.44
13:I:66:THR:HG22	13:I:67:GLN:H	1.82	0.44
19:O:237:ARG:O	19:O:241:GLU:HG2	2.16	0.44
29:Y:386:PRO:HB3	32:b:274:ILE:HD12	1.99	0.44
30:Z:61:PHE:CD2	32:b:228:LEU:HD22	2.51	0.44
37:g:61:ASN:HA	37:g:86:ARG:HH12	1.82	0.44
37:g:65:GLY:N	37:g:86:ARG:O	2.48	0.44
40:j:93:TRP:CE3	40:j:94:PRO:HD2	2.52	0.44
44:n:53:ILE:HD12	56:z:626:LEU:CD2	2.47	0.44
48:r:99:LEU:C	48:r:101:ALA:N	2.74	0.44
48:r:108:ASN:O	48:r:112:VAL:HG13	2.17	0.44
48:r:159:ASP:HB3	48:r:164:GLY:O	2.17	0.44
48:r:950:VAL:HG23	48:r:951:GLU:N	2.30	0.44
48:r:1273:TRP:CG	48:r:1314:ARG:HD2	2.52	0.44
51:u:70:HIS:NE2	51:u:74:LYS:HD3	2.31	0.44
55:y:49:VAL:O	55:y:53:LYS:HG2	2.17	0.44
55:y:111:LYS:HA	55:y:111:LYS:HD2	1.59	0.44
56:z:721:LEU:HD11	56:z:736:TRP:CE3	2.51	0.44
1:0:567:HIS:CD2	4:3:218:ARG:HG2	2.52	0.44
2:1:891:LEU:HD23	2:1:891:LEU:HA	1.75	0.44
3:2:185:GLU:O	3:2:188:SER:N	2.42	0.44
3:2:290:PHE:HE2	3:2:341:LEU:HD21	1.83	0.44
5:A:466:LYS:HG2	5:A:524:MET:HE1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:585:LEU:HD12	12:H:47:ILE:HD13	1.99	0.44
5:A:1313:GLN:HG3	5:A:1317:LYS:O	2.17	0.44
9:E:27:LEU:H	9:E:64:HIS:HB2	1.82	0.44
13:I:50:ASN:OD1	13:I:51:SER:N	2.50	0.44
13:I:66:THR:HG22	13:I:67:GLN:N	2.32	0.44
22:R:97:LEU:O	22:R:137:TYR:HE1	1.99	0.44
22:R:214:GLU:HA	22:R:217:GLN:HB3	1.99	0.44
27:W:121:TYR:OH	27:W:486:PRO:CA	2.52	0.44
27:W:347:SER:HA	27:W:374:TRP:CH2	2.52	0.44
28:X:48:LYS:O	28:X:52:LEU:HB2	2.17	0.44
29:Y:381:ARG:HD3	32:b:256:PHE:HB2	1.96	0.44
30:Z:46:ARG:NE	32:b:53:ARG:HB2	2.20	0.44
30:Z:215:PHE:HB3	30:Z:216:MET:HE2	1.99	0.44
32:b:68:ARG:HD2	32:b:118:LEU:HD13	1.99	0.44
40:j:251:LEU:HD23	40:j:251:LEU:H	1.82	0.44
40:j:569:ILE:HG23	40:j:583:ARG:CA	2.47	0.44
41:k:19:MET:CG	41:k:177:ALA:HA	2.47	0.44
44:n:49:GLU:O	44:n:53:ILE:HG12	2.17	0.44
45:o:99:ARG:NH2	47:q:35:ARG:HB2	2.32	0.44
48:r:230:PHE:CD1	48:r:230:PHE:O	2.70	0.44
49:s:102:LYS:HB3	49:s:102:LYS:HE3	1.83	0.44
51:u:133:GLN:HA	51:u:136:LYS:CB	2.41	0.44
52:v:125:ARG:HH21	52:v:126:SER:HA	1.81	0.44
1:0:588:THR:HB	1:0:596:MET:SD	2.57	0.44
1:0:702:ASP:OD1	1:0:702:ASP:N	2.49	0.44
2:1:363:ARG:HG3	2:1:364:GLY:H	1.81	0.44
2:1:596:HIS:O	2:1:598:TRP:N	2.51	0.44
4:3:216:ASP:HB3	4:3:219:HIS:CD2	2.52	0.44
5:A:192:ARG:HE	5:A:199:TYR:HB2	1.82	0.44
5:A:350:VAL:O	5:A:355:MET:HG2	2.17	0.44
6:B:161:CYS:SG	6:B:162:LEU:N	2.91	0.44
7:C:47:ILE:HB	7:C:69:GLY:HA2	2.00	0.44
10:F:112:ASP:OD1	10:F:113:GLY:N	2.50	0.44
11:G:81:LYS:HG3	11:G:148:VAL:C	2.42	0.44
13:I:40:ARG:NH2	23:S:171:LEU:HD13	2.32	0.44
20:P:163:PRO:HD3	20:P:325:PHE:CD2	2.52	0.44
30:Z:101:LEU:HB2	30:Z:105:LEU:HB2	2.00	0.44
30:Z:122:LEU:O	32:b:100:LYS:CB	2.65	0.44
30:Z:414:SER:O	30:Z:439:ARG:NH1	2.45	0.44
35:e:132:TRP:HD1	36:f:1:MET:HE3	1.82	0.44
35:e:177:TRP:CD1	35:e:215:GLY:H	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:96:VAL:HG13	36:f:101:PRO:HG3	1.98	0.44
36:f:218:LEU:HB2	36:f:252:MET:HE1	1.99	0.44
38:h:122:LYS:HG3	38:h:123:GLN:N	2.32	0.44
38:h:157:GLU:OE2	39:i:53:THR:OG1	2.31	0.44
40:j:224:VAL:O	40:j:225:ILE:HD13	2.16	0.44
40:j:565:ASN:HA	48:r:637:PHE:CZ	2.52	0.44
43:m:113:ASP:HB3	47:q:178:ASN:ND2	2.32	0.44
44:n:39:MET:HE2	44:n:39:MET:HB3	1.86	0.44
44:n:103:LEU:HG	44:n:104:TYR:H	1.81	0.44
48:r:54:LEU:CD2	53:w:131:ILE:HG23	2.47	0.44
49:s:99:GLU:O	49:s:102:LYS:HE3	2.17	0.44
53:w:88:ASN:C	53:w:90:GLU:OE2	2.61	0.44
55:y:60:ASP:O	55:y:63:TYR:HB2	2.18	0.44
1:0:796:LYS:H	1:0:796:LYS:HG2	1.40	0.44
2:1:476:LEU:HD13	2:1:476:LEU:HA	1.88	0.44
2:1:1220:SER:OG	2:1:1221:ILE:N	2.50	0.44
3:2:21:TYR:HB3	56:z:748:PHE:CD2	2.52	0.44
3:2:208:ASN:OD1	3:2:212:ARG:HG2	2.18	0.44
3:2:218:CYS:O	3:2:222:ILE:HG13	2.17	0.44
3:2:472:ASN:HA	3:2:475:THR:HG22	1.98	0.44
3:2:553:LYS:O	3:2:553:LYS:HD3	2.18	0.44
3:2:946:PHE:CE2	3:2:949:PHE:HB2	2.53	0.44
5:A:264:VAL:HG23	5:A:272:ASN:HB3	2.00	0.44
5:A:375:ILE:HG22	5:A:485:ASN:HD22	1.81	0.44
5:A:601:ASN:HD22	5:A:988:TRP:CD1	2.36	0.44
5:A:1165:THR:H	5:A:1168:LYS:NZ	2.06	0.44
17:M:27:ASP:HA	17:M:30:LEU:HB2	2.00	0.44
17:M:38:VAL:HG22	18:N:27:GLN:OE1	2.17	0.44
17:M:322:ASP:N	17:M:322:ASP:OD1	2.51	0.44
25:U:18:DG:H5'	25:U:18:DG:C8	2.52	0.44
27:W:613:THR:HB	27:W:614:SER:HB3	1.98	0.44
28:X:75:ARG:NH2	28:X:235:GLU:OE2	2.51	0.44
28:X:118:HIS:CD2	28:X:121:VAL:HG23	2.53	0.44
30:Z:400:ARG:CZ	33:c:61:MET:CE	2.95	0.44
37:g:84:GLN:HB3	37:g:92:VAL:HG11	1.98	0.44
39:i:111:CYS:CA	47:q:159:ILE:HD11	2.41	0.44
40:j:152:SER:OG	43:m:58:ASN:ND2	2.51	0.44
40:j:457:ASP:O	40:j:458:PRO:C	2.60	0.44
42:l:155:SER:HG	44:n:287:PHE:HE2	1.64	0.44
48:r:99:LEU:O	48:r:101:ALA:N	2.50	0.44
48:r:490:ILE:HB	48:r:491:PRO:HD3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:570:PHE:O	48:r:612:ALA:HA	2.17	0.44
48:r:885:LEU:HD11	48:r:1186:LEU:HD22	2.00	0.44
55:y:49:VAL:O	55:y:50:ASN:C	2.59	0.44
55:y:81:TYR:C	55:y:85:ARG:NH2	2.76	0.44
1:0:225:ASN:HD22	1:0:225:ASN:HA	1.56	0.44
1:0:263:LEU:HD11	1:0:309:TRP:CZ3	2.53	0.44
2:1:431:HIS:CD2	2:1:483:THR:HG23	2.52	0.44
2:1:1240:LYS:O	2:1:1281:VAL:HG23	2.17	0.44
3:2:85:PHE:CD1	3:2:97:LEU:HD21	2.52	0.44
3:2:509:SER:C	3:2:511:VAL:H	2.25	0.44
3:2:568:LYS:HG3	3:2:569:LEU:H	1.82	0.44
17:M:45:LEU:HA	17:M:48:ASN:ND2	2.32	0.44
18:N:90:VAL:HG12	18:N:93:VAL:HG22	1.98	0.44
18:N:95:ILE:H	18:N:95:ILE:HD12	1.82	0.44
19:O:8:ASP:OD1	19:O:9:ALA:N	2.50	0.44
20:P:222:THR:CG2	26:V:79:DT:O4'	2.65	0.44
23:S:44:GLN:HB3	24:T:9:LEU:HD13	1.99	0.44
24:T:20:LEU:HD12	24:T:21:VAL:H	1.83	0.44
28:X:573:ASP:HB2	28:X:576:GLU:HB2	2.00	0.44
29:Y:372:ILE:CB	31:a:54:ARG:HD2	2.39	0.44
29:Y:386:PRO:O	32:b:253:ALA:HA	2.18	0.44
30:Z:407:VAL:HG11	30:Z:448:HIS:HB2	1.98	0.44
37:g:130:PHE:HA	38:h:49:PHE:CE2	2.52	0.44
43:m:130:LEU:O	43:m:133:GLU:N	2.49	0.44
46:p:136:HIS:O	46:p:137:SER:OG	2.28	0.44
48:r:82:LYS:O	48:r:86:VAL:HG22	2.18	0.44
48:r:154:ILE:N	48:r:155:PRO:CD	2.81	0.44
48:r:174:ARG:HA	48:r:177:ILE:CG2	2.47	0.44
48:r:324:VAL:HG21	48:r:337:LEU:HD13	1.98	0.44
48:r:431:ILE:HB	48:r:437:ALA:CB	2.47	0.44
48:r:440:VAL:O	48:r:452:LEU:HB3	2.17	0.44
48:r:657:LEU:O	48:r:661:LEU:HB2	2.17	0.44
50:t:31:ALA:HA	50:t:32:PRO:HD2	1.73	0.44
52:v:106:LYS:HA	52:v:109:LEU:HB3	2.00	0.44
53:w:90:GLU:OE2	53:w:90:GLU:N	2.37	0.44
54:x:112:ASP:O	54:x:115:LEU:HD11	2.18	0.44
56:z:736:TRP:HH2	56:z:776:TRP:CD1	2.36	0.44
1:0:341:ILE:H	1:0:341:ILE:HD12	1.83	0.44
1:0:812:ARG:NH2	46:p:90:ASN:CG	2.69	0.44
2:1:349:PHE:N	2:1:350:PRO:HD2	2.33	0.44
2:1:434:ARG:HG3	2:1:484:ASN:CG	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:447:ILE:HG13	2:1:455:HIS:ND1	2.33	0.44
2:1:628:HIS:CE1	2:1:677:SER:HB2	2.52	0.44
2:1:1014:MET:HE2	2:1:1014:MET:HB2	1.86	0.44
5:A:102:LYS:O	5:A:106:VAL:HG12	2.17	0.44
5:A:109:CYS:O	5:A:110:VAL:HG13	2.18	0.44
5:A:213:LYS:HE3	5:A:213:LYS:HB2	1.77	0.44
5:A:618:TYR:OH	12:H:29:HIS:HE1	2.00	0.44
5:A:787:VAL:HG12	5:A:824:GLU:HA	1.98	0.44
5:A:931:ARG:O	5:A:932:ARG:HB3	2.17	0.44
5:A:1313:GLN:HE22	5:A:1333:GLU:N	2.16	0.44
5:A:1620:PRO:HB2	38:h:104:VAL:CG1	2.45	0.44
6:B:686:GLU:HG3	6:B:687:VAL:N	2.31	0.44
6:B:759:VAL:HG12	6:B:999:ALA:HB2	1.99	0.44
8:D:124:ASP:HA	8:D:127:LEU:HB3	1.98	0.44
11:G:143:ILE:HD13	11:G:170:LEU:HD22	1.98	0.44
13:I:44:TYR:CE1	13:I:46:GLN:HB3	2.53	0.44
20:P:181:LYS:HA	20:P:181:LYS:HD2	1.86	0.44
27:W:469:THR:HG21	27:W:634:ARG:NH1	1.97	0.44
27:W:519:TYR:O	33:c:22:TYR:CZ	2.69	0.44
28:X:308:PRO:CD	28:X:308:PRO:O	2.65	0.44
29:Y:482:ASN:HA	29:Y:492:LYS:NZ	2.32	0.44
30:Z:403:PHE:CZ	33:c:54:GLN:HA	2.53	0.44
35:e:224:ARG:HA	35:e:227:GLU:HG2	2.00	0.44
39:i:87:ARG:HH21	40:j:299:GLN:NE2	2.15	0.44
40:j:186:GLU:OE1	40:j:291:TRP:CE3	2.71	0.44
40:j:438:ILE:O	40:j:438:ILE:HG22	2.17	0.44
43:m:134:TYR:CE2	47:q:157:LYS:CG	3.01	0.44
46:p:161:LEU:O	46:p:165:LYS:HE2	2.18	0.44
48:r:113:GLU:O	48:r:116:ALA:N	2.50	0.44
48:r:657:LEU:HD23	48:r:682:ILE:HD12	1.92	0.44
48:r:1297:ASN:HA	48:r:1300:ILE:HD12	1.99	0.44
49:s:97:GLU:HA	49:s:100:VAL:HG22	2.00	0.44
49:s:127:GLN:HB3	49:s:131:LYS:HZ1	1.83	0.44
50:t:78:LEU:HD12	50:t:81:LEU:HB3	1.99	0.44
50:t:154:GLN:HE21	50:t:155:LYS:HD3	1.83	0.44
52:v:70:TYR:CD1	52:v:75:ARG:HB2	2.53	0.44
52:v:90:ALA:O	52:v:94:GLN:HG2	2.18	0.44
52:v:100:ASP:HA	52:v:103:LYS:CE	2.48	0.44
1:0:49:MET:HB3	1:0:63:HIS:CE1	2.52	0.44
1:0:132:VAL:HG13	1:0:182:VAL:O	2.17	0.44
1:0:137:LEU:HD23	1:0:137:LEU:HA	1.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:572:PRO:HG2	1:0:574:LYS:HE3	1.99	0.44
2:1:37:LEU:HD22	2:1:82:CYS:SG	2.58	0.44
2:1:507:ILE:HG12	2:1:518:GLY:HA2	2.00	0.44
5:A:517:GLU:HG3	10:F:66:LEU:HD12	2.00	0.44
5:A:1254:LYS:HD3	5:A:1255:LEU:HD23	1.98	0.44
5:A:1471:PHE:CZ	10:F:61:GLU:HA	2.52	0.44
7:C:78:ILE:HG21	7:C:127:VAL:HG13	2.00	0.44
23:S:163:GLU:OE1	23:S:167:ARG:HD3	2.17	0.44
27:W:336:GLY:HA3	27:W:488:LEU:HD13	1.99	0.44
28:X:493:MET:HE3	28:X:676:LEU:HD11	1.98	0.44
31:a:59:ARG:NH2	31:a:235:HIS:O	2.48	0.44
36:f:102:ARG:HG3	36:f:103:ILE:HD12	1.99	0.44
37:g:25:ASN:O	37:g:28:SER:N	2.45	0.44
39:i:69:TYR:HA	39:i:72:GLN:OE1	2.18	0.44
40:j:465:SER:HA	44:n:205:ARG:HH12	1.83	0.44
48:r:313:LEU:HA	48:r:316:ILE:HG22	1.99	0.44
49:s:100:VAL:HA	49:s:103:ARG:HE	1.83	0.44
49:s:118:GLU:O	49:s:119:GLN:C	2.57	0.44
49:s:128:ALA:O	49:s:131:LYS:HB2	2.18	0.44
50:t:91:ASP:C	50:t:94:ASP:H	2.24	0.44
50:t:118:HIS:O	50:t:119:VAL:C	2.60	0.44
51:u:120:SER:O	51:u:124:GLN:NE2	2.49	0.44
52:v:80:TYR:O	52:v:81:THR:C	2.61	0.44
54:x:8:LEU:CD2	54:x:75:SER:CB	2.92	0.44
55:y:84:PHE:O	55:y:85:ARG:C	2.59	0.44
55:y:124:GLN:HA	55:y:127:ASN:HD22	1.81	0.44
1:0:96:LEU:HB3	1:0:108:TRP:HB2	2.00	0.44
2:1:74:LYS:HE3	2:1:74:LYS:HB3	1.65	0.44
2:1:240:SER:HB2	2:1:1217:HIS:NE2	2.33	0.44
2:1:423:PHE:HB3	2:1:476:LEU:HD11	2.00	0.44
2:1:424:ALA:O	2:1:427:CYS:HB2	2.18	0.44
2:1:770:MET:HE3	2:1:771:SER:H	1.83	0.44
3:2:127:ALA:O	3:2:131:LEU:HD13	2.17	0.44
3:2:678:LEU:HB3	3:2:683:THR:HB	2.00	0.44
3:2:965:LYS:HZ3	3:2:968:LEU:HB3	1.83	0.44
5:A:480:SER:HB2	6:B:1059:ILE:HD11	1.99	0.44
5:A:589:LYS:HE3	12:H:120:GLY:HA3	2.00	0.44
5:A:605:THR:HG23	5:A:609:HIS:ND1	2.33	0.44
5:A:677:ASN:HD21	6:B:787:GLY:HA3	1.82	0.44
5:A:805:ARG:HG2	5:A:812:LYS:HA	1.99	0.44
5:A:1369:LEU:HD23	9:E:139:ILE:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:29:ALA:CB	11:G:5:ILE:HG22	2.48	0.44
8:D:93:HIS:CD2	8:D:94:LYS:H	2.35	0.44
13:I:103:ARG:HD2	13:I:103:ARG:O	2.18	0.44
20:P:186:ARG:HE	20:P:244:LEU:HA	1.83	0.44
23:S:168:ASN:OD1	23:S:169:LYS:N	2.51	0.44
24:T:175:ARG:HB2	24:T:209:PRO:HD3	2.00	0.44
27:W:105:GLU:HG2	27:W:487:LYS:CD	2.45	0.44
29:Y:504:LYS:CA	29:Y:507:PRO:CG	2.96	0.44
32:b:147:MET:HB3	32:b:157:MET:HE1	1.99	0.44
35:e:182:GLU:HG2	35:e:183:LEU:N	2.33	0.44
38:h:146:MET:O	38:h:150:LEU:HG	2.17	0.44
42:l:76:PHE:CD1	42:l:86:ILE:HG23	2.52	0.44
43:m:47:GLN:HG3	43:m:48:VAL:H	1.83	0.44
44:n:311:GLN:O	48:r:543:THR:OG1	2.34	0.44
46:p:92:GLN:O	46:p:93:LYS:HB2	2.18	0.44
46:p:157:TYR:HB3	46:p:158:PRO:HD3	2.00	0.44
48:r:93:ARG:HA	48:r:96:PHE:HB2	1.99	0.44
48:r:114:LYS:O	48:r:117:MET:HB3	2.18	0.44
48:r:520:LEU:HB3	48:r:522:LEU:HG	1.98	0.44
48:r:743:ARG:HB2	48:r:805:TYR:HE2	1.83	0.44
48:r:1205:SER:O	48:r:1208:GLU:N	2.50	0.44
49:s:86:GLN:O	49:s:90:HIS:CB	2.65	0.44
50:t:75:LYS:CD	54:x:79:GLU:HB3	2.48	0.44
50:t:137:VAL:O	50:t:141:VAL:HG22	2.18	0.44
51:u:111:PRO:HB2	51:u:112:GLU:OE1	2.18	0.44
53:w:95:LYS:HB2	53:w:96:PHE:CD2	2.53	0.44
55:y:16:LEU:C	55:y:18:PHE:N	2.74	0.44
55:y:27:CYS:C	55:y:29:ALA:N	2.74	0.44
1:0:111:ALA:HB2	1:0:119:GLU:HB3	1.99	0.44
1:0:484:THR:HG23	1:0:486:TYR:H	1.81	0.44
4:3:45:GLU:OE2	4:3:51:PRO:HD3	2.17	0.44
4:3:170:VAL:O	4:3:173:ILE:HG22	2.18	0.44
5:A:1177:TYR:CE2	5:A:1179:PRO:HG3	2.53	0.44
5:A:1215:GLU:HB3	5:A:1255:LEU:HG	2.00	0.44
5:A:1481:LYS:HZ3	48:r:331:ALA:HB3	1.81	0.44
6:B:98:HIS:O	6:B:105:PRO:HA	2.18	0.44
6:B:1167:ILE:O	6:B:1169:PRO:HD3	2.18	0.44
10:F:84:GLU:HG2	10:F:95:LYS:NZ	2.33	0.44
17:M:39:LEU:O	17:M:42:LEU:HG	2.18	0.44
17:M:315:ASN:HA	17:M:318:ASP:HA	1.99	0.44
17:M:333:ASN:ND2	18:N:93:VAL:HA	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:12:ARG:HE	19:O:23:LEU:HD12	1.82	0.44
27:W:612:ASP:HA	27:W:613:THR:HA	1.68	0.44
27:W:624:ILE:HG12	27:W:660:TYR:HB2	1.99	0.44
28:X:309:VAL:CG2	28:X:402:ASN:CG	2.88	0.44
31:a:59:ARG:NH1	31:a:236:VAL:O	2.42	0.44
35:e:174:VAL:CG1	35:e:179:ARG:HG3	2.48	0.44
37:g:99:TYR:O	37:g:106:TYR:N	2.33	0.44
38:h:114:ASP:HB3	38:h:117:VAL:HG23	2.00	0.44
40:j:377:LEU:HD13	47:q:177:ARG:HB2	2.00	0.44
44:n:139:GLN:HG3	47:q:39:GLU:HG2	2.00	0.44
44:n:245:HIS:HD2	44:n:295:THR:O	2.00	0.44
48:r:874:ASP:O	48:r:875:THR:OG1	2.36	0.44
50:t:121:HIS:O	50:t:124:ASN:HB2	2.18	0.44
50:t:142:GLN:C	50:t:146:ARG:NE	2.75	0.44
50:t:146:ARG:NH1	54:x:97:ASN:HB3	2.28	0.44
50:t:152:ARG:HH11	50:t:152:ARG:C	2.25	0.44
51:u:122:ARG:HB3	51:u:126:ARG:NE	2.33	0.44
52:v:7:HIS:ND1	52:v:11:HIS:CD2	2.86	0.44
52:v:30:GLN:O	52:v:32:SER:N	2.51	0.44
52:v:89:LEU:O	52:v:91:LYS:N	2.51	0.44
52:v:112:GLU:O	52:v:113:LEU:C	2.60	0.44
53:w:82:ASN:O	53:w:84:ILE:N	2.51	0.44
54:x:74:ASP:O	54:x:75:SER:C	2.58	0.44
55:y:31:PRO:O	55:y:34:LEU:CA	2.65	0.44
55:y:35:ASN:HA	55:y:38:ALA:HB3	2.00	0.44
55:y:127:ASN:C	55:y:130:GLY:H	2.26	0.44
1:0:459:PRO:HD3	1:0:494:HIS:CD2	2.52	0.43
1:0:579:ARG:O	1:0:582:GLU:HG3	2.18	0.43
2:1:427:CYS:SG	2:1:480:ALA:HB2	2.57	0.43
2:1:485:SER:HA	2:1:488:PHE:HE1	1.81	0.43
3:2:181:ALA:O	3:2:185:GLU:HG2	2.18	0.43
3:2:357:CYS:HB3	3:2:405:PRO:HG3	2.00	0.43
3:2:498:LEU:HD13	3:2:665:ILE:HG23	2.00	0.43
3:2:909:SER:CB	3:2:952:VAL:HG21	2.48	0.43
5:A:14:PRO:HG2	11:G:12:LEU:CD1	2.48	0.43
5:A:549:THR:HG21	5:A:640:LEU:HD13	2.00	0.43
5:A:1148:ALA:O	5:A:1334:TRP:HD1	2.00	0.43
5:A:1338:THR:HG22	5:A:1339:ASP:H	1.83	0.43
5:A:1362:ILE:HG22	5:A:1411:LEU:HD21	2.00	0.43
5:A:1624:PRO:CG	38:h:107:ASP:OD2	2.66	0.43
6:B:364:PHE:O	6:B:368:MET:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:138:ARG:HA	8:D:140:PHE:CE1	2.52	0.43
10:F:49:GLN:O	10:F:50:LYS:HE2	2.18	0.43
19:O:12:ARG:NE	19:O:23:LEU:HD12	2.32	0.43
20:P:169:VAL:HG11	25:U:15:DA:C2	2.53	0.43
20:P:302:LEU:HD11	20:P:312:LEU:HG	2.00	0.43
22:R:229:ASP:HA	22:R:232:LYS:HE2	1.99	0.43
24:T:42:LYS:HG3	24:T:42:LYS:O	2.18	0.43
24:T:194:HIS:HB2	24:T:197:TYR:CE1	2.53	0.43
29:Y:504:LYS:C	29:Y:508:PHE:CD2	2.90	0.43
30:Z:65:PRO:HB2	30:Z:107:GLY:HA3	2.00	0.43
39:i:81:GLY:HA2	41:k:45:ASN:ND2	2.34	0.43
40:j:247:ILE:HD12	40:j:252:GLU:HA	1.99	0.43
40:j:464:TRP:CD2	40:j:475:VAL:HG23	2.52	0.43
41:k:130:VAL:CG1	41:k:149:PHE:HB2	2.46	0.43
41:k:193:LEU:HD13	41:k:197:VAL:CG1	2.47	0.43
42:l:148:VAL:O	42:l:149:VAL:C	2.61	0.43
48:r:104:LYS:HB3	53:w:108:PHE:HE2	1.81	0.43
49:s:119:GLN:O	49:s:123:THR:HG23	2.18	0.43
49:s:145:SER:HA	49:s:148:ILE:HG12	2.00	0.43
49:s:149:ILE:C	49:s:151:TYR:N	2.74	0.43
49:s:191:ASN:O	49:s:192:ASN:C	2.61	0.43
50:t:124:ASN:O	50:t:125:GLU:C	2.58	0.43
52:v:60:ASP:OD1	52:v:60:ASP:O	2.35	0.43
54:x:18:GLN:NE2	54:x:68:ASP:HB2	2.27	0.43
55:y:81:TYR:O	55:y:82:GLU:C	2.60	0.43
55:y:116:GLN:OE1	55:y:119:LEU:CD1	2.66	0.43
1:0:62:ILE:HG13	1:0:78:SER:HB3	1.99	0.43
1:0:236:ALA:H	1:0:266:ARG:CZ	2.30	0.43
1:0:792:THR:HG22	44:n:40:ARG:C	2.42	0.43
2:1:584:PHE:CD1	2:1:588:LEU:HD23	2.52	0.43
3:2:414:GLU:HB3	3:2:415:PRO:HD3	1.99	0.43
3:2:957:LYS:HA	3:2:957:LYS:HD2	1.91	0.43
4:3:45:GLU:C	4:3:47:PHE:N	2.75	0.43
5:A:316:THR:HG21	5:A:329:MET:HE2	1.98	0.43
5:A:962:ASP:OD2	5:A:1043:ILE:HG12	2.18	0.43
5:A:1203:ASP:HB3	5:A:1266:GLU:OE2	2.18	0.43
6:B:53:MET:O	6:B:53:MET:HG2	2.18	0.43
6:B:285:LEU:HD21	6:B:305:LEU:HD11	1.99	0.43
6:B:1143:LYS:HZ2	11:G:151:ARG:NE	2.16	0.43
7:C:256:LEU:HD22	15:K:91:ILE:HG13	1.99	0.43
8:D:126:GLU:HG2	8:D:127:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:88:PHE:HD1	12:H:146:LYS:HB2	1.83	0.43
17:M:360:LEU:HD21	17:M:365:TYR:HD2	1.82	0.43
18:N:35:GLN:O	18:N:39:GLN:HG2	2.18	0.43
19:O:244:LEU:O	19:O:246:PRO:HD3	2.18	0.43
20:P:172:VAL:HG22	20:P:253:PHE:HA	2.00	0.43
21:Q:12:ALA:O	21:Q:16:ARG:HG2	2.18	0.43
28:X:532:PRO:CB	31:a:204:GLU:O	2.66	0.43
30:Z:433:PHE:CE1	33:c:42:HIS:CG	2.89	0.43
30:Z:442:VAL:HG11	33:c:9:LEU:HD23	1.94	0.43
32:b:19:PRO:HD2	32:b:64:ILE:HG23	2.00	0.43
36:f:185:GLU:O	36:f:188:ARG:HB3	2.18	0.43
37:g:82:ARG:CZ	37:g:94:PRO:HG3	2.48	0.43
37:g:99:TYR:OH	38:h:78:PRO:HB3	2.18	0.43
40:j:183:PHE:CD1	40:j:228:THR:OG1	2.68	0.43
40:j:314:GLU:OE1	40:j:427:LEU:N	2.51	0.43
40:j:414:ASP:HA	40:j:418:ILE:HB	2.00	0.43
42:l:68:ASN:CB	42:l:190:MET:HE2	2.48	0.43
48:r:1233:ASN:HB3	48:r:1243:LYS:HG2	1.99	0.43
50:t:79:ARG:HA	50:t:82:ASN:OD1	2.18	0.43
50:t:105:ARG:HB2	50:t:106:GLU:H	1.57	0.43
50:t:127:ARG:NH2	54:x:9:GLN:OE1	2.43	0.43
52:v:80:TYR:HA	52:v:83:GLU:HG3	2.00	0.43
52:v:124:TYR:CE1	52:v:127:ILE:HD12	2.52	0.43
54:x:129:GLN:HA	54:x:132:THR:CB	2.48	0.43
55:y:21:GLU:HB2	55:y:58:TRP:HZ2	1.81	0.43
55:y:35:ASN:C	55:y:38:ALA:H	2.26	0.43
1:0:730:ASP:HB3	1:0:779:ILE:HG13	2.00	0.43
1:0:812:ARG:NE	46:p:90:ASN:CB	2.72	0.43
4:3:123:GLN:HA	4:3:123:GLN:HE21	1.78	0.43
4:3:124:LEU:HD12	4:3:124:LEU:HA	1.61	0.43
5:A:575:PRO:HG3	5:A:594:LEU:HD11	1.99	0.43
5:A:1189:ASP:HB2	5:A:1192:TRP:CD1	2.52	0.43
5:A:1218:ARG:HH22	5:A:1248:ASN:HD21	1.67	0.43
8:D:78:GLU:O	38:h:51:LEU:CD2	2.66	0.43
8:D:129:GLN:CG	38:h:65:HIS:CE1	2.89	0.43
9:E:94:MET:HE3	9:E:94:MET:HB3	1.96	0.43
20:P:194:PRO:HB2	24:T:176:ALA:HB2	2.01	0.43
22:R:184:ALA:O	22:R:189:ILE:HG23	2.19	0.43
27:W:159:CYS:O	27:W:163:TYR:CE2	2.67	0.43
27:W:398:ASP:N	27:W:398:ASP:OD1	2.51	0.43
27:W:516:PRO:CD	33:c:18:GLN:OE1	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:533:ASP:OD2	31:a:205:VAL:HA	2.19	0.43
28:X:616:ARG:O	28:X:676:LEU:N	2.51	0.43
29:Y:372:ILE:HD13	31:a:54:ARG:NH1	2.33	0.43
30:Z:300:THR:HG22	30:Z:302:HIS:H	1.84	0.43
30:Z:440:LEU:HD13	33:c:36:GLN:CG	2.48	0.43
31:a:189:LEU:HD22	31:a:194:ILE:HG21	2.01	0.43
31:a:249:LEU:CB	32:b:289:PHE:HE1	2.27	0.43
34:d:246:TYR:CD1	35:e:119:LEU:HD21	2.53	0.43
38:h:31:CYS:HA	38:h:34:GLU:OE2	2.18	0.43
39:i:78:PRO:CB	40:j:197:ARG:CD	2.93	0.43
39:i:78:PRO:HG3	40:j:197:ARG:HD2	1.78	0.43
39:i:87:ARG:NE	40:j:296:GLU:OE2	2.51	0.43
40:j:336:PHE:CZ	40:j:500:GLU:CA	2.98	0.43
40:j:647:SER:OG	40:j:648:PRO:HD2	2.17	0.43
47:q:96:TYR:HA	47:q:99:CYS:SG	2.58	0.43
48:r:68:VAL:O	48:r:69:LEU:C	2.60	0.43
48:r:130:VAL:HG23	48:r:131:ASP:OD1	2.18	0.43
48:r:168:ARG:HD2	48:r:168:ARG:H	1.82	0.43
48:r:233:THR:O	48:r:248:LEU:HD12	2.19	0.43
48:r:243:VAL:HA	48:r:244:PRO:HD2	1.81	0.43
48:r:452:LEU:HA	48:r:467:LEU:HD13	2.00	0.43
48:r:1318:HIS:HB3	48:r:1436:PHE:CD1	2.54	0.43
50:t:133:GLU:O	50:t:137:VAL:HG22	2.18	0.43
52:v:71:ILE:HG22	52:v:76:ASN:HA	2.00	0.43
52:v:99:ILE:C	52:v:103:LYS:HZ1	2.26	0.43
54:x:118:ILE:HG13	54:x:119:GLN:H	1.79	0.43
54:x:126:ALA:O	54:x:129:GLN:NE2	2.51	0.43
55:y:46:LYS:C	55:y:48:PHE:N	2.74	0.43
55:y:73:LEU:O	55:y:75:MET:N	2.51	0.43
55:y:83:HIS:HA	55:y:86:LYS:HG2	1.99	0.43
55:y:120:ALA:HA	55:y:123:GLN:OE1	2.18	0.43
1:0:43:ASN:ND2	1:0:489:TRP:HB3	2.33	0.43
1:0:570:ASN:OD1	1:0:572:PRO:HD2	2.18	0.43
1:0:796:LYS:HA	1:0:834:TRP:O	2.17	0.43
2:1:883:TYR:HB3	2:1:974:PHE:CE1	2.53	0.43
2:1:1167:ARG:HD3	2:1:1167:ARG:HA	1.77	0.43
2:1:1235:LEU:HD12	2:1:1235:LEU:HA	1.80	0.43
3:2:554:VAL:O	3:2:558:VAL:HG22	2.18	0.43
4:3:71:PHE:HB3	4:3:82:VAL:CG1	2.49	0.43
5:A:88:ILE:HD12	5:A:253:LEU:HD23	2.00	0.43
5:A:1161:LEU:CB	5:A:1307:VAL:HG11	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1349:GLU:HG2	5:A:1350:LYS:N	2.33	0.43
5:A:1443:ALA:HB2	6:B:1167:ILE:HG23	2.00	0.43
6:B:309:PHE:HZ	13:I:25:TYR:HE2	1.66	0.43
6:B:400:LEU:HD21	6:B:448:LEU:HD11	2.01	0.43
19:O:154:ARG:HH21	19:O:197:LEU:HD11	1.84	0.43
20:P:191:GLU:HG3	20:P:201:ILE:HB	1.99	0.43
23:S:167:ARG:HG2	23:S:168:ASN:N	2.31	0.43
27:W:339:VAL:HG21	27:W:470:LEU:HG	2.01	0.43
30:Z:254:MET:HE2	30:Z:258:LEU:HB3	2.01	0.43
30:Z:403:PHE:CE2	33:c:54:GLN:HA	2.53	0.43
37:g:130:PHE:CE2	43:m:62:HIS:HB3	2.52	0.43
39:i:17:ILE:HD11	39:i:59:VAL:HG22	2.01	0.43
40:j:198:LYS:HB3	43:m:88:LEU:CD2	2.35	0.43
40:j:367:HIS:CD2	40:j:438:ILE:HG22	2.52	0.43
42:l:9:MET:SD	42:l:10:PRO:HD2	2.59	0.43
42:l:72:PRO:O	42:l:73:LEU:HD22	2.17	0.43
42:l:129:VAL:HG21	42:l:200:ILE:HG12	1.99	0.43
43:m:29:ILE:CD1	43:m:68:ILE:HG23	2.48	0.43
48:r:105:TRP:HE1	53:w:108:PHE:HB2	1.83	0.43
48:r:138:SER:O	48:r:139:LEU:C	2.59	0.43
48:r:509:ILE:HD12	48:r:509:ILE:HA	1.78	0.43
49:s:128:ALA:O	49:s:129:LYS:C	2.61	0.43
49:s:140:LYS:C	49:s:142:ALA:H	2.23	0.43
50:t:32:PRO:C	55:y:18:PHE:CE1	2.96	0.43
51:u:92:SER:O	51:u:96:GLU:HG2	2.19	0.43
53:w:92:ALA:CA	53:w:95:LYS:HD2	2.45	0.43
54:x:69:ILE:O	54:x:72:LEU:HB2	2.18	0.43
55:y:26:GLN:NE2	55:y:68:LYS:H	2.15	0.43
1:0:593:ASP:HB2	1:0:690:PHE:CD2	2.53	0.43
2:1:385:GLN:HE22	2:1:483:THR:HG22	1.84	0.43
2:1:946:GLN:NE2	2:1:947:ILE:O	2.51	0.43
2:1:1043:CYS:O	2:1:1044:LEU:C	2.61	0.43
3:2:74:SER:HB2	3:2:77:SER:H	1.83	0.43
3:2:183:LEU:HD23	3:2:979:ARG:HH11	1.83	0.43
5:A:95:PHE:HB2	5:A:311:GLN:NE2	2.33	0.43
6:B:17:ILE:HG22	6:B:18:THR:H	1.84	0.43
9:E:82:VAL:O	9:E:111:THR:HG23	2.18	0.43
18:N:56:VAL:HG12	18:N:57:ASN:N	2.33	0.43
18:N:90:VAL:CG1	18:N:93:VAL:HG22	2.48	0.43
19:O:105:ARG:HG2	19:O:107:MET:HG2	1.99	0.43
19:O:143:LYS:HA	19:O:146:TYR:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:130:ILE:HD12	22:R:140:LYS:HG3	1.99	0.43
22:R:165:GLY:HA2	22:R:169:GLU:OE1	2.18	0.43
29:Y:432:THR:O	29:Y:435:SER:OG	2.31	0.43
35:e:79:ASP:HB3	35:e:90:VAL:HB	2.00	0.43
35:e:94:MET:SD	35:e:146:ASP:HB3	2.59	0.43
35:e:231:THR:HG23	35:e:252:PHE:H	1.84	0.43
36:f:11:TRP:HE1	36:f:157:HIS:HD2	1.66	0.43
36:f:235:SER:O	36:f:236:LEU:HD12	2.18	0.43
37:g:119:VAL:O	37:g:123:VAL:HG23	2.19	0.43
39:i:82:SER:HB3	40:j:211:SER:CB	2.49	0.43
40:j:381:GLU:O	40:j:385:GLN:HG2	2.19	0.43
40:j:410:PRO:HB3	41:k:111:SER:N	2.33	0.43
40:j:443:ARG:HE	40:j:518:GLU:HG2	1.83	0.43
40:j:492:GLN:NE2	40:j:507:ARG:NE	2.65	0.43
46:p:160:TYR:O	46:p:163:VAL:HG12	2.19	0.43
47:q:163:LEU:HA	47:q:163:LEU:HD12	1.77	0.43
48:r:128:LEU:HD11	50:t:105:ARG:HE	1.83	0.43
48:r:169:LEU:HD23	48:r:175:ASP:OD2	2.18	0.43
48:r:640:VAL:HG13	48:r:641:LEU:CD2	2.49	0.43
49:s:122:ALA:O	49:s:123:THR:C	2.62	0.43
49:s:128:ALA:O	49:s:131:LYS:CB	2.67	0.43
50:t:113:LYS:O	50:t:117:VAL:HG13	2.17	0.43
52:v:39:GLN:OE1	52:v:42:ASN:HB3	2.19	0.43
52:v:92:ASN:HA	52:v:95:VAL:CG1	2.47	0.43
52:v:109:LEU:O	52:v:112:GLU:HG3	2.18	0.43
54:x:52:GLU:OE2	54:x:55:ALA:HB3	2.17	0.43
55:y:35:ASN:O	55:y:38:ALA:N	2.49	0.43
55:y:83:HIS:O	55:y:87:GLU:OE2	2.36	0.43
56:z:721:LEU:HD11	56:z:736:TRP:CZ3	2.53	0.43
56:z:731:ALA:HA	56:z:766:LYS:HZ3	1.84	0.43
1:0:170:LEU:HD13	1:0:174:LYS:O	2.18	0.43
1:0:625:VAL:HG11	1:0:659:MET:HE2	1.99	0.43
1:0:696:LEU:HG	1:0:708:GLU:OE2	2.19	0.43
1:0:780:ASP:HA	1:0:804:VAL:O	2.17	0.43
1:0:800:ARG:N	1:0:800:ARG:HD2	2.34	0.43
2:1:292:GLN:NE2	2:1:293:HIS:HB2	2.34	0.43
2:1:1060:PRO:O	2:1:1062:VAL:N	2.50	0.43
2:1:1229:LYS:HE2	2:1:1229:LYS:HB2	1.72	0.43
3:2:118:ILE:HD11	3:2:184:GLU:OE2	2.18	0.43
3:2:290:PHE:HE1	3:2:359:CYS:SG	2.40	0.43
4:3:113:LEU:HD12	4:3:113:LEU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:468:SER:O	5:A:468:SER:OG	2.34	0.43
5:A:962:ASP:O	5:A:966:LEU:HB2	2.19	0.43
6:B:816:GLU:HG2	6:B:867:ILE:HG21	2.01	0.43
7:C:45:ILE:HD13	7:C:128:ILE:HD11	2.01	0.43
7:C:67:ARG:NH2	14:J:2:ILE:HG23	2.33	0.43
8:D:141:GLN:HB3	43:m:67:ASN:CG	2.44	0.43
11:G:149:GLY:O	11:G:160:ILE:HG12	2.18	0.43
15:K:36:ASN:OD1	15:K:70:LYS:NZ	2.49	0.43
23:S:49:ARG:NE	23:S:50:ASP:OD1	2.50	0.43
24:T:207:LYS:HD2	24:T:207:LYS:HA	1.78	0.43
26:V:40:DT:P	27:W:610:VAL:HG12	2.58	0.43
28:X:328:HIS:HE1	34:d:107:PHE:HB2	1.83	0.43
31:a:60:HIS:CD2	31:a:163:THR:HG21	2.54	0.43
38:h:74:GLN:O	38:h:76:ILE:N	2.37	0.43
39:i:20:GLU:HG2	39:i:58:HIS:HD2	1.82	0.43
39:i:83:SER:O	39:i:83:SER:OG	2.25	0.43
40:j:544:MET:HB3	45:o:89:ARG:HD3	2.00	0.43
42:l:111:GLU:OE2	42:l:113:ARG:HB2	2.19	0.43
45:o:68:THR:O	45:o:69:ASP:C	2.61	0.43
47:q:139:ARG:CG	47:q:140:ARG:HD3	2.49	0.43
48:r:78:ASP:O	48:r:81:ARG:HB2	2.18	0.43
48:r:111:LYS:O	48:r:112:VAL:C	2.62	0.43
48:r:141:ARG:O	48:r:142:ASP:C	2.60	0.43
48:r:330:HIS:C	48:r:332:GLY:H	2.26	0.43
48:r:471:ASP:C	48:r:473:ALA:H	2.26	0.43
48:r:794:LEU:O	48:r:797:PHE:O	2.37	0.43
48:r:869:LEU:HD13	48:r:869:LEU:HA	1.75	0.43
49:s:64:GLN:HE21	49:s:68:LEU:HD11	1.83	0.43
49:s:109:GLN:HG3	49:s:110:LEU:H	1.83	0.43
50:t:119:VAL:O	50:t:120:HIS:C	2.59	0.43
52:v:61:ILE:O	52:v:62:THR:C	2.61	0.43
54:x:90:LEU:O	54:x:94:GLU:N	2.51	0.43
55:y:61:PRO:O	55:y:62:GLU:C	2.60	0.43
1:0:207:CYS:SG	3:2:680:GLN:HB3	2.58	0.43
1:0:213:VAL:HG23	1:0:213:VAL:O	2.19	0.43
1:0:521:VAL:HG21	4:3:153:LEU:HD13	2.01	0.43
2:1:423:PHE:HZ	2:1:457:PHE:HB3	1.82	0.43
2:1:765:ARG:O	2:1:769:SER:OG	2.23	0.43
3:2:80:THR:O	3:2:84:LYS:HG2	2.18	0.43
5:A:112:PHE:O	5:A:113:PHE:HB2	2.18	0.43
5:A:311:GLN:HA	5:A:314:VAL:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:540:ASP:OD2	6:B:784:SER:HB2	2.18	0.43
5:A:800:PHE:CE1	5:A:820:ARG:HD2	2.54	0.43
5:A:1052:ARG:HE	5:A:1056:GLU:CD	2.27	0.43
6:B:374:LEU:HD22	6:B:379:ARG:HG3	2.00	0.43
7:C:124:SER:CB	7:C:127:VAL:HB	2.48	0.43
10:F:61:GLU:CD	10:F:108:ARG:HH21	2.26	0.43
11:G:90:THR:OG1	11:G:91:GLN:N	2.51	0.43
19:O:30:GLY:O	19:O:45:VAL:N	2.50	0.43
20:P:166:GLN:OE1	26:V:81:DA:OP1	2.37	0.43
24:T:81:HIS:ND1	24:T:82:PRO:HD2	2.33	0.43
24:T:211:VAL:HG12	25:U:20:DG:H3'	2.00	0.43
28:X:319:VAL:HG11	28:X:324:ARG:HH21	1.84	0.43
28:X:542:TYR:O	28:X:546:GLU:HB2	2.19	0.43
30:Z:409:TYR:CB	30:Z:412:PHE:HZ	2.23	0.43
37:g:83:LYS:HA	37:g:83:LYS:HD2	1.69	0.43
39:i:104:LEU:HA	39:i:107:VAL:HG22	1.99	0.43
40:j:323:PRO:HG3	48:r:455:PHE:CD2	2.54	0.43
40:j:486:GLN:CD	40:j:486:GLN:C	2.85	0.43
41:k:84:HIS:HE1	41:k:107:ASP:HB3	1.84	0.43
44:n:17:ALA:CB	46:p:120:LEU:HD21	2.49	0.43
44:n:113:TRP:CZ3	44:n:117:LEU:HD22	2.54	0.43
45:o:66:ASN:HD22	48:r:883:ASN:HB3	1.83	0.43
47:q:72:GLN:O	47:q:76:THR:HG23	2.19	0.43
48:r:51:LEU:HB3	48:r:52:SER:H	1.58	0.43
48:r:135:ARG:CZ	50:t:109:LEU:HB3	2.49	0.43
48:r:401:LEU:O	48:r:405:VAL:HG13	2.19	0.43
48:r:726:PHE:HB2	48:r:805:TYR:CE2	2.54	0.43
48:r:893:LEU:HD13	48:r:1295:LYS:HB3	2.01	0.43
48:r:919:ARG:HD3	48:r:919:ARG:N	2.26	0.43
48:r:940:ALA:O	48:r:950:VAL:HG13	2.19	0.43
48:r:1209:ARG:HH21	48:r:1259:GLN:HB3	1.83	0.43
48:r:1363:MET:O	48:r:1387:ILE:HA	2.19	0.43
50:t:26:ILE:O	50:t:27:GLN:C	2.60	0.43
51:u:130:GLU:HA	51:u:133:GLN:OE1	2.19	0.43
52:v:60:ASP:O	52:v:61:ILE:C	2.61	0.43
52:v:79:LEU:O	52:v:82:LYS:HB2	2.19	0.43
52:v:110:ILE:HA	52:v:113:LEU:HB3	2.00	0.43
54:x:117:LYS:C	54:x:120:SER:HG	2.12	0.43
55:y:26:GLN:HE22	55:y:68:LYS:H	1.66	0.43
55:y:76:LEU:O	55:y:80:GLN:HB3	2.19	0.43
55:y:77:GLU:H	55:y:77:GLU:HG2	1.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:564:VAL:HG21	2:1:955:TYR:CD2	2.54	0.43
2:1:1292:ASP:HB2	2:1:1293:PRO:HD3	2.01	0.43
3:2:175:ARG:O	3:2:178:LEU:HB3	2.19	0.43
3:2:622:ALA:HB2	3:2:673:MET:HE1	2.00	0.43
3:2:734:THR:O	3:2:738:MET:HB3	2.19	0.43
3:2:945:GLN:CB	3:2:949:PHE:HD2	2.31	0.43
5:A:31:LEU:HD22	5:A:254:PRO:HG3	2.00	0.43
5:A:544:ALA:HB1	5:A:676:ILE:HG22	2.01	0.43
5:A:1282:ASP:OD2	13:I:26:PRO:HB2	2.19	0.43
5:A:1419:VAL:HG21	5:A:1432:PHE:CE2	2.54	0.43
6:B:665:ILE:HD11	6:B:695:HIS:NE2	2.34	0.43
6:B:721:ARG:HD3	6:B:721:ARG:HA	1.81	0.43
12:H:99:ILE:O	12:H:99:ILE:HG13	2.19	0.43
15:K:77:THR:HG21	15:K:81:TYR:HB3	2.01	0.43
17:M:44:THR:O	17:M:47:GLU:HG3	2.19	0.43
17:M:311:GLU:OE2	20:P:235:ARG:HD2	2.19	0.43
21:Q:172:ASP:N	21:Q:172:ASP:OD1	2.51	0.43
22:R:111:ILE:O	22:R:114:LYS:N	2.51	0.43
27:W:522:TYR:HE1	27:W:534:TYR:HD2	1.67	0.43
29:Y:471:LEU:CD1	29:Y:502:VAL:HG13	2.49	0.43
35:e:64:LYS:HG3	36:f:159:ILE:HD11	2.01	0.43
38:h:115:PRO:O	38:h:118:GLU:HB2	2.19	0.43
40:j:479:ILE:HG23	40:j:529:MET:SD	2.56	0.43
42:l:28:LEU:HD21	42:l:124:VAL:HG13	2.01	0.43
48:r:61:ARG:HH22	48:r:65:GLU:CG	2.32	0.43
48:r:735:SER:C	48:r:737:ARG:H	2.26	0.43
49:s:103:ARG:HD2	51:u:121:LEU:HD22	2.00	0.43
50:t:16:GLN:OE1	50:t:19:LYS:NZ	2.36	0.43
52:v:23:GLY:O	52:v:26:VAL:N	2.51	0.43
52:v:86:GLU:HB2	52:v:87:ARG:HH11	1.82	0.43
54:x:11:ALA:HB1	54:x:72:LEU:CD2	2.48	0.43
54:x:16:ALA:HA	54:x:19:PHE:CD2	2.53	0.43
54:x:26:LEU:H	54:x:26:LEU:HD12	1.84	0.43
54:x:52:GLU:C	54:x:55:ALA:H	2.27	0.43
54:x:104:LEU:O	54:x:105:GLU:C	2.61	0.43
55:y:26:GLN:HB3	55:y:68:LYS:NZ	2.34	0.43
55:y:65:LYS:HG3	55:y:66:TYR:CZ	2.54	0.43
1:0:144:ALA:HB3	1:0:160:SER:OG	2.18	0.43
1:0:167:SER:O	1:0:168:LEU:HB2	2.19	0.43
1:0:405:PHE:CG	1:0:405:PHE:O	2.69	0.43
1:0:482:MET:HG3	1:0:529:MET:SD	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:199:LEU:HD21	3:2:203:LEU:HD22	2.01	0.43
3:2:965:LYS:NZ	3:2:968:LEU:HB3	2.34	0.43
4:3:37:LYS:O	4:3:42:PRO:HD2	2.18	0.43
5:A:41:ILE:HD11	5:A:88:ILE:HD11	2.01	0.43
5:A:220:ARG:NE	22:R:226:ASP:HB2	2.33	0.43
5:A:1231:ILE:O	5:A:1235:ILE:HG12	2.19	0.43
5:A:1307:VAL:HA	5:A:1338:THR:HA	2.01	0.43
5:A:1473:LEU:CB	11:G:59:ILE:HD11	2.49	0.43
6:B:711:ILE:HG21	6:B:722:ASN:OD1	2.18	0.43
6:B:795:ILE:HG12	6:B:947:ILE:HG22	2.00	0.43
7:C:100:GLU:HG3	7:C:164:TYR:CE1	2.53	0.43
7:C:115:VAL:O	7:C:150:ILE:HG22	2.17	0.43
8:D:94:LYS:H	8:D:94:LYS:HG3	1.64	0.43
9:E:63:ALA:HB2	9:E:71:GLN:HA	2.01	0.43
10:F:69:ARG:HA	10:F:69:ARG:HD2	1.75	0.43
17:M:371:ILE:HG23	18:N:55:ARG:HH12	1.84	0.43
21:Q:53:LYS:O	22:R:199:LYS:HE2	2.18	0.43
23:S:114:LYS:HA	23:S:144:TYR:HB3	2.00	0.43
27:W:511:TRP:HH2	30:Z:348:ARG:NH1	2.16	0.43
28:X:25:MET:SD	28:X:55:LEU:HB2	2.59	0.43
29:Y:523:SER:OG	31:a:269:PRO:HD3	2.17	0.43
30:Z:58:ARG:CD	32:b:241:LEU:CD2	2.69	0.43
31:a:289:TYR:OH	32:b:251:TYR:CE2	2.72	0.43
34:d:113:VAL:HG12	34:d:115:LEU:H	1.84	0.43
34:d:193:PRO:HG2	34:d:196:LEU:HD12	1.99	0.43
35:e:239:ASP:O	35:e:239:ASP:CG	2.62	0.43
36:f:163:PRO:HA	36:f:166:PRO:HG2	1.99	0.43
36:f:195:LEU:O	36:f:198:ILE:HG22	2.19	0.43
37:g:30:LEU:HA	37:g:33:PHE:CE2	2.54	0.43
40:j:475:VAL:HG12	40:j:495:LEU:HB2	2.01	0.43
40:j:482:GLN:OE1	43:m:137:SER:CB	2.67	0.43
41:k:118:LEU:HD22	41:k:123:PHE:CE2	2.54	0.43
42:l:92:ASP:O	42:l:96:VAL:HG23	2.19	0.43
43:m:26:ILE:O	43:m:29:ILE:HG22	2.19	0.43
44:n:70:LEU:HD12	44:n:70:LEU:HA	1.90	0.43
45:o:57:ALA:HA	45:o:60:VAL:HG12	2.01	0.43
48:r:97:VAL:O	48:r:98:ARG:C	2.60	0.43
48:r:193:HIS:O	48:r:197:GLN:HG2	2.18	0.43
49:s:114:LEU:HD12	54:x:122:LEU:HD21	2.01	0.43
49:s:132:LEU:O	49:s:133:LYS:C	2.62	0.43
50:t:16:GLN:CD	50:t:17:TYR:HD1	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:22:THR:O	50:t:25:ASN:N	2.52	0.43
52:v:34:GLN:O	52:v:38:ASN:N	2.22	0.43
52:v:95:VAL:HG13	52:v:96:LYS:N	2.34	0.43
54:x:3:ASP:O	54:x:4:ARG:C	2.61	0.43
54:x:111:GLY:O	54:x:112:ASP:C	2.59	0.43
55:y:28:LEU:HD23	55:y:33:TYR:CE2	2.54	0.43
55:y:82:GLU:HA	55:y:85:ARG:CZ	2.48	0.43
56:z:678:LEU:HD12	56:z:678:LEU:HA	1.77	0.43
1:0:170:LEU:HG	1:0:172:GLY:H	1.84	0.43
1:0:287:ALA:HB3	1:0:290:MET:HB3	2.01	0.43
2:1:488:PHE:C	2:1:491:PRO:HD2	2.44	0.43
2:1:1057:GLU:N	2:1:1057:GLU:OE2	2.51	0.43
2:1:1074:ARG:NH2	2:1:1087:PHE:HE1	2.16	0.43
3:2:631:LEU:HD23	3:2:631:LEU:HA	1.89	0.43
5:A:931:ARG:C	5:A:933:THR:H	2.27	0.43
8:D:142:TYR:OH	43:m:20:LYS:C	2.62	0.43
8:D:142:TYR:CD2	43:m:25:ASP:OD1	2.72	0.43
9:E:26:TYR:CE2	9:E:72:MET:HB2	2.54	0.43
24:T:24:PRO:HG2	24:T:27:LEU:HD22	2.01	0.43
24:T:40:VAL:O	24:T:43:LEU:HD13	2.18	0.43
26:V:49:DG:H2"	26:V:50:DA:C8	2.53	0.43
27:W:134:SER:O	27:W:138:GLU:HB2	2.18	0.43
27:W:165:LYS:CD	27:W:181:HIS:CE1	3.02	0.43
28:X:170:LEU:HD21	28:X:194:LEU:HD21	2.01	0.43
29:Y:140:GLU:O	29:Y:144:ALA:HB2	2.19	0.43
31:a:282:PRO:O	31:a:282:PRO:CD	2.66	0.43
37:g:20:TRP:HB2	37:g:32:TYR:HE1	1.83	0.43
40:j:394:HIS:NE2	41:k:78:ARG:HG3	2.14	0.43
40:j:426:GLY:HA3	40:j:429:GLU:OE2	2.19	0.43
40:j:647:SER:O	40:j:649:CYS:N	2.52	0.43
43:m:119:LEU:HD12	45:o:139:TRP:CE3	2.54	0.43
48:r:80:GLU:OE2	48:r:80:GLU:N	2.40	0.43
48:r:232:ALA:CB	48:r:250:LEU:CG	2.96	0.43
48:r:391:LYS:HD2	48:r:391:LYS:N	2.34	0.43
49:s:133:LYS:HG3	49:s:137:LYS:HZ2	1.84	0.43
50:t:141:VAL:HA	50:t:144:ARG:CB	2.49	0.43
50:t:150:ALA:O	50:t:151:GLU:C	2.61	0.43
55:y:78:LEU:HA	55:y:84:PHE:CE1	2.53	0.43
55:y:87:GLU:C	55:y:89:VAL:H	2.27	0.43
1:0:395:HIS:O	1:0:396:ARG:HB3	2.19	0.42
1:0:573:ASP:HA	4:3:189:PRO:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:209:VAL:O	2:1:257:PRO:HG3	2.19	0.42
2:1:706:SER:OG	2:1:708:GLN:OE1	2.26	0.42
2:1:1083:SER:HB3	2:1:1084:PRO:HD3	2.00	0.42
3:2:803:ASP:HB2	3:2:804:PRO:HD3	2.01	0.42
3:2:894:ARG:NE	3:2:894:ARG:HA	2.34	0.42
5:A:841:MET:HG2	6:B:501:LEU:HD23	2.00	0.42
5:A:906:LEU:HD21	5:A:966:LEU:HD11	2.00	0.42
5:A:1426:PRO:HD2	5:A:1449:ASP:HB2	2.01	0.42
5:A:1651:SER:HA	5:A:1652:PRO:HD3	1.57	0.42
6:B:297:MET:HE1	6:B:370:HIS:CD2	2.54	0.42
6:B:761:THR:HG23	6:B:1001:PRO:HD3	2.00	0.42
6:B:815:LYS:HG3	6:B:918:PHE:HE1	1.83	0.42
6:B:873:LEU:N	6:B:888:THR:O	2.32	0.42
8:D:64:THR:HG21	11:G:46:ILE:HD12	2.00	0.42
19:O:204:THR:HG22	19:O:205:SER:N	2.33	0.42
21:Q:188:TYR:O	21:Q:191:LEU:HG	2.19	0.42
22:R:78:LEU:O	22:R:82:VAL:HG23	2.18	0.42
24:T:226:LYS:HE2	25:U:29:DC:H3'	1.98	0.42
27:W:612:ASP:N	27:W:612:ASP:OD1	2.52	0.42
30:Z:409:TYR:HD1	33:c:4:VAL:HG12	1.84	0.42
34:d:305:PHE:CD1	34:d:305:PHE:N	2.85	0.42
38:h:130:ARG:NH2	38:h:131:ILE:HA	2.34	0.42
39:i:12:ARG:HH21	39:i:15:GLU:HG3	1.83	0.42
40:j:373:HIS:HB3	47:q:173:MET:HE1	2.00	0.42
40:j:399:PRO:CD	41:k:107:ASP:OD2	2.63	0.42
41:k:85:LEU:HD11	41:k:114:LEU:HD22	2.01	0.42
42:l:128:THR:O	42:l:128:THR:OG1	2.33	0.42
45:o:65:VAL:HG13	48:r:844:CYS:SG	2.59	0.42
45:o:69:ASP:HB3	45:o:72:GLU:OE1	2.19	0.42
48:r:54:LEU:HD23	53:w:131:ILE:HG23	2.01	0.42
48:r:61:ARG:HH22	48:r:65:GLU:HG3	1.84	0.42
48:r:70:THR:CG2	53:w:151:GLY:HA3	2.50	0.42
48:r:122:LEU:O	48:r:123:ASP:C	2.61	0.42
49:s:126:TYR:HA	49:s:129:LYS:HE2	2.01	0.42
49:s:131:LYS:O	49:s:134:SER:OG	2.36	0.42
50:t:94:ASP:O	50:t:96:LEU:N	2.52	0.42
50:t:117:VAL:HA	50:t:120:HIS:CD2	2.54	0.42
52:v:32:SER:C	52:v:34:GLN:N	2.76	0.42
56:z:685:LEU:HA	56:z:685:LEU:HD23	1.65	0.42
1:0:61:MET:CG	1:0:76:ILE:O	2.65	0.42
1:0:394:VAL:HG12	1:0:396:ARG:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:443:LEU:O	1:0:454:VAL:HA	2.18	0.42
1:0:733:PRO:O	1:0:735:SER:N	2.52	0.42
2:1:98:CYS:SG	2:1:137:LEU:HD21	2.59	0.42
2:1:757:LYS:HD3	2:1:832:TYR:CZ	2.54	0.42
2:1:1076:VAL:HG11	2:1:1145:TRP:NE1	2.34	0.42
2:1:1239:VAL:HG23	2:1:1244:GLN:HB3	2.01	0.42
2:1:1278:LEU:HA	2:1:1281:VAL:HG12	2.00	0.42
2:1:1302:LYS:HE3	2:1:1332:ILE:O	2.19	0.42
3:2:90:ARG:N	3:2:90:ARG:HD2	2.34	0.42
3:2:183:LEU:HD21	3:2:974:SER:HA	2.00	0.42
3:2:217:GLN:O	3:2:221:LEU:HG	2.19	0.42
3:2:350:LYS:HB2	3:2:350:LYS:HE3	1.60	0.42
3:2:736:LEU:HD11	3:2:741:VAL:HG12	2.02	0.42
3:2:954:GLU:O	3:2:958:VAL:HG13	2.20	0.42
5:A:31:LEU:HA	5:A:34:MET:HE2	2.00	0.42
5:A:430:ARG:NE	19:O:28:ARG:HH21	2.17	0.42
5:A:883:ILE:HG13	5:A:1423:ASP:OD1	2.19	0.42
5:A:1172:ASN:HA	13:I:57:LYS:C	2.44	0.42
6:B:30:ILE:HG21	6:B:702:MET:HE3	2.01	0.42
6:B:203:ASN:O	6:B:571:GLY:HA3	2.19	0.42
6:B:584:MET:SD	6:B:603:MET:HB3	2.59	0.42
10:F:82:GLU:OE1	10:F:82:GLU:N	2.50	0.42
20:P:280:PHE:HB2	20:P:293:TYR:CE1	2.53	0.42
21:Q:44:LYS:HA	21:Q:44:LYS:HD3	1.85	0.42
21:Q:44:LYS:HB2	21:Q:47:ASP:OD1	2.19	0.42
27:W:165:LYS:CG	27:W:181:HIS:CE1	2.99	0.42
27:W:172:HIS:HA	27:W:434:GLU:CG	2.41	0.42
27:W:319:TYR:CD1	27:W:501:TYR:CE2	3.08	0.42
28:X:438:MET:HE2	28:X:438:MET:HB3	1.91	0.42
36:f:181:LEU:HD21	36:f:187:LEU:CD1	2.49	0.42
39:i:107:VAL:HG12	47:q:162:GLN:CB	2.48	0.42
40:j:165:GLU:O	40:j:169:LYS:HG2	2.18	0.42
40:j:336:PHE:CZ	40:j:500:GLU:HA	2.54	0.42
40:j:463:HIS:CD2	43:m:128:TYR:HD1	2.26	0.42
40:j:557:LEU:HD11	48:r:680:HIS:CE1	2.54	0.42
47:q:91:LYS:O	47:q:95:VAL:HG22	2.19	0.42
47:q:92:LEU:HA	47:q:95:VAL:HG22	2.01	0.42
48:r:53:THR:HG22	52:v:60:ASP:OD2	2.18	0.42
48:r:415:GLU:O	48:r:419:ILE:HG13	2.19	0.42
49:s:95:VAL:HA	49:s:98:LYS:CD	2.48	0.42
49:s:142:ALA:N	49:s:144:SER:OG	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:111:PRO:HD2	51:u:112:GLU:CD	2.43	0.42
51:u:119:GLN:HA	51:u:122:ARG:HD3	2.01	0.42
52:v:15:PHE:N	52:v:15:PHE:CD1	2.87	0.42
52:v:108:LEU:CD1	54:x:62:ILE:HD12	2.49	0.42
54:x:129:GLN:HA	54:x:132:THR:OG1	2.19	0.42
55:y:15:ARG:HA	55:y:18:PHE:HD2	1.83	0.42
55:y:53:LYS:O	55:y:56:LEU:N	2.51	0.42
1:0:36:ALA:O	1:0:47:PHE:HA	2.19	0.42
1:0:355:ALA:HB3	1:0:383:ALA:HB3	2.01	0.42
1:0:824:ILE:HG23	4:3:104:MET:HE3	2.01	0.42
2:1:777:ILE:HG22	2:1:810:VAL:HG22	2.01	0.42
3:2:51:MET:HG2	3:2:85:PHE:CE1	2.54	0.42
3:2:223:ARG:O	3:2:226:PRO:HD2	2.19	0.42
3:2:767:LEU:HD23	3:2:767:LEU:HA	1.85	0.42
3:2:818:LEU:HD23	3:2:818:LEU:HA	1.90	0.42
3:2:957:LYS:O	3:2:960:ALA:HB2	2.18	0.42
5:A:458:PHE:CE2	5:A:484:LEU:HD13	2.54	0.42
5:A:782:SER:O	5:A:786:ALA:HB3	2.19	0.42
5:A:1175:ILE:HG12	5:A:1212:LEU:HD13	2.01	0.42
6:B:853:LEU:O	16:L:46:LYS:NZ	2.53	0.42
6:B:954:MET:HE2	6:B:963:PRO:O	2.19	0.42
9:E:110:MET:HB2	9:E:115:LYS:HZ3	1.85	0.42
9:E:172:ARG:HD3	9:E:210:GLN:HG2	2.00	0.42
11:G:99:THR:N	11:G:106:CYS:O	2.52	0.42
20:P:181:LYS:NZ	20:P:185:LEU:HB3	2.34	0.42
24:T:134:GLU:C	24:T:136:SER:N	2.77	0.42
24:T:168:LYS:HA	24:T:168:LYS:HD2	1.59	0.42
27:W:361:CYS:HB3	27:W:405:VAL:HG22	1.99	0.42
27:W:511:TRP:CH2	30:Z:348:ARG:NH1	2.86	0.42
27:W:519:TYR:C	33:c:22:TYR:CD1	2.97	0.42
29:Y:377:LYS:HB2	32:b:286:GLU:HG3	1.99	0.42
35:e:267:ASP:OD1	35:e:268:LEU:N	2.52	0.42
40:j:486:GLN:OE1	40:j:486:GLN:HA	2.19	0.42
40:j:550:SER:CB	48:r:713:GLN:HG2	2.49	0.42
42:l:174:ALA:O	42:l:177:GLY:N	2.48	0.42
44:n:17:ALA:HB1	46:p:120:LEU:HD21	2.01	0.42
48:r:100:LEU:HD23	52:v:16:VAL:HG11	2.01	0.42
48:r:165:SER:C	48:r:167:PRO:CD	2.92	0.42
48:r:799:GLU:HG3	48:r:816:LYS:CE	2.13	0.42
49:s:152:ALA:N	49:s:155:ILE:HD12	2.34	0.42
50:t:156:HIS:ND1	50:t:156:HIS:C	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:161:ILE:O	50:t:164:ILE:HG13	2.19	0.42
52:v:98:LYS:HE3	52:v:98:LYS:HA	2.02	0.42
54:x:111:GLY:O	54:x:115:LEU:HG	2.19	0.42
55:y:67:LEU:HD11	55:y:72:CYS:SG	2.58	0.42
55:y:73:LEU:HD12	55:y:74:HIS:N	2.35	0.42
55:y:118:ALA:HA	55:y:121:GLU:CD	2.44	0.42
2:1:304:LEU:HD23	2:1:304:LEU:HA	1.89	0.42
2:1:539:LEU:O	2:1:542:SER:OG	2.30	0.42
2:1:606:GLU:OE1	2:1:956:PHE:N	2.29	0.42
2:1:1186:TYR:CZ	3:2:238:LYS:HE3	2.54	0.42
3:2:188:SER:O	3:2:192:ILE:HG23	2.19	0.42
3:2:204:ALA:HA	3:2:212:ARG:NH1	2.35	0.42
3:2:509:SER:O	3:2:511:VAL:N	2.53	0.42
3:2:548:ARG:HH11	3:2:548:ARG:HG3	1.84	0.42
3:2:567:MET:HG2	3:2:568:LYS:N	2.33	0.42
5:A:733:LEU:HD12	5:A:733:LEU:HA	1.89	0.42
5:A:841:MET:HB3	5:A:841:MET:HE2	1.75	0.42
5:A:871:VAL:HG12	5:A:881:ASN:HB3	2.01	0.42
5:A:1144:LEU:HD12	5:A:1145:GLY:H	1.84	0.42
5:A:1203:ASP:OD2	5:A:1206:ARG:NH1	2.52	0.42
5:A:1622:TYR:CD2	5:A:1622:TYR:O	2.72	0.42
6:B:138:GLU:H	6:B:138:GLU:CD	2.27	0.42
6:B:1125:MET:O	6:B:1127:ILE:N	2.46	0.42
11:G:22:LEU:O	11:G:26:VAL:HG23	2.19	0.42
13:I:12:VAL:O	13:I:13:GLY:C	2.62	0.42
21:Q:74:CYS:SG	21:Q:92:TYR:HA	2.59	0.42
22:R:90:GLN:HE22	22:R:176:PRO:HG3	1.84	0.42
28:X:117:ILE:HG23	28:X:185:ARG:HE	1.85	0.42
28:X:562:GLN:HE21	28:X:567:LEU:HD12	1.84	0.42
30:Z:408:LEU:HD11	33:c:44:PHE:CE2	2.10	0.42
35:e:284:ILE:HA	35:e:288:GLN:NE2	2.34	0.42
40:j:248:PRO:C	40:j:250:ASP:H	2.27	0.42
41:k:99:HIS:HA	41:k:201:LYS:HZ2	1.85	0.42
42:l:28:LEU:HD21	42:l:124:VAL:CG1	2.49	0.42
45:o:42:SER:O	45:o:42:SER:OG	2.32	0.42
45:o:83:LYS:HB3	45:o:83:LYS:HE2	1.82	0.42
48:r:53:THR:HA	48:r:56:GLU:HG2	2.00	0.42
48:r:61:ARG:O	48:r:65:GLU:HB2	2.16	0.42
48:r:84:GLU:HA	48:r:87:GLN:HB3	2.01	0.42
48:r:99:LEU:O	48:r:100:LEU:C	2.61	0.42
48:r:165:SER:CB	48:r:167:PRO:HD3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:194:GLN:O	48:r:198:ILE:HG12	2.19	0.42
48:r:570:PHE:HB2	48:r:615:LYS:HZ3	1.83	0.42
49:s:69:LEU:HD13	49:s:72:ARG:NH1	2.35	0.42
49:s:88:LYS:HD3	49:s:88:LYS:HA	1.64	0.42
49:s:102:LYS:HZ2	49:s:103:ARG:N	2.18	0.42
50:t:30:LEU:O	50:t:32:PRO:HD3	2.20	0.42
50:t:133:GLU:OE1	50:t:136:ARG:HB2	2.20	0.42
52:v:11:HIS:CG	52:v:12:LEU:H	2.34	0.42
54:x:24:GLY:O	54:x:27:GLN:NE2	2.52	0.42
54:x:66:ALA:C	54:x:68:ASP:N	2.77	0.42
55:y:38:ALA:O	55:y:39:GLN:C	2.60	0.42
1:0:537:SER:O	1:0:539:CYS:N	2.53	0.42
2:1:420:THR:HG21	2:1:530:SER:O	2.19	0.42
2:1:834:PHE:HB2	2:1:885:ILE:HD11	2.01	0.42
2:1:958:ASN:HD21	2:1:961:LEU:HG	1.84	0.42
3:2:788:LEU:HA	3:2:788:LEU:HD23	1.75	0.42
3:2:949:PHE:C	3:2:951:THR:N	2.78	0.42
5:A:34:MET:SD	6:B:1124:ILE:HG21	2.59	0.42
5:A:97:VAL:HB	5:A:315:ALA:HB1	2.02	0.42
5:A:338:SER:O	5:A:339:LEU:C	2.62	0.42
5:A:350:VAL:HG21	5:A:1435:THR:OG1	2.19	0.42
5:A:689:ILE:HG13	6:B:981:LEU:HB3	2.01	0.42
5:A:1191:GLU:CD	5:A:1191:GLU:H	2.27	0.42
5:A:1202:PHE:CD2	5:A:1203:ASP:HB2	2.55	0.42
5:A:1244:ASN:OD1	5:A:1245:CYS:N	2.47	0.42
5:A:1285:LEU:HA	5:A:1285:LEU:HD23	1.84	0.42
17:M:326:GLN:O	17:M:328:LEU:HG	2.19	0.42
18:N:71:VAL:HG12	18:N:98:CYS:SG	2.60	0.42
20:P:271:GLU:O	20:P:275:LEU:HD23	2.20	0.42
23:S:173:HIS:CD2	23:S:176:ILE:HG13	2.55	0.42
24:T:31:TRP:HD1	24:T:62:LEU:HD23	1.84	0.42
25:U:25:DG:N2	26:V:70:DC:O2	2.51	0.42
30:Z:87:THR:HG23	30:Z:96:TRP:HZ3	1.84	0.42
40:j:308:PHE:HE2	48:r:319:ARG:HH22	1.66	0.42
40:j:478:LEU:C	40:j:478:LEU:CD2	2.86	0.42
48:r:122:LEU:HD13	52:v:91:LYS:CB	2.49	0.42
48:r:175:ASP:C	48:r:177:ILE:N	2.75	0.42
48:r:536:ASN:HD22	48:r:554:MET:CG	2.31	0.42
48:r:691:LYS:HA	48:r:692:GLY:HA2	1.75	0.42
48:r:888:VAL:HA	48:r:889:PRO:HD3	1.91	0.42
49:s:96:LEU:HD13	49:s:96:LEU:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:u:68:LEU:HD13	51:u:90:LEU:HD11	2.00	0.42
52:v:114:SER:O	52:v:116:VAL:O	2.38	0.42
55:y:119:LEU:HA	55:y:122:GLN:OE1	2.19	0.42
1:0:68:GLU:OE2	1:0:737:GLY:HA3	2.19	0.42
2:1:57:GLU:OE1	2:1:57:GLU:N	2.45	0.42
2:1:753:ARG:NH2	2:1:828:ASP:O	2.51	0.42
2:1:1278:LEU:HD22	2:1:1298:LEU:HD11	2.01	0.42
3:2:172:THR:HG23	3:2:986:ILE:HB	2.01	0.42
3:2:181:ALA:HB1	3:2:185:GLU:OE1	2.20	0.42
4:3:183:VAL:HG12	4:3:221:VAL:HG13	2.01	0.42
5:A:540:ASP:OD1	5:A:680:LEU:HD21	2.20	0.42
5:A:794:GLU:N	5:A:845:GLU:OE2	2.52	0.42
5:A:1307:VAL:HG23	5:A:1338:THR:OG1	2.19	0.42
6:B:229:SER:OG	6:B:231:PRO:HD3	2.20	0.42
6:B:541:ILE:HG12	6:B:596:ILE:CG2	2.49	0.42
6:B:712:PRO:HG2	6:B:939:HIS:CE1	2.55	0.42
6:B:875:GLU:OE2	6:B:888:THR:HG21	2.19	0.42
9:E:28:VAL:HG22	9:E:32:GLU:HB3	2.01	0.42
10:F:53:THR:OG1	10:F:116:GLU:OE2	2.25	0.42
11:G:4:HIS:O	11:G:4:HIS:CG	2.72	0.42
18:N:44:ILE:HG22	18:N:48:LEU:HD22	2.02	0.42
19:O:142:PHE:O	19:O:146:TYR:HD1	2.03	0.42
22:R:187:ASP:HB2	22:R:189:ILE:HG22	2.02	0.42
22:R:228:MET:O	22:R:232:LYS:HG3	2.20	0.42
22:R:231:GLU:OE1	22:R:231:GLU:HA	2.18	0.42
24:T:7:LEU:HD22	24:T:103:LYS:HG3	2.01	0.42
24:T:85:LEU:HD11	24:T:112:GLN:HG3	2.02	0.42
27:W:292:LEU:CD2	27:W:294:GLU:CD	2.79	0.42
31:a:169:ILE:HB	31:a:198:VAL:HG22	2.01	0.42
36:f:268:GLU:N	36:f:268:GLU:OE1	2.52	0.42
37:g:61:ASN:C	37:g:86:ARG:HH12	2.27	0.42
40:j:142:GLN:CD	40:j:142:GLN:H	2.27	0.42
40:j:191:ARG:CD	43:m:88:LEU:HG	2.48	0.42
40:j:309:ALA:HB1	48:r:318:GLU:OE1	2.19	0.42
40:j:402:HIS:ND1	40:j:402:HIS:O	2.53	0.42
42:l:66:MET:HE1	42:l:193:TYR:HB3	2.01	0.42
44:n:60:LEU:HD23	44:n:60:LEU:HA	1.80	0.42
47:q:105:GLY:C	47:q:106:MET:HE2	2.45	0.42
48:r:71:ASP:O	48:r:74:PRO:HD2	2.19	0.42
48:r:154:ILE:HD12	48:r:157:ALA:HB3	2.00	0.42
48:r:201:HIS:NE2	49:s:111:GLN:CG	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:201:HIS:CD2	49:s:111:GLN:HG3	2.47	0.42
48:r:300:CYS:O	48:r:304:GLN:HG3	2.20	0.42
48:r:438:LEU:O	48:r:438:LEU:HD23	2.20	0.42
49:s:120:ILE:C	49:s:122:ALA:N	2.77	0.42
49:s:150:LYS:HA	49:s:153:HIS:HB2	2.02	0.42
50:t:154:GLN:C	50:t:158:GLU:OE2	2.63	0.42
52:v:51:ILE:O	52:v:52:ASP:C	2.63	0.42
52:v:108:LEU:HA	52:v:111:GLN:HB2	2.00	0.42
53:w:90:GLU:O	53:w:91:GLN:C	2.59	0.42
55:y:79:LEU:C	55:y:85:ARG:CZ	2.92	0.42
1:0:69:HIS:HD2	1:0:799:THR:HG23	1.85	0.42
2:1:356:LEU:HD21	2:1:372:LEU:HD11	2.02	0.42
2:1:407:GLU:HG3	2:1:408:TYR:N	2.33	0.42
2:1:509:LEU:HD21	2:1:955:TYR:HE1	1.85	0.42
2:1:699:ASP:O	2:1:1222:GLY:HA3	2.20	0.42
3:2:181:ALA:C	3:2:185:GLU:HG2	2.45	0.42
3:2:317:LEU:HB3	3:2:372:LEU:HD11	2.01	0.42
3:2:658:PHE:HB3	3:2:661:GLU:CD	2.44	0.42
5:A:367:ILE:HD13	5:A:501:MET:CE	2.50	0.42
5:A:591:ILE:HD13	5:A:591:ILE:HA	1.79	0.42
5:A:1411:LEU:HD12	5:A:1411:LEU:HA	1.90	0.42
7:C:1:MET:HB2	15:K:93:ASP:OD1	2.19	0.42
7:C:77:ASP:O	7:C:78:ILE:HD13	2.19	0.42
8:D:76:ASN:ND2	8:D:80:ILE:HG23	2.34	0.42
8:D:83:VAL:HG23	8:D:134:ILE:HD13	2.02	0.42
13:I:79:PRO:HB2	13:I:96:PHE:CE2	2.55	0.42
19:O:154:ARG:HD2	19:O:190:GLU:OE2	2.20	0.42
19:O:304:PHE:HB3	19:O:306:PHE:CE1	2.53	0.42
20:P:317:VAL:HG23	20:P:320:GLU:H	1.84	0.42
21:Q:104:LYS:HE3	21:Q:191:LEU:HB2	2.01	0.42
22:R:109:LEU:HD23	22:R:109:LEU:H	1.84	0.42
26:V:48:DC:H2'	26:V:49:DG:C8	2.54	0.42
30:Z:99:GLN:O	30:Z:107:GLY:N	2.53	0.42
31:a:166:GLU:HA	31:a:195:ARG:O	2.20	0.42
31:a:379:LEU:CD1	32:b:138:ALA:HB1	2.47	0.42
32:b:268:CYS:CB	32:b:271:CYS:SG	2.90	0.42
38:h:75:VAL:O	38:h:77:ILE:N	2.52	0.42
39:i:27:ASN:O	39:i:31:VAL:HG23	2.20	0.42
39:i:56:VAL:HG11	43:m:30:MET:SD	2.59	0.42
40:j:335:PRO:O	40:j:336:PHE:C	2.62	0.42
40:j:558:GLY:N	40:j:559:PRO:HD3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:112:GLU:H	41:k:112:GLU:CD	2.27	0.42
41:k:171:LEU:HD21	41:k:189:PHE:CD2	2.54	0.42
43:m:33:PHE:HA	43:m:36:ILE:HG22	2.02	0.42
45:o:107:PRO:O	45:o:111:ILE:HG23	2.20	0.42
48:r:854:GLN:HB3	48:r:910:SER:C	2.44	0.42
48:r:885:LEU:HB3	48:r:904:PHE:HD2	1.84	0.42
49:s:36:ASP:HA	49:s:39:VAL:HG12	2.00	0.42
49:s:118:GLU:O	49:s:120:ILE:N	2.53	0.42
49:s:119:GLN:O	49:s:122:ALA:HB3	2.20	0.42
50:t:75:LYS:H	50:t:75:LYS:HG2	1.46	0.42
50:t:122:LEU:HA	50:t:125:GLU:OE1	2.19	0.42
52:v:82:LYS:C	52:v:85:LEU:HB3	2.44	0.42
52:v:124:TYR:O	52:v:125:ARG:C	2.58	0.42
53:w:89:LEU:O	53:w:92:ALA:HB3	2.19	0.42
54:x:129:GLN:HA	54:x:132:THR:HB	2.01	0.42
55:y:31:PRO:HG2	55:y:32:ASN:H	1.85	0.42
55:y:35:ASN:O	55:y:36:PHE:C	2.62	0.42
55:y:46:LYS:C	55:y:49:VAL:H	2.22	0.42
55:y:73:LEU:C	55:y:75:MET:N	2.73	0.42
55:y:81:TYR:C	55:y:83:HIS:N	2.76	0.42
1:0:113:HIS:CD2	4:3:104:MET:HE2	2.55	0.42
1:0:196:SER:HB2	1:0:198:GLN:OE1	2.20	0.42
2:1:844:ASN:O	2:1:847:ILE:HG22	2.20	0.42
2:1:1046:ASP:OD1	2:1:1047:THR:N	2.49	0.42
3:2:442:MET:O	3:2:447:SER:HB2	2.20	0.42
4:3:17:ASP:OD1	4:3:17:ASP:N	2.47	0.42
5:A:189:PRO:HB3	5:A:202:TRP:CD1	2.55	0.42
5:A:823:VAL:HG22	5:A:835:GLU:HG2	2.01	0.42
5:A:1313:GLN:H	5:A:1313:GLN:CD	2.28	0.42
7:C:13:GLU:OE2	7:C:14:LEU:N	2.53	0.42
7:C:149:LEU:HD22	7:C:152:LYS:HE2	2.02	0.42
9:E:113:SER:O	9:E:116:GLN:HG3	2.20	0.42
9:E:185:ILE:HG13	9:E:189:GLN:OE1	2.19	0.42
19:O:18:HIS:CE1	19:O:37:CYS:HB2	2.51	0.42
20:P:180:LEU:HD13	20:P:215:SER:HA	2.02	0.42
20:P:255:ILE:HG13	20:P:255:ILE:O	2.20	0.42
21:Q:154:CYS:HB3	21:Q:157:CYS:O	2.19	0.42
28:X:365:VAL:O	28:X:367:ILE:N	2.52	0.42
30:Z:297:ALA:O	30:Z:382:VAL:CG1	2.49	0.42
30:Z:368:LEU:CB	30:Z:383:LEU:CD1	2.70	0.42
35:e:101:ILE:HD12	35:e:145:LEU:HD21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:7:GLN:HE21	36:f:85:MET:HE2	1.83	0.42
36:f:71:PHE:CG	36:f:75:MET:HE3	2.55	0.42
37:g:75:GLU:CD	37:g:76:PRO:HD3	2.44	0.42
38:h:122:LYS:O	38:h:126:THR:HG22	2.19	0.42
40:j:261:ILE:HB	40:j:368:LEU:HD23	2.00	0.42
40:j:366:ASP:C	40:j:369:TYR:H	2.28	0.42
40:j:525:LEU:HD23	40:j:525:LEU:HA	1.75	0.42
48:r:248:LEU:HD23	48:r:248:LEU:HA	1.40	0.42
48:r:286:GLU:CD	48:r:287:LYS:H	2.28	0.42
48:r:553:GLU:OE1	48:r:567:LYS:HB2	2.20	0.42
48:r:749:TYR:OH	48:r:769:ASP:OD2	2.32	0.42
49:s:149:ILE:C	49:s:151:TYR:H	2.28	0.42
51:u:123:GLU:O	51:u:124:GLN:C	2.63	0.42
52:v:37:LEU:O	52:v:40:LYS:HB2	2.20	0.42
52:v:64:PRO:C	52:v:68:PHE:HD2	2.28	0.42
52:v:68:PHE:C	52:v:70:TYR:N	2.75	0.42
54:x:73:ILE:O	54:x:77:PRO:HD3	2.20	0.42
54:x:108:VAL:CG2	54:x:109:TYR:N	2.82	0.42
54:x:115:LEU:HD13	54:x:119:GLN:HE22	1.76	0.42
55:y:124:GLN:OE1	55:y:125:GLN:HG3	2.19	0.42
1:0:40:SER:OG	1:0:41:CYS:N	2.50	0.42
1:0:217:ASP:OD1	1:0:218:ILE:N	2.53	0.42
1:0:259:ILE:HG12	3:2:633:LEU:HB2	2.02	0.42
1:0:710:ASP:O	1:0:713:LEU:N	2.51	0.42
2:1:148:ILE:HD13	2:1:160:LEU:HD13	2.02	0.42
2:1:374:TRP:HH2	2:1:479:ASN:HD21	1.68	0.42
2:1:487:CYS:SG	2:1:488:PHE:N	2.93	0.42
3:2:694:THR:C	3:2:696:PRO:HD3	2.45	0.42
5:A:380:VAL:HG11	5:A:450:MET:HE1	2.02	0.42
5:A:470:MET:HG2	5:A:524:MET:SD	2.60	0.42
5:A:675:VAL:HG12	5:A:676:ILE:HD13	2.01	0.42
5:A:1162:GLU:OE1	5:A:1307:VAL:N	2.53	0.42
5:A:1343:LEU:HA	5:A:1346:VAL:HG22	2.02	0.42
6:B:245:GLN:HG3	6:B:250:SER:H	1.85	0.42
6:B:246:GLY:HA3	23:S:166:ARG:NH2	2.33	0.42
6:B:403:LEU:O	6:B:407:MET:HG2	2.20	0.42
6:B:712:PRO:HG3	6:B:938:ARG:NH2	2.34	0.42
6:B:856:PRO:HA	6:B:904:VAL:HG12	2.02	0.42
6:B:1066:PRO:HB2	6:B:1075:MET:HE3	2.00	0.42
7:C:118:ARG:HD3	7:C:133:ARG:NH2	2.35	0.42
8:D:78:GLU:CD	38:h:51:LEU:HD23	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:142:TYR:OH	43:m:20:LYS:O	2.37	0.42
8:D:142:TYR:C	43:m:70:ARG:NH2	2.76	0.42
9:E:121:MET:HB3	9:E:121:MET:HE3	1.73	0.42
19:O:10:LEU:HG	21:Q:156:PHE:O	2.20	0.42
20:P:257:ASN:OD1	20:P:258:MET:N	2.53	0.42
24:T:191:PHE:HD1	24:T:191:PHE:HA	1.75	0.42
24:T:236:LYS:HD3	24:T:237:PRO:HD2	2.02	0.42
27:W:109:ARG:CZ	27:W:492:ASN:HB2	2.50	0.42
27:W:134:SER:O	27:W:138:GLU:CB	2.68	0.42
27:W:280:LEU:HG	27:W:291:LEU:HD11	2.02	0.42
28:X:251:LEU:HD22	28:X:433:LEU:HD23	2.01	0.42
29:Y:377:LYS:H	32:b:285:CYS:HA	1.85	0.42
29:Y:505:LEU:C	29:Y:507:PRO:HD3	2.45	0.42
29:Y:540:GLN:O	29:Y:544:LEU:HG	2.20	0.42
30:Z:442:VAL:CG1	33:c:9:LEU:HB2	2.50	0.42
35:e:64:LYS:HD2	36:f:115:VAL:HG13	2.01	0.42
36:f:198:ILE:HD11	36:f:255:MET:HG2	2.01	0.42
37:g:120:LEU:HB2	43:m:52:THR:HG22	2.00	0.42
38:h:173:PHE:CE1	41:k:198:HIS:HB2	2.55	0.42
39:i:103:LYS:HA	39:i:103:LYS:HD3	1.81	0.42
40:j:197:ARG:O	40:j:204:LEU:HB3	2.20	0.42
43:m:134:TYR:CZ	47:q:157:LYS:HB2	2.55	0.42
44:n:45:LEU:CD2	56:z:630:ARG:NH2	2.82	0.42
48:r:150:PRO:CG	54:x:9:GLN:HE22	2.32	0.42
48:r:173:ILE:O	48:r:174:ARG:C	2.63	0.42
48:r:208:LEU:HB2	48:r:212:LEU:CD1	2.45	0.42
48:r:800:VAL:HG22	48:r:810:LEU:HD22	2.02	0.42
48:r:930:SER:O	48:r:931:ARG:C	2.62	0.42
49:s:127:GLN:HA	49:s:130:GLU:CD	2.45	0.42
49:s:151:TYR:C	49:s:155:ILE:HD12	2.44	0.42
50:t:123:ILE:HG13	50:t:124:ASN:H	1.84	0.42
52:v:2:ALA:O	52:v:5:PHE:HB2	2.20	0.42
52:v:73:GLN:OE1	52:v:73:GLN:HA	2.20	0.42
53:w:95:LYS:C	53:w:96:PHE:CD1	2.97	0.42
54:x:76:LEU:HD23	54:x:76:LEU:HA	1.85	0.42
55:y:45:ASP:O	55:y:48:PHE:CD2	2.73	0.42
1:0:99:ALA:HB2	1:0:134:LEU:HD21	2.02	0.42
1:0:565:ARG:HH12	4:3:218:ARG:HH11	1.68	0.42
1:0:620:TRP:O	1:0:621:VAL:C	2.63	0.42
1:0:746:GLN:OE1	1:0:746:GLN:N	2.48	0.42
2:1:245:PRO:HB3	2:1:287:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:571:LEU:HD23	2:1:571:LEU:HA	1.82	0.42
3:2:568:LYS:O	3:2:569:LEU:HG	2.20	0.42
5:A:64:VAL:HG11	5:A:78:MET:HA	2.01	0.42
6:B:94:SER:HB3	6:B:123:PRO:HG2	2.00	0.42
6:B:117:ASN:HD22	6:B:189:GLY:HA3	1.84	0.42
6:B:744:MET:HE1	6:B:920:LYS:O	2.19	0.42
6:B:1054:MET:HE3	6:B:1054:MET:HB2	1.97	0.42
9:E:47:LYS:HB2	9:E:48:PRO:HD3	2.02	0.42
12:H:148:LEU:C	12:H:150:PHE:N	2.78	0.42
13:I:33:ARG:O	13:I:34:ILE:HD13	2.20	0.42
19:O:119:LYS:HE2	19:O:119:LYS:HB2	1.86	0.42
20:P:201:ILE:CD1	26:V:78:DT:OP1	2.68	0.42
20:P:288:PHE:HA	20:P:289:PRO:HD3	1.87	0.42
21:Q:76:MET:HG3	21:Q:89:HIS:C	2.45	0.42
21:Q:104:LYS:O	21:Q:107:LEU:HG	2.20	0.42
23:S:24:LYS:HA	24:T:99:SER:HA	2.00	0.42
24:T:91:GLN:NE2	24:T:94:THR:HG23	2.34	0.42
27:W:159:CYS:SG	27:W:163:TYR:HE2	2.42	0.42
27:W:184:VAL:O	27:W:188:LEU:HB2	2.20	0.42
28:X:524:LEU:HD11	28:X:595:ILE:HD11	2.02	0.42
29:Y:389:ILE:HD11	32:b:259:ARG:CG	2.42	0.42
29:Y:415:THR:OG1	32:b:112:VAL:HG13	2.20	0.42
35:e:100:VAL:HG23	35:e:310:PRO:HG3	2.01	0.42
35:e:143:LEU:HD22	35:e:151:LEU:HD21	2.02	0.42
37:g:43:ARG:O	37:g:45:CYS:N	2.52	0.42
37:g:66:ILE:HA	37:g:85:GLN:HA	2.02	0.42
40:j:340:GLN:OE1	40:j:340:GLN:N	2.53	0.42
40:j:398:ALA:HB2	41:k:84:HIS:CE1	2.55	0.42
48:r:111:LYS:HA	48:r:114:LYS:HE2	2.02	0.42
48:r:485:ASP:OD1	48:r:486:MET:N	2.53	0.42
48:r:489:ILE:HG23	48:r:490:ILE:HD13	2.01	0.42
48:r:683:ARG:CZ	48:r:683:ARG:HB2	2.50	0.42
48:r:732:ASN:OD1	48:r:743:ARG:NH1	2.52	0.42
49:s:103:ARG:O	49:s:104:ASP:C	2.62	0.42
50:t:130:GLN:O	50:t:131:ALA:C	2.62	0.42
51:u:126:ARG:O	51:u:130:GLU:HG2	2.19	0.42
51:u:132:LEU:O	51:u:136:LYS:HG2	2.19	0.42
53:w:95:LYS:H	53:w:95:LYS:HG3	1.53	0.42
55:y:65:LYS:HE2	55:y:66:TYR:CE1	2.55	0.42
2:1:5:LEU:HG	2:1:9:PHE:CE2	2.55	0.41
2:1:931:LYS:HA	2:1:951:TYR:OH	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1025:LYS:HD2	2:1:1025:LYS:HA	1.64	0.41
2:1:1187:PRO:HA	2:1:1190:LEU:CD2	2.50	0.41
2:1:1205:CYS:HB2	2:1:1247:TYR:HE2	1.83	0.41
3:2:85:PHE:HB3	3:2:130:TRP:NE1	2.29	0.41
3:2:491:LEU:HD12	3:2:662:ARG:HH22	1.85	0.41
3:2:612:LYS:O	3:2:613:VAL:C	2.62	0.41
3:2:957:LYS:CD	3:2:967:VAL:HG21	2.50	0.41
5:A:479:TRP:HA	15:K:2:ASN:O	2.20	0.41
5:A:920:PHE:CD2	5:A:959:MET:HE1	2.55	0.41
6:B:601:VAL:O	6:B:601:VAL:HG13	2.20	0.41
6:B:629:GLU:HB2	6:B:634:LEU:HD21	2.02	0.41
6:B:707:CYS:SG	6:B:730:LYS:HG2	2.60	0.41
6:B:712:PRO:HG3	6:B:938:ARG:HH21	1.85	0.41
6:B:851:ASP:HB2	16:L:15:MET:SD	2.60	0.41
7:C:56:SER:HB2	7:C:158:GLU:H	1.84	0.41
7:C:101:PHE:N	7:C:163:ALA:O	2.45	0.41
13:I:65:LEU:HD11	13:I:124:THR:HG22	2.02	0.41
19:O:157:ASP:HB2	19:O:185:ARG:NH2	2.35	0.41
22:R:229:ASP:HA	22:R:232:LYS:HG3	2.02	0.41
27:W:473:GLU:HG3	27:W:632:SER:OG	2.18	0.41
28:X:118:HIS:HD2	28:X:121:VAL:HG23	1.84	0.41
28:X:497:ARG:HB3	28:X:709:THR:HA	2.02	0.41
29:Y:464:LEU:HG	29:Y:513:ARG:NH2	2.35	0.41
30:Z:400:ARG:HD2	33:c:61:MET:HE1	2.02	0.41
36:f:218:LEU:HD23	36:f:218:LEU:HA	1.80	0.41
37:g:50:VAL:HG13	37:g:55:LEU:HB2	2.02	0.41
40:j:99:ARG:HD3	40:j:103:ARG:NH2	2.35	0.41
40:j:191:ARG:CG	40:j:196:LEU:HD13	2.10	0.41
40:j:398:ALA:HB1	40:j:399:PRO:HD2	2.02	0.41
40:j:415:LYS:HA	42:l:70:GLU:O	2.19	0.41
40:j:432:ILE:HD13	40:j:432:ILE:HA	1.69	0.41
40:j:439:PHE:CZ	40:j:443:ARG:HD2	2.55	0.41
40:j:639:MET:HE3	40:j:639:MET:HB3	1.81	0.41
42:l:181:ASP:OD1	42:l:181:ASP:N	2.47	0.41
47:q:84:GLN:O	47:q:88:LEU:HG	2.20	0.41
48:r:87:GLN:O	48:r:88:PHE:C	2.61	0.41
48:r:100:LEU:O	48:r:104:LYS:N	2.53	0.41
48:r:325:GLN:OE1	48:r:325:GLN:N	2.53	0.41
48:r:555:LEU:HD23	48:r:565:SER:OG	2.19	0.41
48:r:669:GLN:OE1	48:r:683:ARG:CG	2.66	0.41
48:r:1209:ARG:O	48:r:1213:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:49:GLN:O	52:v:53:LYS:HG2	2.20	0.41
52:v:68:PHE:O	52:v:70:TYR:N	2.52	0.41
1:0:16:ALA:HB3	1:0:454:VAL:HB	2.02	0.41
1:0:388:ASP:OD1	1:0:389:GLY:N	2.53	0.41
2:1:57:GLU:HG2	2:1:58:GLN:N	2.34	0.41
2:1:89:THR:HG22	2:1:89:THR:O	2.20	0.41
2:1:213:ARG:HH12	2:1:259:ASP:HA	1.85	0.41
2:1:786:PRO:O	2:1:788:LEU:HG	2.20	0.41
2:1:959:VAL:HG22	2:1:962:ARG:NH2	2.35	0.41
2:1:1068:TYR:CE2	2:1:1125:ALA:HB1	2.54	0.41
3:2:272:ARG:CD	3:2:936:GLU:HG3	2.36	0.41
3:2:552:THR:HG23	3:2:554:VAL:HG22	2.02	0.41
4:3:118:LEU:HD23	4:3:118:LEU:HA	1.90	0.41
5:A:354:LEU:HD12	6:B:1158:LEU:HD13	2.02	0.41
5:A:514:GLU:O	5:A:518:LEU:HB2	2.21	0.41
5:A:578:ALA:O	12:H:92:MET:HA	2.20	0.41
5:A:727:PRO:HG3	5:A:733:LEU:HD13	2.03	0.41
5:A:734:ARG:NH2	13:I:108:MET:HB2	2.36	0.41
5:A:1625:THR:HG22	55:y:89:VAL:HG22	2.01	0.41
6:B:166:LEU:HB3	6:B:170:ASP:HB2	2.02	0.41
6:B:584:MET:HE3	6:B:588:ARG:HH11	1.85	0.41
9:E:71:GLN:HB2	9:E:99:ILE:HG22	2.02	0.41
12:H:13:LYS:HE3	12:H:31:GLU:OE1	2.20	0.41
17:M:46:TRP:CZ3	17:M:47:GLU:HB3	2.56	0.41
19:O:265:SER:OG	19:O:266:ALA:N	2.53	0.41
20:P:223:GLY:HA2	26:V:80:DT:H5'	2.02	0.41
21:Q:77:ARG:HG3	21:Q:79:GLU:H	1.85	0.41
22:R:86:LYS:HZ2	22:R:140:LYS:HD2	1.83	0.41
24:T:84:VAL:HG22	24:T:85:LEU:H	1.85	0.41
24:T:180:LYS:HB2	24:T:180:LYS:HE2	1.82	0.41
27:W:495:GLU:O	27:W:499:ASN:HB2	2.20	0.41
27:W:689:VAL:O	30:Z:393:LEU:CD1	2.68	0.41
29:Y:509:GLN:O	29:Y:513:ARG:HG3	2.20	0.41
30:Z:440:LEU:HB3	33:c:38:ILE:HG21	2.01	0.41
31:a:314:SER:HB3	31:a:317:HIS:CD2	2.55	0.41
40:j:469:ASP:CG	44:n:231:TRP:HD1	2.19	0.41
41:k:60:LEU:HD23	41:k:62:GLY:H	1.85	0.41
41:k:156:ASN:CG	41:k:158:ASP:H	2.27	0.41
42:l:187:ALA:O	42:l:191:VAL:HG23	2.20	0.41
43:m:105:LEU:HD23	43:m:105:LEU:HA	1.88	0.41
44:n:274:ILE:HD12	44:n:274:ILE:HA	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:91:GLY:C	46:p:93:LYS:H	2.27	0.41
48:r:155:PRO:O	48:r:156:TYR:C	2.61	0.41
49:s:146:GLU:HA	49:s:149:ILE:HG13	2.02	0.41
52:v:116:VAL:O	52:v:118:PRO:CD	2.68	0.41
54:x:18:GLN:C	54:x:20:CYS:H	2.27	0.41
54:x:68:ASP:O	54:x:69:ILE:C	2.62	0.41
55:y:60:ASP:HB2	55:y:63:TYR:CB	2.49	0.41
1:0:228:VAL:HG23	1:0:242:TYR:O	2.19	0.41
1:0:359:LEU:HD12	1:0:360:PRO:HD2	2.01	0.41
2:1:726:ASN:O	2:1:873:SER:OG	2.35	0.41
2:1:753:ARG:HH21	2:1:832:TYR:HB2	1.86	0.41
2:1:1105:LEU:HD12	2:1:1151:LEU:HB3	2.01	0.41
3:2:157:GLN:O	3:2:160:MET:HE2	2.19	0.41
4:3:172:GLN:HA	4:3:175:GLU:HG3	2.02	0.41
4:3:193:LEU:O	4:3:197:LYS:HB2	2.19	0.41
5:A:107:LEU:HD23	5:A:107:LEU:HA	1.82	0.41
5:A:860:ILE:H	5:A:860:ILE:HD12	1.84	0.41
5:A:868:MET:HE2	5:A:868:MET:HB3	1.84	0.41
5:A:1313:GLN:NE2	5:A:1333:GLU:H	2.18	0.41
6:B:261:PRO:HB2	6:B:346:GLU:HB3	2.03	0.41
6:B:699:HIS:ND1	6:B:701:SER:HB3	2.35	0.41
7:C:149:LEU:CD2	7:C:152:LYS:HE2	2.49	0.41
8:D:18:SER:O	8:D:117:SER:HB3	2.20	0.41
10:F:102:ILE:HA	10:F:103:PRO:HD3	1.85	0.41
12:H:75:TYR:CD2	12:H:77:PRO:HD3	2.55	0.41
17:M:334:VAL:HG12	18:N:94:LYS:HE3	2.02	0.41
19:O:12:ARG:HH21	19:O:23:LEU:HB2	1.85	0.41
19:O:42:GLY:O	19:O:43:ASP:HB2	2.20	0.41
19:O:52:TRP:N	19:O:52:TRP:CD1	2.87	0.41
19:O:175:ARG:HD2	19:O:179:GLU:OE2	2.21	0.41
27:W:105:GLU:CB	27:W:487:LYS:NZ	2.82	0.41
29:Y:506:CYS:O	29:Y:510:GLU:HG3	2.21	0.41
30:Z:400:ARG:CD	33:c:61:MET:HE1	2.49	0.41
31:a:293:GLN:HB2	31:a:310:LEU:HD22	2.03	0.41
35:e:231:THR:HG21	35:e:250:LYS:O	2.20	0.41
38:h:74:GLN:H	38:h:74:GLN:CD	2.28	0.41
38:h:150:LEU:HD21	39:i:45:LEU:HD13	2.01	0.41
39:i:11:LEU:O	39:i:15:GLU:HG2	2.19	0.41
40:j:387:LEU:O	40:j:387:LEU:HD23	2.19	0.41
41:k:153:VAL:CG1	41:k:156:ASN:HB3	2.50	0.41
43:m:75:LEU:HD12	43:m:75:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:n:10:ASN:HD21	44:n:78:GLY:HA3	1.85	0.41
44:n:225:ASP:O	44:n:227:LYS:N	2.48	0.41
48:r:82:LYS:HG2	48:r:82:LYS:H	1.54	0.41
48:r:176:LYS:C	48:r:176:LYS:HD3	2.45	0.41
48:r:230:PHE:O	48:r:230:PHE:CG	2.73	0.41
48:r:640:VAL:HG22	48:r:641:LEU:HD22	2.02	0.41
49:s:133:LYS:C	49:s:137:LYS:HZ2	2.28	0.41
50:t:151:GLU:HA	50:t:154:GLN:CD	2.46	0.41
50:t:159:ARG:NH1	50:t:160:VAL:HB	2.34	0.41
54:x:26:LEU:HG	54:x:58:PHE:CZ	2.55	0.41
54:x:69:ILE:HA	54:x:72:LEU:HG	2.02	0.41
55:y:35:ASN:ND2	55:y:94:ALA:HB2	2.34	0.41
55:y:113:MET:HB3	55:y:114:ARG:NH1	2.35	0.41
1:0:19:CYS:O	1:0:19:CYS:SG	2.77	0.41
1:0:112:ASP:OD1	1:0:112:ASP:N	2.50	0.41
1:0:521:VAL:HG22	4:3:151:TYR:HE2	1.85	0.41
1:0:568:PHE:CD2	1:0:570:ASN:HB3	2.55	0.41
3:2:22:GLN:HA	3:2:25:ILE:HG12	2.02	0.41
3:2:691:GLY:O	3:2:693:ASP:N	2.53	0.41
4:3:36:ARG:HA	4:3:40:LEU:HB2	2.03	0.41
4:3:153:LEU:HD23	4:3:154:PRO:O	2.21	0.41
5:A:466:LYS:HZ1	6:B:1097:HIS:HA	1.85	0.41
5:A:692:SER:O	5:A:828:LEU:HD22	2.20	0.41
5:A:928:ARG:HD2	12:H:106:THR:HG23	2.02	0.41
5:A:1162:GLU:H	5:A:1304:ILE:CD1	2.32	0.41
5:A:1480:CYS:SG	11:G:18:PHE:HB3	2.61	0.41
6:B:531:TYR:HB3	6:B:622:CYS:SG	2.60	0.41
6:B:1098:GLY:HA3	10:F:60:TYR:HE1	1.85	0.41
7:C:42:VAL:HA	7:C:43:PRO:HD3	1.93	0.41
7:C:59:LEU:HD13	7:C:63:PHE:CD2	2.55	0.41
8:D:112:LYS:HE3	8:D:112:LYS:HB3	1.89	0.41
8:D:135:GLN:HE22	8:D:138:ARG:HE	1.68	0.41
9:E:47:LYS:N	9:E:47:LYS:HD3	2.36	0.41
17:M:17:VAL:O	17:M:21:VAL:N	2.42	0.41
18:N:42:LYS:C	18:N:42:LYS:HD3	2.44	0.41
21:Q:188:TYR:O	21:Q:192:ARG:HG2	2.20	0.41
23:S:114:LYS:HE3	23:S:142:ASN:HD22	1.85	0.41
27:W:562:ALA:HB3	27:W:568:LEU:HD13	2.01	0.41
30:Z:122:LEU:HG	32:b:50:PHE:HE1	1.69	0.41
30:Z:409:TYR:HD1	33:c:4:VAL:CG1	2.34	0.41
35:e:119:LEU:HD12	35:e:119:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:72:LYS:HA	36:f:72:LYS:HD3	1.83	0.41
36:f:218:LEU:CD2	36:f:228:MET:HE2	2.49	0.41
40:j:225:ILE:HG22	40:j:226:LYS:H	1.85	0.41
40:j:393:PRO:HD2	41:k:137:ARG:NH2	2.18	0.41
40:j:464:TRP:CE3	40:j:475:VAL:CG2	3.04	0.41
40:j:595:GLN:HG2	40:j:621:PRO:O	2.20	0.41
42:l:154:TRP:CZ2	42:l:158:LEU:HD13	2.55	0.41
43:m:115:LYS:HB2	45:o:146:ILE:CD1	2.50	0.41
44:n:251:LEU:HA	44:n:251:LEU:HD23	1.80	0.41
44:n:258:MET:HE2	44:n:260:ASP:HB3	2.00	0.41
44:n:276:LEU:HA	44:n:297:ARG:NH2	2.35	0.41
48:r:113:GLU:O	48:r:114:LYS:C	2.64	0.41
48:r:226:VAL:HG13	48:r:228:GLY:H	1.85	0.41
48:r:234:LEU:HB3	48:r:246:ARG:C	2.46	0.41
48:r:909:GLN:OE1	48:r:915:ARG:HD2	2.21	0.41
48:r:933:VAL:HB	48:r:1176:ILE:HG22	2.02	0.41
48:r:1280:VAL:HA	48:r:1283:LYS:HD2	2.02	0.41
49:s:91:HIS:O	49:s:95:VAL:HG13	2.21	0.41
49:s:149:ILE:O	49:s:150:LYS:C	2.63	0.41
50:t:17:TYR:HA	50:t:19:LYS:HG2	2.01	0.41
50:t:78:LEU:O	50:t:82:ASN:OD1	2.37	0.41
50:t:154:GLN:HG3	50:t:155:LYS:N	2.34	0.41
52:v:76:ASN:N	52:v:76:ASN:HD22	2.18	0.41
52:v:116:VAL:O	52:v:117:PHE:C	2.63	0.41
54:x:119:GLN:HG3	54:x:119:GLN:H	1.04	0.41
55:y:55:LEU:O	55:y:58:TRP:CD1	2.74	0.41
1:0:264:PHE:CD1	1:0:265:MET:N	2.85	0.41
1:0:618:LEU:HD22	1:0:662:ILE:HD11	2.01	0.41
1:0:788:GLY:H	56:z:635:ASN:HD22	1.68	0.41
2:1:608:PHE:CE2	2:1:615:ILE:HG13	2.55	0.41
3:2:28:LYS:HD3	3:2:33:LYS:HG3	2.03	0.41
3:2:317:LEU:HD23	3:2:317:LEU:HA	1.92	0.41
3:2:422:LYS:HD3	3:2:423:THR:OG1	2.20	0.41
4:3:23:GLU:HG3	4:3:28:LEU:HD23	2.02	0.41
5:A:1288:ILE:O	5:A:1292:MET:HE2	2.21	0.41
6:B:1136:GLU:HG2	6:B:1143:LYS:HG2	2.03	0.41
10:F:83:LEU:HD12	10:F:83:LEU:H	1.86	0.41
12:H:60:ILE:HA	12:H:142:TYR:O	2.20	0.41
22:R:189:ILE:HB	22:R:204:ASN:HB2	2.03	0.41
23:S:20:LYS:NZ	24:T:32:ALA:HA	2.35	0.41
23:S:52:SER:HB3	23:S:99:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:43:LEU:HD12	24:T:58:LEU:HA	2.01	0.41
26:V:40:DT:OP1	27:W:610:VAL:HG12	2.20	0.41
28:X:310:LEU:HB3	28:X:311:PRO:CD	2.50	0.41
28:X:335:ARG:HH22	34:d:75:ARG:HD3	1.84	0.41
28:X:493:MET:HE2	28:X:493:MET:HB3	1.96	0.41
29:Y:428:SER:O	30:Z:64:GLN:NE2	2.53	0.41
29:Y:471:LEU:HD22	29:Y:502:VAL:CG2	2.49	0.41
29:Y:488:GLU:O	29:Y:492:LYS:HG3	2.20	0.41
35:e:41:LYS:O	35:e:88:SER:HA	2.21	0.41
35:e:83:HIS:ND1	35:e:84:LYS:N	2.67	0.41
37:g:47:ASN:OD1	37:g:48:GLU:N	2.53	0.41
37:g:84:GLN:HB3	37:g:92:VAL:CG1	2.50	0.41
40:j:463:HIS:CG	43:m:131:GLU:OE1	2.74	0.41
40:j:481:SER:OG	40:j:636:VAL:CG2	2.68	0.41
40:j:487:ILE:HD12	40:j:487:ILE:HA	1.60	0.41
40:j:551:PHE:CB	40:j:569:ILE:O	2.69	0.41
42:l:106:LYS:NZ	42:l:108:SER:HB3	2.35	0.41
44:n:21:ILE:HG12	46:p:116:LEU:HD22	2.02	0.41
48:r:52:SER:H	52:v:60:ASP:CA	2.23	0.41
48:r:90:SER:C	48:r:92:THR:N	2.76	0.41
48:r:104:LYS:HB3	53:w:108:PHE:CE2	2.55	0.41
48:r:160:VAL:CA	48:r:164:GLY:H	2.20	0.41
48:r:270:GLN:HG2	48:r:271:ILE:H	1.85	0.41
48:r:545:LEU:HD12	48:r:545:LEU:O	2.20	0.41
49:s:147:GLU:O	49:s:151:TYR:N	2.53	0.41
50:t:139:MET:HB2	54:x:97:ASN:OD1	2.21	0.41
50:t:149:THR:O	50:t:150:ALA:C	2.61	0.41
52:v:25:ILE:HG23	52:v:37:LEU:HD21	2.02	0.41
52:v:33:SER:O	52:v:37:LEU:N	2.42	0.41
53:w:128:ARG:NH1	53:w:131:ILE:C	2.78	0.41
54:x:69:ILE:O	54:x:70:ASP:C	2.63	0.41
54:x:93:LEU:O	54:x:96:GLU:HB2	2.20	0.41
55:y:52:LEU:C	55:y:56:LEU:HG	2.45	0.41
55:y:55:LEU:O	55:y:56:LEU:C	2.62	0.41
55:y:97:ILE:HD12	55:y:97:ILE:C	2.46	0.41
1:0:169:THR:O	1:0:170:LEU:HB2	2.19	0.41
1:0:238:PRO:HD3	1:0:264:PHE:CE2	2.56	0.41
1:0:239:VAL:HG22	1:0:263:LEU:O	2.20	0.41
1:0:792:THR:O	44:n:48:ARG:NH2	2.53	0.41
2:1:425:MET:O	2:1:428:ILE:HG12	2.20	0.41
2:1:515:MET:O	2:1:557:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:581:ILE:O	2:1:585:ILE:HG12	2.20	0.41
2:1:611:ARG:HD3	2:1:911:HIS:CD2	2.56	0.41
2:1:729:SER:N	2:1:875:GLU:OE1	2.53	0.41
4:3:132:ARG:C	4:3:134:GLN:N	2.78	0.41
5:A:57:LEU:HD23	5:A:57:LEU:H	1.86	0.41
5:A:262:PRO:HD3	6:B:1070:LEU:HD13	2.02	0.41
5:A:423:ASN:OD1	5:A:423:ASN:N	2.52	0.41
5:A:921:ARG:HD2	5:A:956:PHE:CD2	2.55	0.41
6:B:84:TYR:CE1	6:B:132:VAL:HG13	2.55	0.41
6:B:554:GLU:HB2	23:S:115:LYS:HD2	2.02	0.41
6:B:584:MET:HG3	6:B:605:ARG:HB2	2.02	0.41
6:B:1131:ARG:CZ	6:B:1131:ARG:HA	2.51	0.41
7:C:116:THR:HB	7:C:146:ASP:HB2	2.03	0.41
10:F:80:MET:HE3	10:F:103:PRO:HG2	2.03	0.41
11:G:127:CYS:SG	11:G:136:VAL:HG23	2.60	0.41
22:R:145:VAL:C	22:R:146:ARG:HD2	2.45	0.41
32:b:255:CYS:SG	32:b:257:CYS:N	2.88	0.41
37:g:130:PHE:HA	38:h:49:PHE:HE2	1.84	0.41
38:h:127:ASP:O	38:h:131:ILE:HG12	2.20	0.41
40:j:409:GLY:C	42:l:74:SER:HG	2.26	0.41
40:j:482:GLN:NE2	40:j:482:GLN:O	2.53	0.41
42:l:149:VAL:HG21	42:l:182:ALA:HA	2.02	0.41
46:p:86:THR:HG21	56:z:628:ASN:HD22	1.83	0.41
47:q:141:GLU:N	47:q:141:GLU:CD	2.79	0.41
48:r:135:ARG:O	48:r:136:LEU:C	2.62	0.41
48:r:185:LYS:C	48:r:185:LYS:HD3	2.45	0.41
48:r:552:VAL:HB	48:r:568:TYR:CD2	2.56	0.41
48:r:1254:SER:O	48:r:1254:SER:OG	2.38	0.41
49:s:107:ILE:HG21	54:x:125:ILE:HD13	2.02	0.41
49:s:152:ALA:O	49:s:153:HIS:C	2.62	0.41
51:u:71:ASN:HA	51:u:74:LYS:HE2	2.02	0.41
52:v:95:VAL:O	52:v:99:ILE:HG12	2.19	0.41
52:v:113:LEU:O	52:v:116:VAL:O	2.39	0.41
53:w:86:HIS:O	53:w:86:HIS:CG	2.74	0.41
55:y:27:CYS:O	55:y:28:LEU:C	2.63	0.41
1:0:531:ALA:HB1	1:0:544:VAL:HG23	2.01	0.41
2:1:229:PRO:HG3	2:1:241:TRP:CD2	2.55	0.41
2:1:642:HIS:O	2:1:646:GLU:HG2	2.20	0.41
2:1:964:LEU:HD12	2:1:964:LEU:HA	1.85	0.41
3:2:125:LEU:HD22	3:2:178:LEU:HG	2.02	0.41
3:2:171:SER:C	3:2:173:LYS:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:28:LEU:HG	4:3:32:PHE:HB2	2.03	0.41
4:3:45:GLU:C	4:3:47:PHE:H	2.28	0.41
5:A:1121:VAL:N	5:A:1122:PRO:HD2	2.36	0.41
5:A:1218:ARG:O	5:A:1222:THR:HB	2.21	0.41
5:A:1624:PRO:HB2	5:A:1627:PRO:CD	2.50	0.41
6:B:128:ILE:HD12	6:B:431:LEU:HD21	2.02	0.41
6:B:222:ARG:HA	6:B:234:THR:HA	2.01	0.41
6:B:625:LEU:HD12	6:B:665:ILE:HD12	2.03	0.41
6:B:755:GLN:NE2	6:B:777:ASN:H	2.17	0.41
6:B:988:LYS:HG2	6:B:1015:LEU:HD11	2.02	0.41
7:C:78:ILE:HG21	7:C:127:VAL:HG22	2.03	0.41
7:C:153:LEU:HB2	7:C:157:GLN:HB2	2.01	0.41
8:D:112:LYS:HE3	8:D:119:GLU:HA	2.02	0.41
11:G:108:ILE:HG22	11:G:161:GLY:HA3	2.02	0.41
18:N:76:LEU:CD1	18:N:95:ILE:HD13	2.49	0.41
21:Q:14:LEU:HD12	21:Q:194:THR:HA	2.02	0.41
23:S:173:HIS:HD2	23:S:176:ILE:HG13	1.86	0.41
25:U:47:DC:H2"	25:U:48:DG:C8	2.56	0.41
27:W:129:VAL:HG23	27:W:334:ARG:NH2	2.36	0.41
27:W:178:GLU:HG2	27:W:269:SER:HB3	2.01	0.41
27:W:295:TYR:CE1	27:W:461:HIS:HB3	2.46	0.41
30:Z:53:LYS:HE3	30:Z:53:LYS:HB2	1.91	0.41
30:Z:400:ARG:CZ	33:c:61:MET:HE1	2.50	0.41
31:a:249:LEU:CD1	32:b:268:CYS:HA	2.49	0.41
35:e:61:ARG:HD2	35:e:157:GLY:O	2.21	0.41
35:e:160:LYS:NZ	36:f:117:GLU:HG3	2.36	0.41
37:g:48:GLU:O	37:g:52:MET:HG2	2.21	0.41
40:j:609:VAL:HG21	56:z:706:LEU:HD21	2.02	0.41
40:j:610:LEU:O	40:j:611:GLN:C	2.63	0.41
44:n:87:HIS:NE2	46:p:134:ALA:HA	2.36	0.41
44:n:95:ASP:O	44:n:97:VAL:N	2.48	0.41
44:n:166:ILE:HD13	44:n:166:ILE:HA	1.87	0.41
46:p:91:GLY:O	46:p:93:LYS:N	2.54	0.41
46:p:103:ASP:HB3	56:z:645:ALA:HB2	2.02	0.41
48:r:504:ARG:NH1	48:r:636:ALA:HA	2.36	0.41
48:r:558:PRO:C	48:r:560:LYS:H	2.29	0.41
48:r:1178:THR:C	48:r:1180:SER:H	2.27	0.41
49:s:129:LYS:O	49:s:130:GLU:C	2.61	0.41
49:s:187:LEU:HD23	49:s:188:GLY:N	2.36	0.41
50:t:95:ILE:HD12	50:t:95:ILE:HA	1.81	0.41
50:t:160:VAL:HA	50:t:163:MET:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:93:GLU:O	52:v:94:GLN:C	2.61	0.41
54:x:112:ASP:HA	54:x:115:LEU:HD21	2.03	0.41
54:x:129:GLN:O	54:x:132:THR:N	2.52	0.41
55:y:27:CYS:O	55:y:33:TYR:HD2	2.04	0.41
55:y:88:LEU:O	55:y:90:ASN:N	2.53	0.41
55:y:117:GLN:O	55:y:121:GLU:HG3	2.21	0.41
2:1:13:VAL:HA	2:1:75:ARG:NH2	2.36	0.41
2:1:676:LEU:HD21	2:1:719:ILE:HG13	2.02	0.41
2:1:977:LEU:HG	2:1:979:PRO:HD2	2.02	0.41
2:1:1261:GLN:HB3	2:1:1262:GLU:OE1	2.21	0.41
3:2:86:ASP:C	3:2:88:PHE:H	2.28	0.41
3:2:434:GLY:O	3:2:438:VAL:HG23	2.20	0.41
3:2:598:ALA:O	3:2:599:PHE:C	2.63	0.41
5:A:430:ARG:NH2	19:O:26:ASP:OD1	2.54	0.41
6:B:528:LEU:HD12	6:B:528:LEU:HA	1.91	0.41
7:C:33:SER:O	7:C:37:VAL:HG22	2.21	0.41
7:C:40:ALA:O	7:C:170:GLY:N	2.49	0.41
17:M:354:LYS:HE2	17:M:354:LYS:HB3	1.72	0.41
21:Q:19:LYS:HA	21:Q:22:ILE:HB	2.03	0.41
22:R:166:ILE:HG22	22:R:167:LEU:N	2.36	0.41
28:X:311:PRO:CD	28:X:410:TYR:HH	2.32	0.41
28:X:464:LEU:HB2	28:X:760:LEU:HD12	2.03	0.41
28:X:653:THR:HG22	28:X:692:LYS:HD2	2.02	0.41
29:Y:430:THR:HB	32:b:225:GLN:HG2	2.03	0.41
36:f:70:VAL:O	36:f:70:VAL:HG12	2.19	0.41
36:f:122:SER:N	36:f:123:PRO:HD2	2.36	0.41
40:j:43:LEU:CD1	48:r:191:THR:HG21	2.49	0.41
40:j:193:HIS:ND1	40:j:292:GLN:NE2	2.67	0.41
40:j:251:LEU:HD12	40:j:298:ALA:O	2.20	0.41
40:j:391:MET:CG	40:j:400:PHE:HD1	2.33	0.41
40:j:406:ARG:O	40:j:409:GLY:N	2.53	0.41
40:j:504:VAL:HG11	40:j:524:PHE:CE2	2.55	0.41
40:j:630:MET:HE2	40:j:630:MET:HB3	1.91	0.41
43:m:26:ILE:HG13	43:m:27:LYS:N	2.36	0.41
44:n:45:LEU:HD21	56:z:630:ARG:NH2	2.35	0.41
45:o:131:LYS:O	45:o:134:THR:OG1	2.32	0.41
48:r:169:LEU:CD1	48:r:173:ILE:HA	2.47	0.41
48:r:609:ARG:HD3	48:r:610:THR:N	2.36	0.41
49:s:141:GLY:C	49:s:143:ILE:N	2.63	0.41
50:t:25:ASN:OD1	50:t:29:GLY:HA3	2.21	0.41
50:t:105:ARG:O	50:t:108:LYS:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:v:7:HIS:C	52:v:11:HIS:HD2	2.28	0.41
52:v:12:LEU:HD12	52:v:15:PHE:CD2	2.56	0.41
54:x:52:GLU:O	54:x:53:GLU:C	2.63	0.41
54:x:65:THR:O	54:x:68:ASP:HB3	2.20	0.41
54:x:79:GLU:OE1	54:x:80:GLU:N	2.53	0.41
55:y:17:ARG:N	55:y:17:ARG:HD3	2.36	0.41
55:y:116:GLN:HA	55:y:119:LEU:HG	2.01	0.41
2:1:8:ILE:HG21	2:1:44:PHE:HE1	1.86	0.41
2:1:196:LEU:HD13	3:2:802:MET:HB2	2.01	0.41
2:1:396:MET:HG3	2:1:429:TRP:HH2	1.86	0.41
2:1:503:GLY:C	2:1:505:MET:H	2.29	0.41
2:1:516:ALA:HA	2:1:557:VAL:HG13	2.03	0.41
2:1:594:LYS:HA	2:1:594:LYS:HD2	1.79	0.41
2:1:608:PHE:HZ	2:1:615:ILE:HG21	1.85	0.41
2:1:905:LYS:HE3	2:1:905:LYS:HB2	1.78	0.41
2:1:975:LEU:HD21	2:1:1016:LEU:HD11	2.03	0.41
2:1:1171:VAL:HG11	2:1:1247:TYR:CZ	2.56	0.41
3:2:484:LYS:HB3	3:2:485:PRO:HD3	2.03	0.41
3:2:553:LYS:HD3	3:2:557:LEU:HB2	2.02	0.41
3:2:574:TRP:HA	3:2:577:ALA:HB3	2.03	0.41
3:2:799:HIS:O	3:2:802:MET:HG2	2.20	0.41
3:2:917:ALA:HA	3:2:921:THR:HG21	2.02	0.41
4:3:67:SER:OG	4:3:124:LEU:HD21	2.21	0.41
4:3:132:ARG:C	4:3:134:GLN:H	2.29	0.41
5:A:280:LEU:O	5:A:284:VAL:HG12	2.21	0.41
5:A:325:LEU:O	5:A:326:PRO:C	2.63	0.41
5:A:330:GLN:HG3	5:A:332:SER:N	2.36	0.41
5:A:402:LEU:HD23	5:A:402:LEU:HA	1.88	0.41
5:A:592:PHE:CD1	5:A:595:ILE:HD11	2.55	0.41
5:A:652:LEU:HD12	5:A:652:LEU:HA	1.94	0.41
5:A:849:ASP:HA	5:A:852:VAL:HG22	2.03	0.41
5:A:1198:GLU:HG3	5:A:1199:MET:H	1.86	0.41
5:A:1284:PHE:O	5:A:1288:ILE:HG13	2.20	0.41
6:B:564:ALA:O	6:B:610:ARG:HB3	2.21	0.41
6:B:1112:ASP:OD1	6:B:1153:TYR:HB3	2.20	0.41
7:C:30:VAL:O	7:C:34:ILE:HG12	2.20	0.41
8:D:83:VAL:HG13	8:D:84:ARG:N	2.35	0.41
8:D:124:ASP:C	8:D:126:GLU:H	2.29	0.41
13:I:40:ARG:CZ	23:S:171:LEU:HB3	2.50	0.41
15:K:13:PHE:H	15:K:16:GLU:HG2	1.86	0.41
21:Q:32:LEU:HD12	21:Q:54:PHE:HZ	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:194:THR:O	21:Q:195:GLU:HG3	2.21	0.41
22:R:166:ILE:HG22	22:R:167:LEU:H	1.86	0.41
23:S:29:MET:HG3	23:S:146:PHE:CD2	2.55	0.41
27:W:103:ILE:HD13	27:W:136:ILE:HG23	2.03	0.41
27:W:568:LEU:HD11	27:W:606:PHE:HB3	2.02	0.41
28:X:145:GLN:HA	28:X:148:HIS:CE1	2.55	0.41
28:X:383:LEU:HD11	28:X:394:PHE:CD2	2.56	0.41
28:X:524:LEU:HD12	28:X:524:LEU:HA	1.91	0.41
29:Y:389:ILE:HG13	32:b:259:ARG:HE	1.85	0.41
29:Y:407:ILE:HD12	32:b:19:PRO:HA	1.97	0.41
30:Z:346:VAL:O	30:Z:394:TRP:CH2	2.74	0.41
31:a:95:TYR:HD2	31:a:104:ILE:HD11	1.85	0.41
31:a:379:LEU:HD11	32:b:138:ALA:CA	2.51	0.41
34:d:74:ILE:HG23	34:d:109:LEU:HD23	2.03	0.41
35:e:125:LEU:HG	35:e:129:HIS:CE1	2.55	0.41
38:h:4:GLU:HG3	38:h:5:GLU:N	2.36	0.41
38:h:58:THR:HA	38:h:61:LYS:HE2	2.03	0.41
38:h:68:THR:O	38:h:69:PRO:C	2.64	0.41
40:j:318:ILE:O	40:j:319:LYS:HB3	2.21	0.41
40:j:542:LYS:HA	40:j:542:LYS:HD3	1.92	0.41
40:j:547:GLN:NE2	40:j:548:VAL:H	2.19	0.41
40:j:569:ILE:CG1	40:j:583:ARG:HG3	2.51	0.41
40:j:620:GLY:HA3	40:j:621:PRO:HD3	1.85	0.41
42:l:47:HIS:HD1	42:l:47:HIS:N	2.18	0.41
42:l:76:PHE:CZ	42:l:86:ILE:CD1	3.04	0.41
43:m:121:ASP:OD2	44:n:186:THR:CB	2.69	0.41
44:n:73:LEU:HA	44:n:73:LEU:HD23	1.80	0.41
44:n:196:LYS:HA	44:n:217:TYR:CG	2.56	0.41
44:n:253:TYR:O	44:n:262:VAL:HG23	2.21	0.41
46:p:172:LYS:HD3	46:p:172:LYS:HA	1.90	0.41
48:r:57:PHE:CD1	48:r:60:HIS:ND1	2.88	0.41
48:r:86:VAL:O	48:r:90:SER:CB	2.68	0.41
48:r:165:SER:H	48:r:168:ARG:NH1	2.17	0.41
48:r:174:ARG:C	48:r:177:ILE:H	2.28	0.41
48:r:307:VAL:O	48:r:310:SER:OG	2.33	0.41
48:r:311:GLN:OE1	48:r:397:ILE:HG22	2.20	0.41
48:r:657:LEU:HD23	48:r:682:ILE:CD1	2.50	0.41
48:r:1249:CYS:SG	48:r:1265:VAL:HG22	2.61	0.41
49:s:102:LYS:HZ2	49:s:102:LYS:C	2.29	0.41
50:t:30:LEU:HD12	50:t:30:LEU:HA	1.78	0.41
50:t:133:GLU:HA	50:t:136:ARG:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:147:LEU:O	50:t:148:GLU:C	2.63	0.41
52:v:11:HIS:O	52:v:14:LYS:N	2.54	0.41
52:v:64:PRO:O	52:v:65:LEU:C	2.64	0.41
52:v:69:GLU:OE2	52:v:72:ASP:HB2	2.21	0.41
52:v:90:ALA:CA	52:v:93:GLU:HG2	2.51	0.41
52:v:93:GLU:N	52:v:93:GLU:OE2	2.54	0.41
52:v:112:GLU:O	52:v:115:LYS:N	2.54	0.41
54:x:53:GLU:O	54:x:54:TYR:C	2.62	0.41
55:y:56:LEU:O	55:y:58:TRP:N	2.54	0.41
56:z:753:HIS:O	56:z:757:THR:HG22	2.20	0.41
1:0:103:GLY:HA3	1:0:126:VAL:O	2.21	0.41
1:0:603:GLU:OE1	1:0:603:GLU:N	2.53	0.41
2:1:130:ASP:O	2:1:134:VAL:HG23	2.21	0.41
2:1:181:TYR:O	2:1:184:VAL:HG12	2.21	0.41
2:1:554:LYS:HE2	2:1:554:LYS:HB2	1.93	0.41
2:1:603:THR:HG22	2:1:953:PRO:HB2	2.02	0.41
2:1:809:ARG:O	2:1:812:GLU:HG2	2.21	0.41
3:2:176:ALA:HB1	3:2:968:LEU:HD13	2.02	0.41
3:2:480:GLU:OE2	3:2:485:PRO:HB2	2.21	0.41
3:2:784:LEU:HG	3:2:904:LEU:HD22	2.02	0.41
5:A:301:HIS:CD2	5:A:302:VAL:HG23	2.55	0.41
5:A:1164:THR:HG22	5:A:1224:ARG:HE	1.85	0.41
5:A:1628:SER:C	5:A:1629:TYR:CG	2.99	0.41
6:B:101:ARG:NH2	19:O:171:GLU:O	2.53	0.41
6:B:286:GLU:OE2	6:B:558:PRO:HB2	2.20	0.41
6:B:332:LYS:O	6:B:336:ILE:HG12	2.21	0.41
6:B:794:VAL:HB	6:B:965:ILE:HG23	2.02	0.41
7:C:7:PRO:HD2	15:K:100:LEU:HD23	2.03	0.41
10:F:57:MET:HE3	10:F:57:MET:HB2	1.89	0.41
11:G:151:ARG:HH22	21:Q:143:GLN:HE22	1.68	0.41
20:P:297:LYS:HE3	20:P:297:LYS:HB3	1.94	0.41
21:Q:110:MET:HE1	22:R:219:LEU:HB3	2.02	0.41
22:R:192:VAL:HG13	22:R:194:ARG:HG2	2.03	0.41
25:U:6:DG:N2	26:V:89:DC:O2	2.54	0.41
27:W:124:TYR:OH	27:W:292:LEU:C	2.58	0.41
27:W:519:TYR:HE2	33:c:22:TYR:CD2	2.38	0.41
27:W:689:VAL:C	30:Z:393:LEU:CD1	2.93	0.41
28:X:517:ILE:HG23	28:X:548:THR:HG23	2.03	0.41
28:X:611:VAL:HG12	28:X:612:HIS:H	1.85	0.41
29:Y:499:ARG:HH22	29:Y:535:LYS:HE3	1.82	0.41
36:f:30:PHE:CD2	36:f:97:MET:HE3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:45:CYS:SG	37:g:46:ASN:N	2.94	0.41
39:i:37:LYS:O	40:j:150:LYS:NZ	2.54	0.41
40:j:569:ILE:CG2	40:j:582:VAL:O	2.64	0.41
40:j:609:VAL:HG11	56:z:682:VAL:CG2	2.49	0.41
42:l:155:SER:O	42:l:159:GLU:HG3	2.21	0.41
44:n:111:TYR:CE1	46:p:136:HIS:HB2	2.52	0.41
44:n:220:ASN:O	44:n:222:TYR:N	2.53	0.41
45:o:105:GLN:O	45:o:107:PRO:HD3	2.21	0.41
47:q:82:LEU:HD23	47:q:85:LEU:HD12	2.03	0.41
48:r:62:ALA:O	48:r:65:GLU:OE2	2.39	0.41
48:r:124:GLN:OE1	48:r:127:ILE:HG13	2.20	0.41
48:r:458:LEU:HA	48:r:458:LEU:HD23	1.74	0.41
49:s:115:LYS:HD3	49:s:115:LYS:HA	1.86	0.41
50:t:16:GLN:CG	50:t:17:TYR:H	2.33	0.41
54:x:85:LEU:C	54:x:87:ALA:N	2.76	0.41
55:y:22:LEU:O	55:y:23:GLU:C	2.64	0.41
55:y:81:TYR:C	55:y:85:ARG:NH1	2.79	0.41
56:z:730:PRO:HB2	56:z:766:LYS:HZ2	1.85	0.41
1:0:90:ASP:HB2	1:0:95:ARG:HB2	2.03	0.40
1:0:283:LEU:HA	1:0:295:LEU:O	2.20	0.40
1:0:713:LEU:HD12	1:0:713:LEU:HA	1.84	0.40
3:2:47:LEU:O	3:2:51:MET:HG3	2.21	0.40
3:2:248:ILE:HD11	3:2:267:LEU:HD11	2.02	0.40
3:2:665:ILE:O	3:2:669:ILE:HG12	2.21	0.40
5:A:72:GLN:C	5:A:74:CYS:N	2.78	0.40
5:A:73:THR:HG22	21:Q:155:THR:HB	2.02	0.40
5:A:1243:LEU:HD11	5:A:1288:ILE:HD13	2.02	0.40
6:B:235:ILE:HG12	6:B:261:PRO:HD3	2.03	0.40
6:B:543:GLU:O	6:B:547:GLU:HG2	2.20	0.40
6:B:584:MET:O	6:B:588:ARG:HG3	2.21	0.40
6:B:712:PRO:HD3	6:B:938:ARG:NE	2.36	0.40
6:B:798:ARG:HA	6:B:801:VAL:HG22	2.03	0.40
7:C:103:LEU:CD1	7:C:119:ASP:HB3	2.51	0.40
8:D:72:SER:HA	8:D:74:PHE:HD1	1.85	0.40
9:E:10:LEU:HD21	9:E:54:ARG:CZ	2.51	0.40
18:N:61:SER:O	18:N:76:LEU:HD23	2.21	0.40
19:O:7:LEU:HB3	19:O:8:ASP:H	1.50	0.40
19:O:9:ALA:HA	21:Q:157:CYS:SG	2.61	0.40
20:P:178:LEU:HA	20:P:178:LEU:HD23	1.80	0.40
23:S:171:LEU:O	23:S:172:ASN:HB2	2.21	0.40
28:X:641:ARG:NH2	28:X:648:GLU:OE1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:11:ARG:H	30:Z:11:ARG:HD3	1.85	0.40
30:Z:17:ARG:NH2	30:Z:221:GLN:OE1	2.51	0.40
30:Z:220:LEU:HD21	30:Z:233:ILE:HG21	2.01	0.40
30:Z:384:PRO:HA	30:Z:385:PRO:HD3	1.82	0.40
30:Z:424:HIS:CD2	30:Z:451:VAL:HG22	2.54	0.40
35:e:263:ALA:HB2	37:g:48:GLU:HG2	2.04	0.40
36:f:198:ILE:HD13	36:f:198:ILE:HG21	1.88	0.40
40:j:263:LYS:HA	40:j:263:LYS:HD3	1.88	0.40
40:j:326:VAL:HG12	40:j:331:ILE:HG23	2.03	0.40
42:l:146:PRO:CB	44:n:236:TYR:CD2	2.90	0.40
47:q:53:GLN:HE22	47:q:56:ARG:NH2	2.19	0.40
48:r:80:GLU:HA	48:r:83:ILE:HG12	2.03	0.40
48:r:152:PHE:CE2	50:t:127:ARG:HG3	2.56	0.40
49:s:76:PHE:HZ	51:u:101:ILE:HD12	1.84	0.40
49:s:109:GLN:O	49:s:110:LEU:C	2.63	0.40
50:t:17:TYR:HD1	50:t:17:TYR:H	1.56	0.40
50:t:152:ARG:O	50:t:153:PHE:C	2.64	0.40
54:x:106:ASP:O	54:x:110:ARG:HG3	2.21	0.40
56:z:768:SER:O	56:z:771:ALA:N	2.52	0.40
1:0:18:VAL:HA	1:0:452:LEU:O	2.21	0.40
1:0:355:ALA:HB2	1:0:434:MET:HG2	2.02	0.40
1:0:377:TYR:O	1:0:378:PRO:C	2.63	0.40
2:1:95:ARG:O	2:1:99:GLU:HG3	2.21	0.40
2:1:408:TYR:OH	2:1:452:ARG:NE	2.52	0.40
2:1:760:VAL:HG21	2:1:829:PHE:CD1	2.56	0.40
2:1:1195:ALA:C	2:1:1197:HIS:H	2.29	0.40
3:2:255:ASN:OD1	3:2:258:GLY:HA3	2.22	0.40
3:2:260:THR:O	3:2:264:VAL:HG23	2.20	0.40
3:2:349:ASP:OD1	3:2:350:LYS:N	2.54	0.40
3:2:481:GLU:HG2	3:2:482:SER:N	2.37	0.40
5:A:1194:ASN:HA	5:A:1197:TYR:CE1	2.56	0.40
6:B:309:PHE:HE2	13:I:40:ARG:HB2	1.86	0.40
6:B:317:ALA:O	6:B:321:ILE:HG13	2.22	0.40
6:B:425:ARG:HH21	6:B:427:LYS:NZ	2.20	0.40
6:B:755:GLN:NE2	6:B:777:ASN:HD22	2.19	0.40
6:B:1075:MET:HG2	6:B:1076:GLU:N	2.37	0.40
7:C:15:THR:HB	7:C:18:ASN:OD1	2.21	0.40
8:D:70:ARG:HA	43:m:20:LYS:CE	2.50	0.40
9:E:82:VAL:HG13	9:E:86:THR:OG1	2.21	0.40
12:H:6:PHE:CE2	12:H:125:LEU:HD11	2.56	0.40
17:M:319:ASP:HB3	20:P:236:LYS:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:18:HIS:CE1	19:O:36:GLU:HG2	2.56	0.40
21:Q:172:ASP:O	21:Q:173:ALA:C	2.64	0.40
22:R:146:ARG:NE	22:R:173:GLU:O	2.54	0.40
24:T:15:ASN:HA	24:T:108:GLY:HA2	2.04	0.40
24:T:131:GLN:O	24:T:135:SER:OG	2.39	0.40
25:U:4:DG:H2"	25:U:5:DG:C8	2.56	0.40
27:W:631:GLY:HA2	27:W:632:SER:HA	1.82	0.40
29:Y:475:PHE:HB3	29:Y:499:ARG:HH21	1.85	0.40
30:Z:74:TRP:HZ2	32:b:229:TRP:CZ2	2.33	0.40
31:a:254:PHE:CE2	32:b:274:ILE:HG23	2.54	0.40
35:e:143:LEU:HD11	35:e:202:ILE:HD13	2.04	0.40
35:e:189:MET:HE2	35:e:189:MET:HB2	1.75	0.40
35:e:257:LEU:HD23	35:e:260:ILE:HD12	2.03	0.40
37:g:121:THR:OG1	40:j:108:GLU:OE2	2.32	0.40
41:k:169:VAL:HG21	41:k:197:VAL:HG21	2.03	0.40
42:l:16:SER:O	42:l:20:THR:N	2.46	0.40
44:n:189:MET:HG2	44:n:203:VAL:HG22	2.02	0.40
44:n:211:ARG:NH2	44:n:230:ILE:O	2.54	0.40
44:n:215:LYS:HE2	44:n:233:LYS:O	2.21	0.40
47:q:73:ASP:O	47:q:77:LYS:HG2	2.21	0.40
48:r:185:LYS:O	48:r:185:LYS:CE	2.69	0.40
48:r:566:TYR:HB3	48:r:568:TYR:HE1	1.85	0.40
52:v:77:PRO:O	52:v:79:LEU:N	2.55	0.40
54:x:86:GLN:NE2	54:x:86:GLN:N	2.69	0.40
55:y:46:LYS:H	55:y:46:LYS:CD	2.33	0.40
55:y:98:ASP:OD1	55:y:98:ASP:N	2.53	0.40
1:0:807:LEU:HD11	1:0:835:ARG:NH1	2.36	0.40
1:0:812:ARG:CZ	46:p:90:ASN:O	2.68	0.40
2:1:160:LEU:HD23	2:1:160:LEU:HA	1.88	0.40
2:1:316:GLU:O	2:1:317:THR:OG1	2.31	0.40
2:1:1186:TYR:CD2	3:2:238:LYS:HB3	2.56	0.40
3:2:343:LYS:HE2	3:2:343:LYS:HB2	1.91	0.40
4:3:40:LEU:O	4:3:44:ILE:HG12	2.21	0.40
5:A:60:PRO:C	5:A:62:GLN:H	2.29	0.40
5:A:380:VAL:HG13	5:A:482:PHE:HE1	1.86	0.40
5:A:988:TRP:O	5:A:992:LYS:HG2	2.20	0.40
5:A:1267:ASN:OD1	5:A:1267:ASN:N	2.54	0.40
6:B:472:ARG:HA	6:B:472:ARG:HD2	1.89	0.40
6:B:552:ASN:O	6:B:556:ILE:HG23	2.21	0.40
6:B:815:LYS:HG3	6:B:918:PHE:CE1	2.56	0.40
7:C:78:ILE:HG22	7:C:82:LEU:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:179:ASP:O	20:P:183:ILE:HG13	2.22	0.40
20:P:323:GLU:HG2	20:P:327:ASN:ND2	2.35	0.40
21:Q:191:LEU:HA	21:Q:194:THR:OG1	2.21	0.40
24:T:147:LYS:HD2	24:T:147:LYS:HA	1.83	0.40
28:X:537:ALA:HB1	28:X:621:PHE:HE2	1.86	0.40
28:X:637:LEU:HD23	28:X:637:LEU:HA	1.88	0.40
29:Y:510:GLU:OE2	29:Y:526:GLU:CG	2.69	0.40
31:a:232:LEU:HD23	31:a:232:LEU:HA	1.89	0.40
35:e:71:HIS:CD2	35:e:72:PRO:HD2	2.56	0.40
35:e:118:MET:HE1	35:e:199:VAL:CG1	2.51	0.40
40:j:336:PHE:HZ	40:j:500:GLU:HA	1.85	0.40
44:n:233:LYS:HD3	44:n:233:LYS:HA	1.80	0.40
44:n:273:TYR:HD1	44:n:276:LEU:HD13	1.87	0.40
46:p:85:ASN:ND2	56:z:641:THR:HG23	2.31	0.40
46:p:103:ASP:C	48:r:944:PHE:CD2	2.97	0.40
48:r:60:HIS:HA	48:r:63:TYR:HB3	2.02	0.40
48:r:528:HIS:CD2	48:r:609:ARG:HD2	2.57	0.40
49:s:92:GLU:O	49:s:96:LEU:HB2	2.20	0.40
50:t:156:HIS:O	50:t:160:VAL:HG12	2.22	0.40
52:v:68:PHE:O	52:v:71:ILE:N	2.54	0.40
52:v:90:ALA:HA	52:v:93:GLU:CG	2.51	0.40
53:w:129:SER:HA	53:w:132:GLU:OE1	2.21	0.40
54:x:115:LEU:HD12	54:x:116:GLU:HG3	2.03	0.40
1:0:309:TRP:CH2	1:0:341:ILE:HG13	2.57	0.40
1:0:585:THR:OG1	1:0:586:LYS:N	2.54	0.40
1:0:609:ASN:ND2	1:0:814:THR:HB	2.37	0.40
1:0:734:ALA:HB3	1:0:802:GLY:HA3	2.04	0.40
1:0:821:GLN:O	4:3:105:GLY:HA2	2.21	0.40
2:1:9:PHE:O	2:1:12:VAL:HG22	2.21	0.40
2:1:98:CYS:HB2	2:1:137:LEU:HD21	2.03	0.40
2:1:507:ILE:HB	2:1:508:PRO:HD2	2.03	0.40
2:1:689:LEU:HD11	2:1:871:MET:HE1	2.03	0.40
2:1:772:ASN:HB2	2:1:776:ILE:HB	2.04	0.40
2:1:972:HIS:CD2	2:1:1008:THR:HG23	2.57	0.40
3:2:113:LYS:HE3	3:2:115:GLU:HG2	2.02	0.40
3:2:286:TRP:CH2	3:2:363:LEU:HD11	2.57	0.40
4:3:16:ALA:O	4:3:64:THR:HA	2.21	0.40
4:3:45:GLU:CA	4:3:48:ASN:O	2.68	0.40
5:A:15:LEU:HD22	6:B:1150:ARG:HG3	2.04	0.40
5:A:130:LEU:HD12	5:A:235:VAL:HG23	2.02	0.40
5:A:279:LYS:HD3	5:A:279:LYS:HA	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:279:LYS:HE2	5:A:336:LEU:HD12	2.03	0.40
5:A:549:THR:O	5:A:589:LYS:HE2	2.22	0.40
6:B:117:ASN:HD22	6:B:117:ASN:HA	1.65	0.40
6:B:591:ARG:O	6:B:598:VAL:HG12	2.22	0.40
6:B:786:THR:HG21	6:B:949:TYR:OH	2.21	0.40
7:C:172:GLU:HB3	7:C:176:TRP:CZ3	2.56	0.40
8:D:142:TYR:CD2	43:m:25:ASP:CA	2.99	0.40
9:E:106:VAL:HG11	9:E:110:MET:HG3	2.04	0.40
13:I:96:PHE:CD1	13:I:110:LEU:HD12	2.57	0.40
20:P:309:LYS:HD3	26:V:83:DA:OP1	2.20	0.40
21:Q:17:LEU:O	21:Q:21:VAL:HG22	2.22	0.40
22:R:133:ILE:HG22	22:R:134:ASP:N	2.36	0.40
22:R:134:ASP:OD1	22:R:135:GLY:N	2.55	0.40
24:T:59:ASN:OD1	24:T:59:ASN:N	2.53	0.40
24:T:124:TYR:O	24:T:128:LYS:HG2	2.21	0.40
25:U:12:DA:N1	26:V:82:DT:N3	2.53	0.40
28:X:72:TYR:OH	28:X:234:ASP:OD2	2.34	0.40
28:X:310:LEU:HB2	28:X:315:LEU:HD21	2.03	0.40
28:X:328:HIS:CE1	34:d:107:PHE:HB2	2.56	0.40
30:Z:228:MET:HE1	30:Z:257:SER:HB2	2.04	0.40
30:Z:384:PRO:HB2	30:Z:387:ILE:CB	2.45	0.40
30:Z:401:LEU:HD23	33:c:16:MET:HE1	2.04	0.40
32:b:256:PHE:CD2	32:b:273:SER:HB2	2.57	0.40
40:j:194:TRP:CE3	40:j:295:LEU:HD13	2.55	0.40
40:j:368:LEU:HD13	40:j:371:LEU:HD13	2.03	0.40
40:j:546:TRP:HZ2	40:j:643:MET:O	2.04	0.40
43:m:66:ALA:O	43:m:69:VAL:HG12	2.21	0.40
43:m:91:PHE:HA	43:m:94:VAL:HG12	2.02	0.40
43:m:140:SER:HA	47:q:146:ASN:CB	2.39	0.40
48:r:232:ALA:CB	48:r:250:LEU:HG	2.51	0.40
48:r:553:GLU:OE2	48:r:555:LEU:N	2.46	0.40
48:r:712:LEU:HD12	48:r:712:LEU:HA	1.88	0.40
49:s:123:THR:HA	49:s:126:TYR:HD2	1.81	0.40
52:v:33:SER:C	52:v:35:ALA:N	2.77	0.40
52:v:53:LYS:C	52:v:56:GLN:HE21	2.28	0.40
52:v:118:PRO:O	52:v:121:MET:HE3	2.22	0.40
55:y:33:TYR:O	55:y:36:PHE:HB2	2.21	0.40
55:y:53:LYS:N	55:y:53:LYS:HD2	2.35	0.40
56:z:711:ASP:HB3	56:z:712:ASP:H	1.70	0.40
1:0:100:ASP:OD1	1:0:100:ASP:N	2.44	0.40
1:0:115:ALA:CB	1:0:834:TRP:CZ3	3.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:207:CYS:SG	1:0:208:ARG:N	2.95	0.40
1:0:286:LEU:HD12	1:0:286:LEU:HA	1.80	0.40
1:0:592:ILE:HG12	1:0:593:ASP:O	2.20	0.40
1:0:667:LEU:HD12	1:0:667:LEU:HA	1.77	0.40
1:0:731:TRP:CE3	1:0:731:TRP:HA	2.57	0.40
1:0:745:LYS:HD2	1:0:745:LYS:C	2.46	0.40
1:0:787:LEU:HD21	1:0:806:MET:SD	2.62	0.40
2:1:445:ILE:HA	2:1:446:PRO:HD3	1.94	0.40
2:1:462:LEU:HD22	2:1:481:TYR:CE2	2.56	0.40
2:1:792:LEU:HB3	2:1:796:MET:HE2	2.03	0.40
3:2:141:ARG:HH21	3:2:154:GLY:HA3	1.87	0.40
4:3:50:GLY:HA2	4:3:51:PRO:HD2	1.63	0.40
5:A:375:ILE:HD13	5:A:669:TYR:HD2	1.86	0.40
5:A:1093:GLN:HE22	6:B:1093:CYS:HA	1.87	0.40
5:A:1625:THR:HG22	55:y:89:VAL:CG2	2.52	0.40
6:B:16:GLU:CG	6:B:637:LYS:HB2	2.51	0.40
6:B:539:SER:OG	6:B:540:PRO:HD3	2.22	0.40
6:B:759:VAL:O	6:B:938:ARG:NH2	2.42	0.40
8:D:104:CYS:N	8:D:105:PRO:HD3	2.36	0.40
17:M:358:MET:SD	17:M:360:LEU:HD23	2.61	0.40
22:R:86:LYS:HZ1	22:R:140:LYS:HD2	1.87	0.40
22:R:121:THR:O	22:R:124:LEU:HB3	2.22	0.40
22:R:163:LEU:CG	22:R:201:LEU:HD21	2.52	0.40
27:W:140:LEU:HD23	27:W:140:LEU:HA	1.95	0.40
27:W:648:LYS:HA	27:W:649:GLY:HA2	1.79	0.40
30:Z:123:LEU:HA	32:b:100:LYS:CG	2.47	0.40
30:Z:409:TYR:HB3	30:Z:412:PHE:CE2	2.54	0.40
32:b:257:CYS:SG	32:b:258:HIS:N	2.94	0.40
35:e:43:ILE:HG12	35:e:59:ALA:HB2	2.03	0.40
37:g:16:VAL:HG12	37:g:104:VAL:HA	2.02	0.40
37:g:74:GLN:N	37:g:78:LEU:O	2.51	0.40
37:g:87:GLN:H	37:g:87:GLN:CD	2.29	0.40
40:j:190:LEU:HD12	40:j:291:TRP:CD2	2.56	0.40
40:j:650:LEU:O	40:j:651:LEU:HB2	2.20	0.40
41:k:137:ARG:HG2	41:k:142:LYS:HG3	2.04	0.40
43:m:45:GLU:HB3	43:m:46:THR:H	1.76	0.40
44:n:60:LEU:HD13	56:z:618:CYS:CB	2.41	0.40
44:n:298:ASP:OD1	44:n:299:PHE:N	2.54	0.40
44:n:307:ASP:N	44:n:307:ASP:OD1	2.54	0.40
48:r:444:GLU:HB3	48:r:445:PRO:HD3	2.02	0.40
48:r:640:VAL:C	48:r:641:LEU:HD22	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:14:PRO:HD3	55:y:42:TYR:CZ	2.56	0.40
50:t:15:MET:HG2	55:y:20:LEU:HD21	2.03	0.40
52:v:101:THR:HG1	52:v:102:MET:H	1.69	0.40
54:x:115:LEU:CD1	54:x:119:GLN:NE2	2.75	0.40
55:y:39:GLN:HG3	55:y:89:VAL:O	2.22	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	740/841 (88%)	619 (84%)	114 (15%)	7 (1%)	14	49
2	1	1313/1368 (96%)	1201 (92%)	108 (8%)	4 (0%)	36	71
3	2	885/989 (90%)	774 (88%)	105 (12%)	6 (1%)	18	55
4	3	189/747 (25%)	167 (88%)	22 (12%)	0	100	100
5	A	1443/1970 (73%)	1316 (91%)	119 (8%)	8 (1%)	21	58
6	B	1134/1174 (97%)	1028 (91%)	103 (9%)	3 (0%)	36	71
7	C	263/275 (96%)	240 (91%)	23 (9%)	0	100	100
8	D	127/142 (89%)	114 (90%)	12 (9%)	1 (1%)	16	52
9	E	208/210 (99%)	190 (91%)	18 (9%)	0	100	100
10	F	84/127 (66%)	80 (95%)	4 (5%)	0	100	100
11	G	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
12	H	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	18	55
13	I	114/125 (91%)	95 (83%)	18 (16%)	1 (1%)	14	49
14	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
15	K	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
16	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	109/376 (29%)	91 (84%)	18 (16%)	0	100	100
18	N	97/109 (89%)	83 (86%)	14 (14%)	0	100	100
19	O	256/316 (81%)	232 (91%)	21 (8%)	3 (1%)	10	42
20	P	183/339 (54%)	178 (97%)	5 (3%)	0	100	100
21	Q	180/439 (41%)	153 (85%)	25 (14%)	2 (1%)	11	45
22	R	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
23	S	123/517 (24%)	97 (79%)	25 (20%)	1 (1%)	16	52
24	T	218/249 (88%)	182 (84%)	33 (15%)	3 (1%)	9	39
27	W	568/782 (73%)	518 (91%)	49 (9%)	1 (0%)	43	78
28	X	758/760 (100%)	666 (88%)	92 (12%)	0	100	100
29	Y	214/548 (39%)	179 (84%)	35 (16%)	0	100	100
30	Z	432/462 (94%)	391 (90%)	39 (9%)	2 (0%)	24	63
31	a	327/395 (83%)	287 (88%)	40 (12%)	0	100	100
32	b	259/308 (84%)	244 (94%)	15 (6%)	0	100	100
33	c	64/71 (90%)	60 (94%)	4 (6%)	0	100	100
34	d	271/309 (88%)	236 (87%)	33 (12%)	2 (1%)	18	55
35	e	294/346 (85%)	277 (94%)	17 (6%)	0	100	100
36	f	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
37	g	128/246 (52%)	111 (87%)	17 (13%)	0	100	100
38	h	152/268 (57%)	133 (88%)	16 (10%)	3 (2%)	6	31
39	i	108/117 (92%)	103 (95%)	5 (5%)	0	100	100
40	j	492/651 (76%)	409 (83%)	72 (15%)	11 (2%)	5	28
41	k	181/208 (87%)	159 (88%)	22 (12%)	0	100	100
42	l	178/212 (84%)	150 (84%)	27 (15%)	1 (1%)	21	58
43	m	121/200 (60%)	118 (98%)	3 (2%)	0	100	100
44	n	277/311 (89%)	225 (81%)	46 (17%)	6 (2%)	5	28
45	o	106/178 (60%)	95 (90%)	9 (8%)	2 (2%)	6	32
46	p	110/200 (55%)	106 (96%)	4 (4%)	0	100	100
47	q	116/178 (65%)	107 (92%)	9 (8%)	0	100	100
48	r	1004/1454 (69%)	819 (82%)	165 (16%)	20 (2%)	6	31
49	s	129/270 (48%)	98 (76%)	27 (21%)	4 (3%)	3	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	t	110/233 (47%)	76 (69%)	32 (29%)	2 (2%)	6	33
51	u	54/146 (37%)	49 (91%)	5 (9%)	0	100	100
52	v	129/135 (96%)	92 (71%)	35 (27%)	2 (2%)	7	37
53	w	31/244 (13%)	21 (68%)	9 (29%)	1 (3%)	3	21
54	x	107/144 (74%)	81 (76%)	26 (24%)	0	100	100
55	y	112/131 (86%)	71 (63%)	36 (32%)	5 (4%)	2	17
56	z	145/788 (18%)	126 (87%)	14 (10%)	5 (3%)	3	20
All	All	15623/21786 (72%)	13748 (88%)	1768 (11%)	107 (1%)	20	55

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	170	LEU
1	0	570	ASN
3	2	687	PHE
5	A	1617	PRO
5	A	1620	PRO
5	A	1622	TYR
24	T	122	GLU
38	h	75	VAL
40	j	318	ILE
48	r	1336	VAL
48	r	1386	PRO
52	v	9	GLU
56	z	702	GLY
1	0	143	LEU
2	1	319	GLU
3	2	87	ASP
5	A	72	GLN
6	B	489	ILE
23	S	152	HIS
34	d	57	ASN
40	j	35	SER
45	o	61	SER
48	r	437	ALA
48	r	438	LEU
48	r	553	GLU
52	v	10	GLU
55	y	65	LYS
56	z	727	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	248	VAL
1	0	266	ARG
5	A	339	LEU
5	A	1626	SER
6	B	145	GLN
13	I	58	ILE
19	O	43	ASP
40	j	195	LYS
40	j	501	GLN
40	j	630	MET
44	n	40	ARG
44	n	229	ASP
48	r	128	LEU
48	r	249	LYS
48	r	804	ASN
48	r	1272	GLN
55	y	70	PRO
56	z	700	ASN
2	1	366	ILE
5	A	73	THR
6	B	144	HIS
12	H	149	ALA
24	T	135	SER
30	Z	381	PRO
38	h	74	GLN
44	n	41	ASN
45	o	70	GLN
48	r	155	PRO
48	r	451	CYS
48	r	798	SER
50	t	25	ASN
1	0	742	LEU
3	2	172	THR
3	2	683	THR
8	D	23	PRO
19	O	12	ARG
34	d	7	PRO
40	j	335	PRO
40	j	472	GLU
44	n	42	LYS
44	n	220	ASN
44	n	221	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	r	69	LEU
48	r	376	PRO
49	s	118	GLU
49	s	144	SER
49	s	146	GLU
53	w	88	ASN
55	y	14	ASN
55	y	88	LEU
2	1	635	GLN
21	Q	78	VAL
21	Q	137	THR
24	T	121	SER
38	h	67	LYS
42	l	168	HIS
48	r	127	ILE
50	t	120	HIS
56	z	712	ASP
19	O	279	GLY
40	j	621	PRO
48	r	552	VAL
2	1	580	GLY
3	2	943	VAL
40	j	399	PRO
48	r	170	PRO
48	r	375	ASP
49	s	193	PRO
56	z	747	PRO
1	0	226	ILE
5	A	1627	PRO
40	j	648	PRO
48	r	182	PRO
55	y	31	PRO
3	2	724	VAL
27	W	477	ILE
30	Z	190	PRO
48	r	950	VAL
40	j	559	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	666/736 (90%)	644 (97%)	22 (3%)	33	55
2	1	1187/1232 (96%)	1183 (100%)	4 (0%)	86	84
3	2	780/864 (90%)	775 (99%)	5 (1%)	78	81
4	3	165/601 (28%)	155 (94%)	10 (6%)	17	39
5	A	1285/1748 (74%)	1278 (100%)	7 (0%)	81	82
6	B	999/1028 (97%)	999 (100%)	0	100	100
7	C	244/252 (97%)	244 (100%)	0	100	100
8	D	119/126 (94%)	119 (100%)	0	100	100
9	E	192/192 (100%)	192 (100%)	0	100	100
10	F	74/111 (67%)	74 (100%)	0	100	100
11	G	152/153 (99%)	152 (100%)	0	100	100
12	H	131/131 (100%)	131 (100%)	0	100	100
13	I	104/112 (93%)	104 (100%)	0	100	100
14	J	56/56 (100%)	56 (100%)	0	100	100
15	K	105/106 (99%)	105 (100%)	0	100	100
16	L	43/55 (78%)	43 (100%)	0	100	100
17	M	105/324 (32%)	105 (100%)	0	100	100
18	N	90/98 (92%)	88 (98%)	2 (2%)	45	64
19	O	222/268 (83%)	222 (100%)	0	100	100
20	P	159/293 (54%)	159 (100%)	0	100	100
21	Q	167/373 (45%)	167 (100%)	0	100	100
22	R	150/261 (58%)	149 (99%)	1 (1%)	76	79
23	S	111/448 (25%)	111 (100%)	0	100	100
24	T	196/218 (90%)	196 (100%)	0	100	100
27	W	508/688 (74%)	497 (98%)	11 (2%)	45	64
28	X	661/664 (100%)	659 (100%)	2 (0%)	86	84
29	Y	162/484 (34%)	162 (100%)	0	100	100
30	Z	372/399 (93%)	365 (98%)	7 (2%)	50	66
31	a	296/352 (84%)	296 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	b	234/272 (86%)	233 (100%)	1 (0%)	84	83
33	c	59/64 (92%)	54 (92%)	5 (8%)	10	29
34	d	210/283 (74%)	210 (100%)	0	100	100
35	e	259/299 (87%)	259 (100%)	0	100	100
36	f	256/296 (86%)	256 (100%)	0	100	100
37	g	115/223 (52%)	115 (100%)	0	100	100
38	h	139/225 (62%)	139 (100%)	0	100	100
39	i	92/98 (94%)	92 (100%)	0	100	100
40	j	452/577 (78%)	426 (94%)	26 (6%)	18	40
41	k	164/183 (90%)	161 (98%)	3 (2%)	51	67
42	l	158/178 (89%)	157 (99%)	1 (1%)	78	81
43	m	118/173 (68%)	118 (100%)	0	100	100
44	n	256/280 (91%)	254 (99%)	2 (1%)	73	78
45	o	102/152 (67%)	102 (100%)	0	100	100
46	p	102/163 (63%)	102 (100%)	0	100	100
47	q	114/155 (74%)	114 (100%)	0	100	100
48	r	905/1271 (71%)	875 (97%)	30 (3%)	33	55
49	s	119/230 (52%)	118 (99%)	1 (1%)	73	78
50	t	110/216 (51%)	109 (99%)	1 (1%)	70	77
51	u	59/133 (44%)	58 (98%)	1 (2%)	53	68
52	v	119/124 (96%)	113 (95%)	6 (5%)	22	43
53	w	34/208 (16%)	33 (97%)	1 (3%)	37	58
54	x	92/119 (77%)	82 (89%)	10 (11%)	6	21
55	y	105/115 (91%)	93 (89%)	12 (11%)	5	19
56	z	135/697 (19%)	129 (96%)	6 (4%)	25	47
All	All	14009/19107 (73%)	13832 (99%)	177 (1%)	59	72

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	13	MET
1	0	14	ASP
1	0	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	18	VAL
1	0	22	GLU
1	0	51	LEU
1	0	59	THR
1	0	60	ARG
1	0	61	MET
1	0	62	ILE
1	0	129	ASP
1	0	132	VAL
1	0	635	GLN
1	0	638	LEU
1	0	639	LEU
1	0	640	ARG
1	0	796	LYS
1	0	801	CYS
1	0	827	CYS
1	0	828	LEU
1	0	832	LEU
1	0	835	ARG
2	1	318	GLU
2	1	676	LEU
2	1	969	ILE
2	1	1193	PHE
3	2	39	ILE
3	2	131	LEU
3	2	248	ILE
3	2	268	THR
3	2	269	MET
4	3	51	PRO
4	3	82	VAL
4	3	83	GLN
4	3	84	CYS
4	3	85	HIS
4	3	122	LEU
4	3	123	GLN
4	3	124	LEU
4	3	128	PHE
4	3	222	LEU
5	A	479	TRP
5	A	521	VAL
5	A	538	VAL
5	A	1616	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1618	THR
5	A	1626	SER
5	A	1651	SER
18	N	5	LEU
18	N	93	VAL
22	R	189	ILE
27	W	165	LYS
27	W	166	VAL
27	W	297	PHE
27	W	298	ARG
27	W	371	VAL
27	W	372	GLU
27	W	374	TRP
27	W	377	GLN
27	W	378	PHE
27	W	504	LYS
27	W	685	TYR
28	X	444	ILE
28	X	678	VAL
30	Z	215	PHE
30	Z	382	VAL
30	Z	391	ILE
30	Z	392	ARG
30	Z	393	LEU
30	Z	395	GLU
30	Z	396	LEU
32	b	157	MET
33	c	2	VAL
33	c	3	ASN
33	c	4	VAL
33	c	5	LEU
33	c	6	LYS
40	j	37	SER
40	j	38	GLN
40	j	47	ILE
40	j	49	PHE
40	j	194	TRP
40	j	432	ILE
40	j	433	LYS
40	j	434	GLN
40	j	469	ASP
40	j	470	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	j	472	GLU
40	j	475	VAL
40	j	476	LYS
40	j	477	VAL
40	j	479	ILE
40	j	481	SER
40	j	485	GLU
40	j	487	ILE
40	j	491	ILE
40	j	499	VAL
40	j	507	ARG
40	j	557	LEU
40	j	614	LYS
40	j	617	HIS
40	j	618	LEU
40	j	627	TRP
41	k	32	LEU
41	k	37	HIS
41	k	193	LEU
42	l	124	VAL
44	n	44	THR
44	n	230	ILE
48	r	169	LEU
48	r	175	ASP
48	r	177	ILE
48	r	184	THR
48	r	185	LYS
48	r	187	GLU
48	r	188	LYS
48	r	221	ARG
48	r	222	VAL
48	r	226	VAL
48	r	227	GLU
48	r	229	GLU
48	r	231	GLU
48	r	233	THR
48	r	234	LEU
48	r	243	VAL
48	r	245	TRP
48	r	246	ARG
48	r	253	LEU
48	r	545	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	r	683	ARG
48	r	693	ILE
48	r	794	LEU
48	r	796	ILE
48	r	797	PHE
48	r	901	TYR
48	r	904	PHE
48	r	1191	THR
48	r	1269	ASN
48	r	1272	GLN
49	s	136	GLU
50	t	24	GLU
51	u	112	GLU
52	v	11	HIS
52	v	48	LEU
52	v	67	VAL
52	v	93	GLU
52	v	100	ASP
52	v	103	LYS
53	w	132	GLU
54	x	5	LEU
54	x	9	GLN
54	x	13	ASN
54	x	15	LEU
54	x	29	CYS
54	x	70	ASP
54	x	115	LEU
54	x	119	GLN
54	x	125	ILE
54	x	132	THR
55	y	92	GLN
55	y	97	ILE
55	y	99	GLU
55	y	100	GLN
55	y	102	ILE
55	y	103	LEU
55	y	105	TRP
55	y	110	ARG
55	y	111	LYS
55	y	112	ARG
55	y	113	MET
55	y	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	z	696	SER
56	z	698	CYS
56	z	701	ASN
56	z	711	ASP
56	z	743	TYR
56	z	746	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (316) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	43	ASN
1	0	63	HIS
1	0	69	HIS
1	0	104	GLN
1	0	392	HIS
1	0	609	ASN
1	0	635	GLN
1	0	643	HIS
1	0	683	GLN
1	0	743	GLN
1	0	751	GLN
1	0	786	HIS
1	0	821	GLN
2	1	6	GLN
2	1	303	GLN
2	1	332	GLN
2	1	433	ASN
2	1	460	GLN
2	1	526	ASN
2	1	541	HIS
2	1	602	HIS
2	1	622	GLN
2	1	759	ASN
2	1	805	GLN
2	1	1106	HIS
2	1	1134	GLN
2	1	1250	HIS
2	1	1280	ASN
2	1	1300	HIS
3	2	26	ASN
3	2	174	ASN
3	2	217	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2	261	GLN
3	2	266	GLN
3	2	370	GLN
3	2	530	GLN
3	2	541	ASN
3	2	645	GLN
3	2	799	HIS
3	2	898	ASN
3	2	922	GLN
3	2	925	GLN
3	2	945	GLN
4	3	38	HIS
4	3	85	HIS
4	3	123	GLN
4	3	139	HIS
4	3	179	HIS
5	A	122	ASN
5	A	204	HIS
5	A	273	GLN
5	A	288	ASN
5	A	296	ASN
5	A	311	GLN
5	A	330	GLN
5	A	353	ASN
5	A	372	ASN
5	A	387	ASN
5	A	461	GLN
5	A	502	ASN
5	A	516	GLN
5	A	539	GLN
5	A	590	GLN
5	A	606	HIS
5	A	620	HIS
5	A	632	ASN
5	A	654	HIS
5	A	685	HIS
5	A	740	GLN
5	A	746	ASN
5	A	757	GLN
5	A	790	GLN
5	A	792	ASN
5	A	982	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	1082	HIS
5	A	1093	GLN
5	A	1146	GLN
5	A	1220	HIS
5	A	1397	HIS
5	A	1410	HIS
5	A	1417	HIS
5	A	1422	GLN
5	A	1462	GLN
6	B	90	GLN
6	B	111	ASN
6	B	117	ASN
6	B	139	GLN
6	B	197	GLN
6	B	245	GLN
6	B	314	GLN
6	B	344	GLN
6	B	370	HIS
6	B	430	ASN
6	B	500	GLN
6	B	503	ASN
6	B	650	ASN
6	B	683	GLN
6	B	755	GLN
6	B	790	GLN
6	B	797	ASN
6	B	825	GLN
6	B	876	ASN
6	B	913	GLN
6	B	930	GLN
6	B	941	GLN
6	B	992	ASN
6	B	1013	ASN
6	B	1053	HIS
6	B	1060	HIS
6	B	1117	HIS
6	B	1142	ASN
7	C	32	ASN
7	C	60	HIS
7	C	217	GLN
8	D	43	HIS
8	D	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	D	135	GLN
9	E	148	HIS
10	F	46	GLN
11	G	14	HIS
11	G	24	ASN
11	G	93	ASN
12	H	29	HIS
13	I	21	ASN
13	I	41	ASN
13	I	46	GLN
13	I	60	HIS
13	I	98	GLN
13	I	100	HIS
16	L	23	HIS
17	M	48	ASN
18	N	8	ASN
18	N	39	GLN
19	O	129	ASN
20	P	164	GLN
20	P	167	ASN
20	P	189	ASN
20	P	257	ASN
20	P	279	GLN
21	Q	64	ASN
21	Q	109	HIS
21	Q	142	ASN
21	Q	183	GLN
22	R	83	ASN
22	R	90	GLN
22	R	157	GLN
23	S	103	ASN
23	S	145	ASN
23	S	152	HIS
23	S	172	ASN
23	S	173	HIS
24	T	143	GLN
24	T	158	ASN
24	T	198	ASN
24	T	229	HIS
27	W	112	HIS
27	W	187	HIS
27	W	377	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	W	459	GLN
27	W	591	GLN
27	W	595	ASN
27	W	598	HIS
27	W	603	ASN
27	W	683	GLN
27	W	714	GLN
28	X	37	HIS
28	X	118	HIS
28	X	201	HIS
28	X	210	HIS
28	X	237	HIS
28	X	238	ASN
28	X	260	GLN
28	X	328	HIS
28	X	348	HIS
28	X	402	ASN
28	X	452	GLN
28	X	613	HIS
28	X	726	GLN
28	X	733	GLN
29	Y	384	HIS
29	Y	442	GLN
29	Y	501	GLN
29	Y	520	ASN
29	Y	524	HIS
30	Z	18	ASN
30	Z	97	HIS
30	Z	181	GLN
30	Z	390	GLN
30	Z	424	HIS
31	a	220	HIS
31	a	256	GLN
31	a	317	HIS
31	a	356	HIS
32	b	18	ASN
32	b	108	ASN
32	b	204	GLN
32	b	248	HIS
33	c	3	ASN
33	c	42	HIS
33	c	64	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	d	117	ASN
34	d	274	HIS
35	e	129	HIS
35	e	130	GLN
35	e	288	GLN
35	e	306	GLN
36	f	3	HIS
36	f	18	GLN
36	f	142	GLN
36	f	247	GLN
37	g	53	GLN
37	g	59	HIS
37	g	62	GLN
37	g	116	ASN
37	g	127	GLN
38	h	35	ASN
38	h	139	GLN
39	i	48	GLN
39	i	58	HIS
39	i	79	HIS
40	j	38	GLN
40	j	142	GLN
40	j	329	ASN
40	j	374	ASN
40	j	383	HIS
40	j	394	HIS
40	j	419	ASN
40	j	422	GLN
40	j	461	GLN
40	j	463	HIS
40	j	492	GLN
40	j	517	GLN
40	j	528	GLN
40	j	532	HIS
40	j	538	GLN
40	j	547	GLN
40	j	565	ASN
40	j	584	ASN
40	j	617	HIS
41	k	30	HIS
41	k	37	HIS
41	k	84	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	k	127	HIS
41	k	134	HIS
42	l	19	GLN
42	l	47	HIS
42	l	90	ASN
43	m	58	ASN
43	m	89	ASN
43	m	104	GLN
44	n	59	ASN
44	n	68	ASN
44	n	109	GLN
44	n	115	ASN
44	n	220	ASN
44	n	237	GLN
44	n	245	HIS
44	n	252	HIS
45	o	70	GLN
45	o	101	GLN
45	o	105	GLN
46	p	81	ASN
46	p	84	GLN
46	p	92	GLN
47	q	29	ASN
47	q	53	GLN
47	q	154	GLN
47	q	171	ASN
47	q	178	ASN
48	r	211	GLN
48	r	304	GLN
48	r	459	HIS
48	r	521	GLN
48	r	528	HIS
48	r	532	ASN
48	r	536	ASN
48	r	607	GLN
48	r	669	GLN
48	r	698	GLN
48	r	717	ASN
48	r	744	HIS
48	r	870	GLN
48	r	898	ASN
48	r	913	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	r	946	ASN
48	r	1426	ASN
49	s	64	GLN
49	s	109	GLN
50	t	74	HIS
50	t	120	HIS
50	t	142	GLN
50	t	154	GLN
51	u	70	HIS
51	u	129	ASN
52	v	11	HIS
52	v	21	GLN
52	v	42	ASN
52	v	56	GLN
52	v	76	ASN
54	x	18	GLN
54	x	27	GLN
54	x	86	GLN
54	x	119	GLN
54	x	127	GLN
54	x	129	GLN
55	y	35	ASN
55	y	127	ASN
56	z	628	ASN
56	z	635	ASN
56	z	636	HIS
56	z	679	GLN
56	z	697	HIS
56	z	701	ASN
56	z	705	HIS
56	z	732	GLN
56	z	753	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	X	1000	28	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
59	SF4	X	1000	28	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

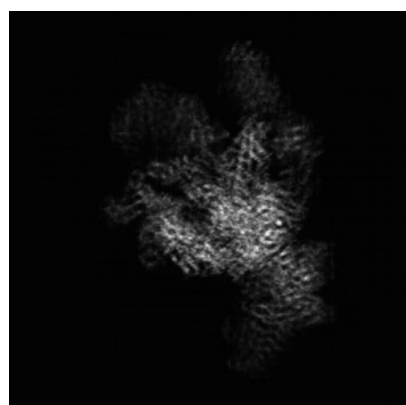
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23255. These allow visual inspection of the internal detail of the map and identification of artifacts.

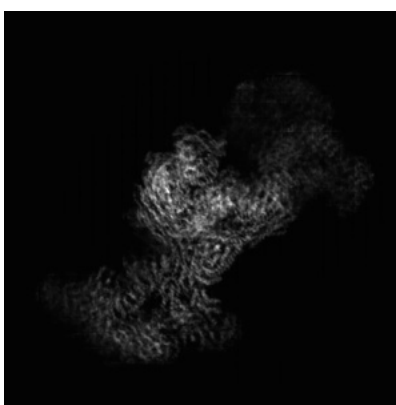
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

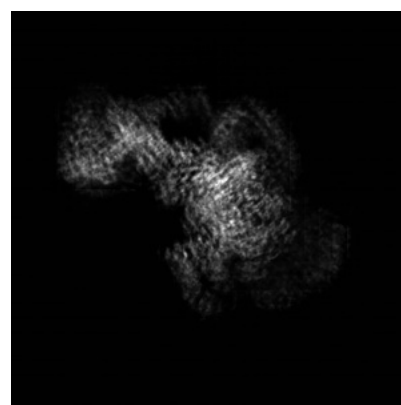
6.1.1 Primary map



X



Y

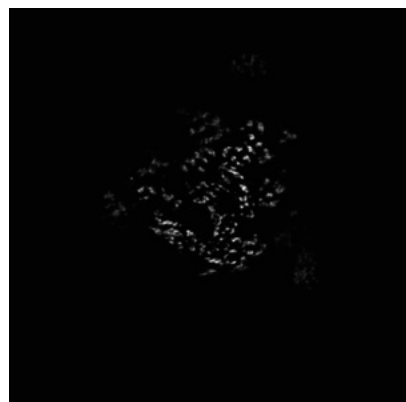


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210



Z Index: 210

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: 221



Y Index: 254

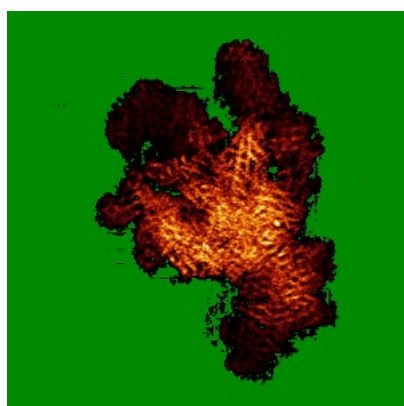


Z Index: 182

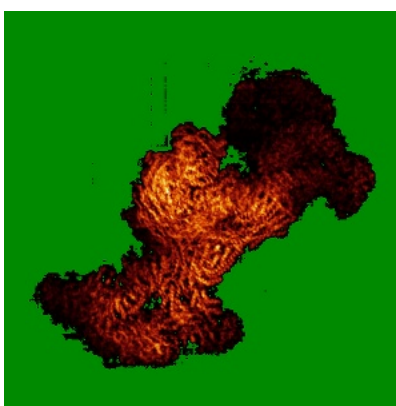
The images above show the largest variance slices of the map in three orthogonal directions.

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

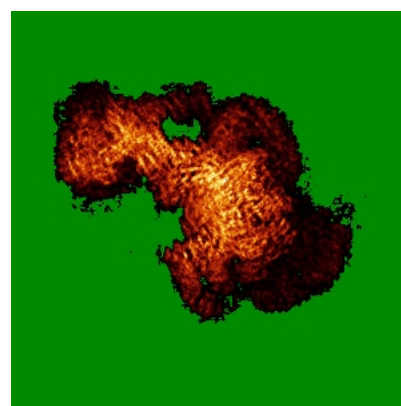
6.4.1 Primary map



X



Y

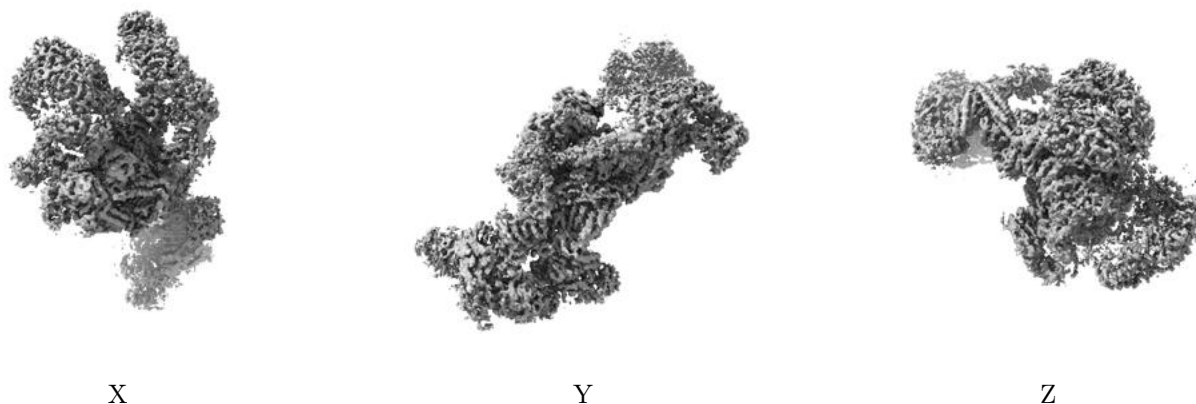


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

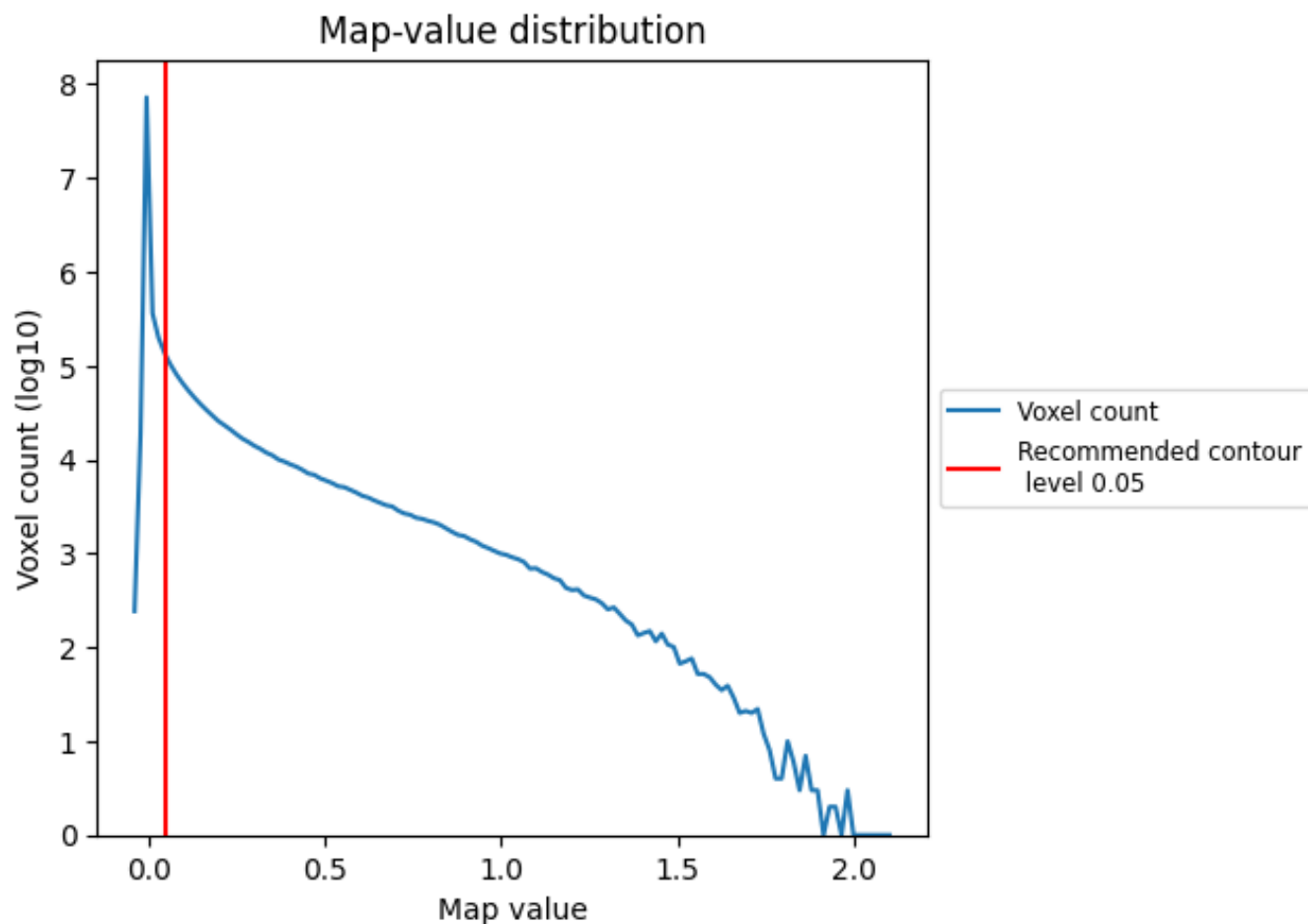
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

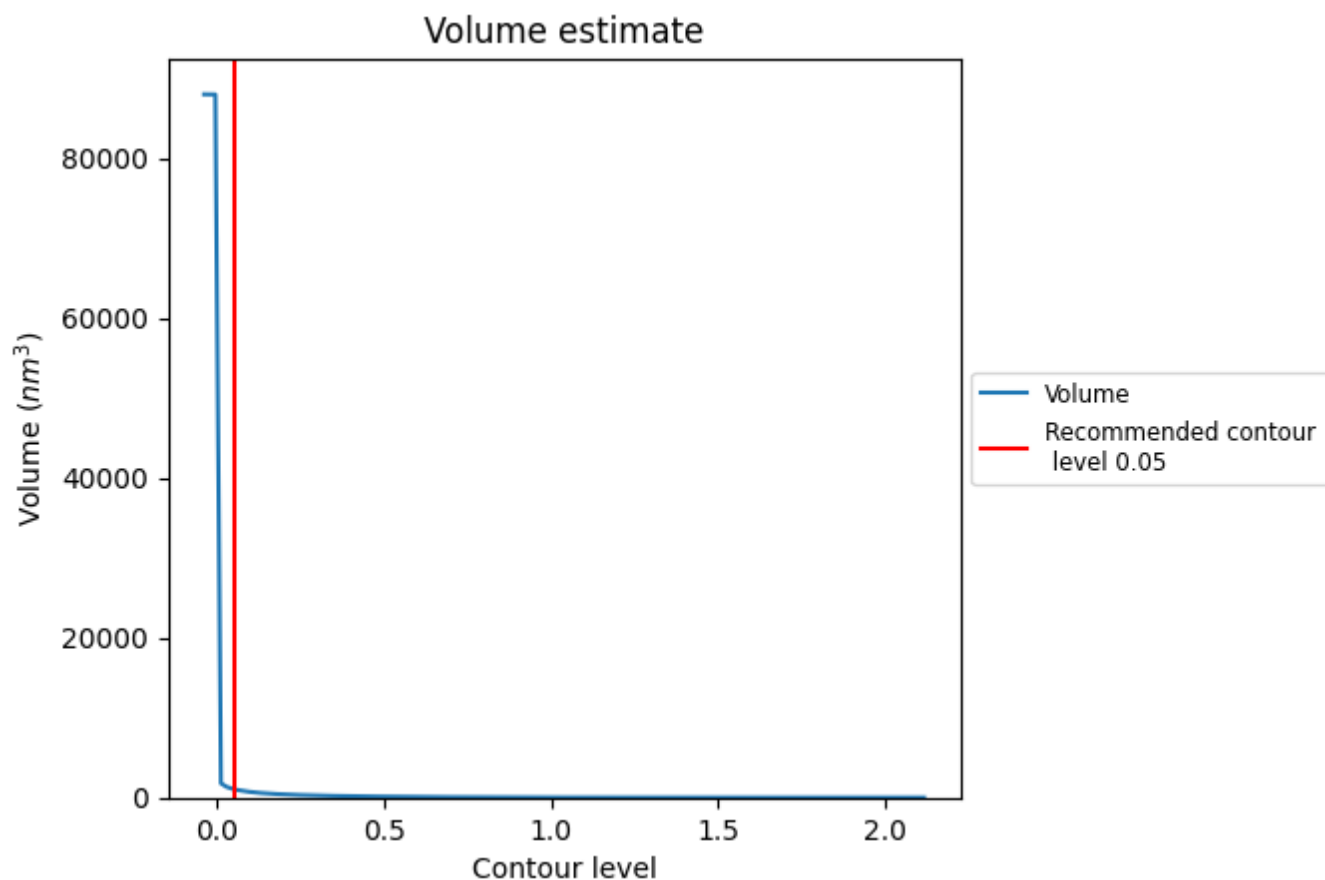
This section contains the results of statistical analysis of the map.

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.

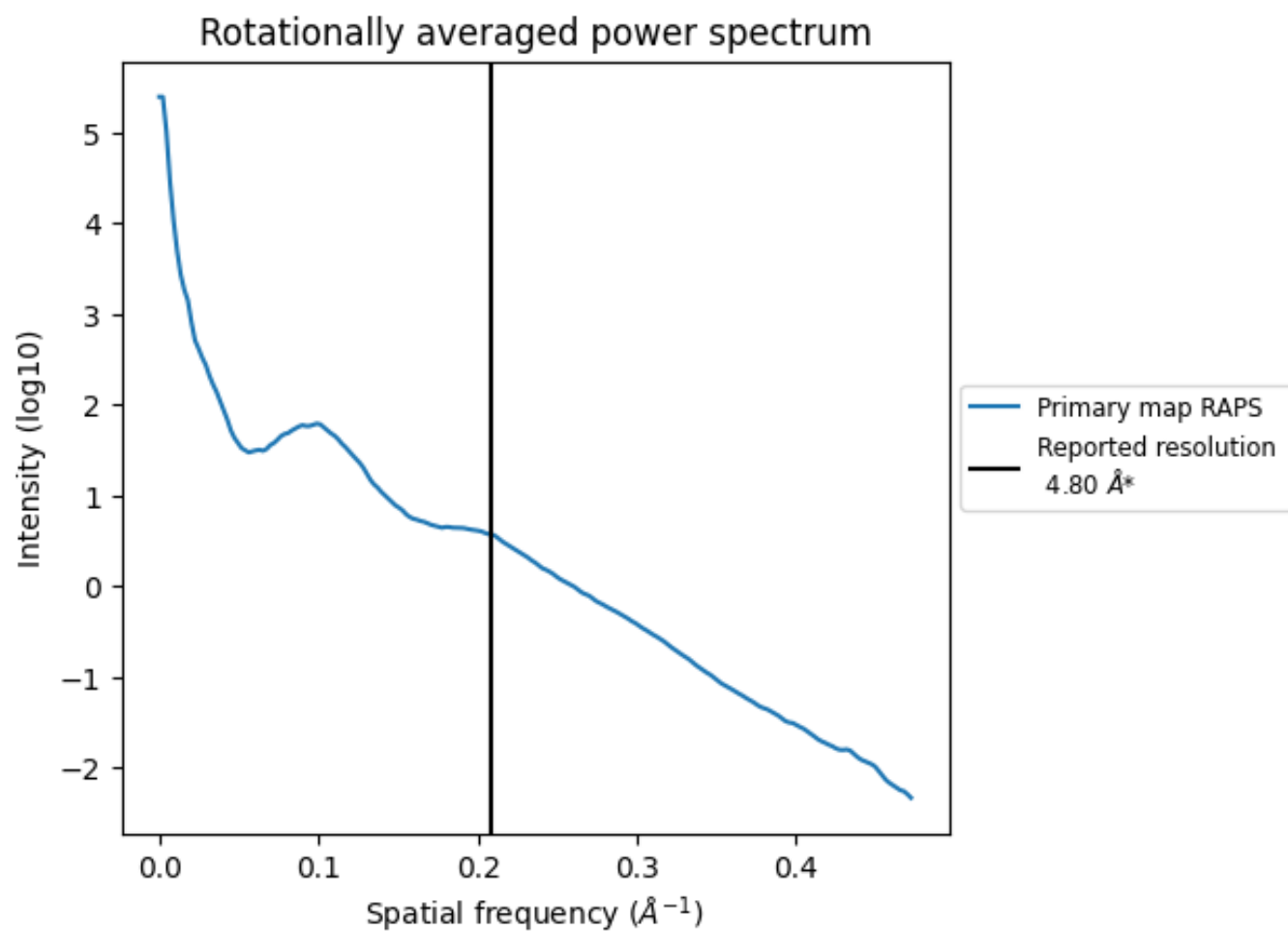
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1055 nm³; this corresponds to an approximate mass of 953 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 0.208 Å⁻¹

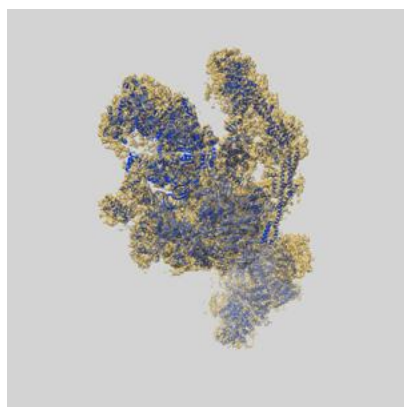
8 Fourier-Shell correlation

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

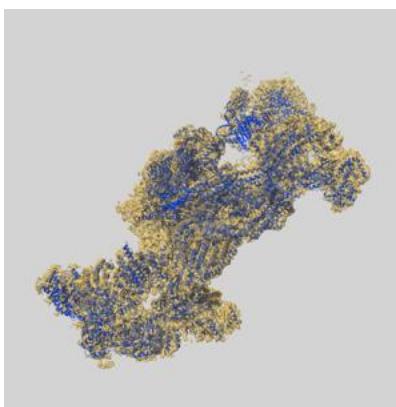
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23255 and PDB model 7LBM. Per-residue inclusion information can be found in section [3](#) on page [16](#).

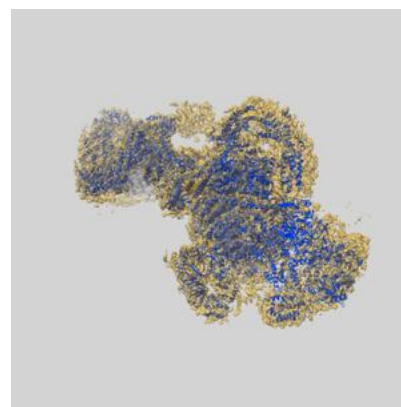
9.1 Map-model overlay [i](#)



X



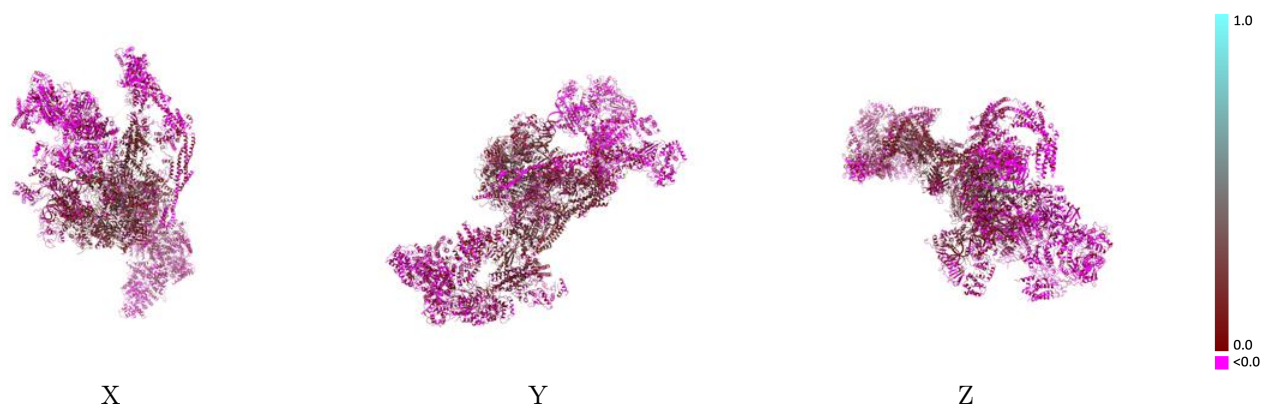
Y



Z

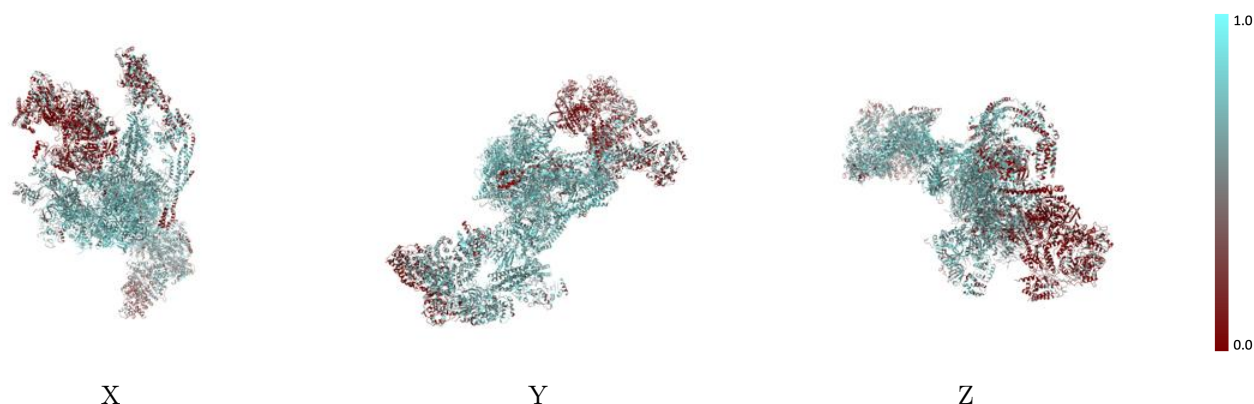
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



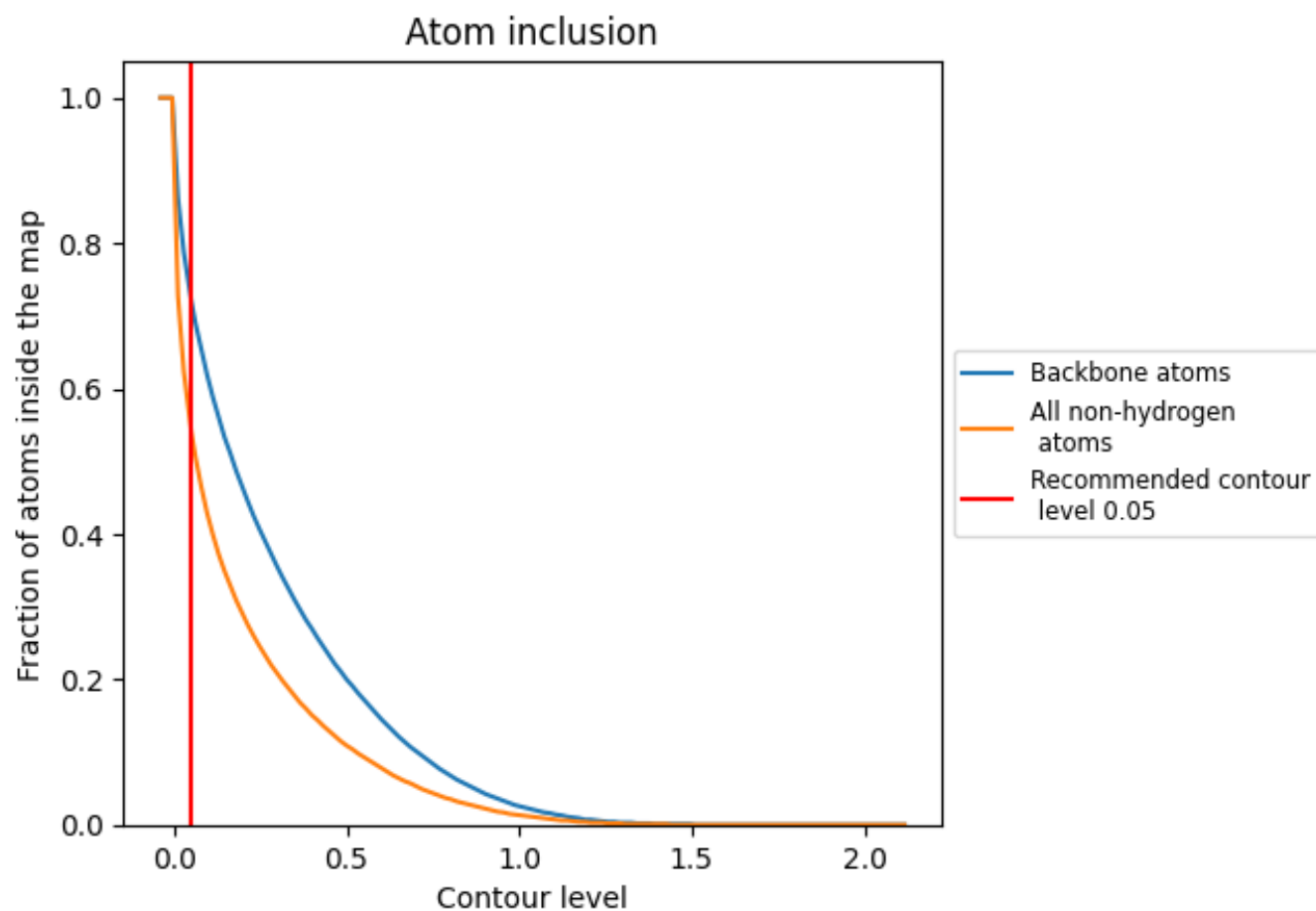
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 54% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5400	 0.0740
0	 0.6280	 0.0650
1	 0.4060	 -0.0060
2	 0.5140	 0.0300
3	 0.5240	 0.0330
A	 0.7150	 0.1930
B	 0.7240	 0.2010
C	 0.6720	 0.1450
D	 0.6640	 0.1400
E	 0.7060	 0.1630
F	 0.7070	 0.2010
G	 0.7280	 0.1730
H	 0.6740	 0.1380
I	 0.7120	 0.1510
J	 0.6810	 0.1180
K	 0.6870	 0.1510
L	 0.7020	 0.1860
M	 0.4900	 -0.0110
N	 0.4860	 0.0020
O	 0.6640	 0.1200
P	 0.6060	 0.0650
Q	 0.6220	 0.0780
R	 0.6070	 0.0470
S	 0.5410	 0.0520
T	 0.5720	 0.0580
U	 0.5970	 0.0640
V	 0.5890	 0.0520
W	 0.0960	 -0.0490
X	 0.3510	 -0.0060
Y	 0.2250	 -0.0660
Z	 0.1720	 -0.0670
a	 0.1290	 -0.0590
b	 0.2200	 -0.0550
c	 0.1850	 -0.0860
d	 0.3580	 -0.0120



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.3920	 -0.0170
f	 0.3390	 -0.0590
g	 0.6910	 0.0790
h	 0.7060	 0.1450
i	 0.7250	 0.1740
j	 0.7350	 0.1960
k	 0.6540	 0.1170
l	 0.6410	 0.1080
m	 0.7310	 0.2080
n	 0.7070	 0.1790
o	 0.6650	 0.1300
p	 0.6440	 0.1040
q	 0.6880	 0.1560
r	 0.6350	 0.1010
s	 0.4180	 0.0040
t	 0.5380	 0.0180
u	 0.3480	 -0.0210
v	 0.4240	 -0.0400
w	 0.3930	 -0.0220
x	 0.5280	 0.0110
y	 0.6030	 0.0470
z	 0.7130	 0.1360