Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 19, 2016 – 02:07 PM EST

PDB ID	:	5GM6
EMDB ID:	:	EMD-9524
Title	:	Cryo-EM structure of the activated spliceosome (Bact complex) at 3.5 angstrom resolution
Authors	:	Yan, C.; Wan, R.; Bai, R.; Huang, G.; Shi, Y.
Deposited on	:	2016-07-12
Resolution	:	3.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

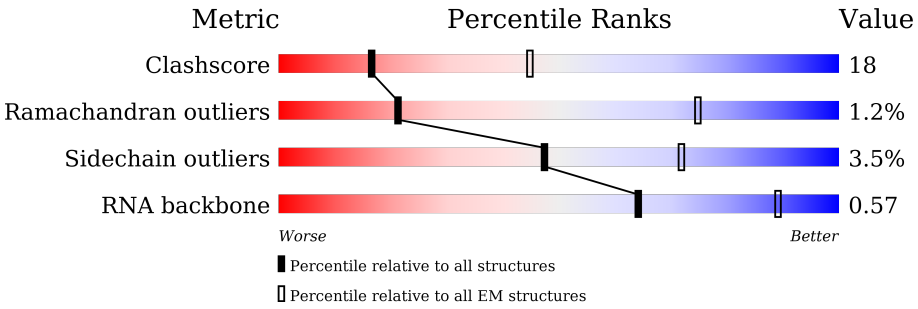
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.50 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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2287	63% 29% • •
2	B	2163	57% 26% 16%
3	C	1008	55% 30% • 13%
4	D	214	36% 14% 5% 45%
5	E	112	54% 32% 6% 8%
6	F	1361	50% 35% • 13%
7	H	436	20% 12% • 65%
8	I	266	27% 9% • 62%

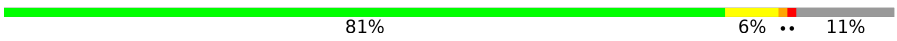
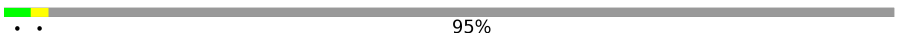
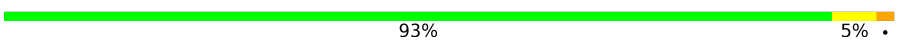
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	107	57% 36%
10	K	85	61% 29% 8%
11	L	1175	94%
12	N	25	28% 48% 24%
13	M	61	28% 28% 26% 18%
14	O	451	48% 24% 25%
15	P	379	43% 18% 35%
16	Q	364	23% 24% 49%
17	R	339	42% 32% 23%
18	S	175	31% 7% 59%
19	T	157	76% 22%
20	U	207	51% 31% 15%
21	V	148	49% 36% 14%
22	W	266	18% 15% 5% 61%
23	Y	876	50% 18% 32%
24	Z	577	58% 15% 23%
25	a	259	46% 53%
26	b	301	49% 50%
27	c	587	68% 29%
28	G	971	58% 30% 10%
29	d	687	79% 21%
30	X	135	10% 10% 80%
31	v	859	64% 34%
32	e	213	62% 8% 30%
33	f	215	47% 53%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	o	503	
34	p	503	
34	q	503	
34	r	503	
35	t	175	
36	n	455	
37	k	196	
38	i	94	
39	h	86	
40	j	77	
41	l	101	
42	m	146	
43	g	94	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 112064 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2200	Total	C	N	O	S	0	0
			18101	11636	3086	3315	64		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	expression tag	UNP P33334

- Molecule 2 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1809	Total	C	N	O	S	0	0
			14504	9283	2414	2750	57		

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	878	Total	C	N	O	S	0	0
			7014	4526	1166	1293	29		

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	117	Total	C	N	O	P	0	0
			2465	1104	414	830	117		

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 6 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	1180	Total	C	N	O	S	0	0
			9380	5996	1580	1753	51		

- Molecule 7 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	151	Total	C	N	O	S	0	0
			1248	804	217	221	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	102	Total	C	N	O	S	0	0
			800	495	150	150	5		

- Molecule 9 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 10 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			693	429	130	132	2		

- Molecule 11 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	66	Total	C	N	O	P	0	0
			1388	622	228	472	66		

- Molecule 12 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	25	Total	C	N	O	P	0	0
			521	234	77	185	25		

- Molecule 13 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	50	Total	C	N	O	P	0	0
			1057	479	191	338	49		

- Molecule 14 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	337	Total	C	N	O	S	0	0
			2646	1669	466	501	10		

- Molecule 15 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	246	Total	C	N	O	S	0	0
			1978	1233	359	380	6		

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	185	Total	C	N	O	S	0	0
			1472	930	256	271	15		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	71	Total	C	N	O	S	0	0
			578	361	117	99	1		

- Molecule 19 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 20 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	176	Total	C	N	O	S	0	0
			1401	877	237	277	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	205	HIS	-	expression tag	UNP Q07930
U	206	HIS	-	expression tag	UNP Q07930
U	207	HIS	-	expression tag	UNP Q07930

- Molecule 21 is a protein called U2 snRNP component IST3.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	128	Total	C	N	O	0	0
			1051	662	181	208		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	104	Total	C	N	O	S	0	0
			842	528	145	167	2		

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	598	Total	C	N	O	S	0	0
			4047	2590	690	752	15		

- Molecule 24 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	447	Total	C	N	O	S	0	0
			3651	2343	602	688	18		

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	123	Total	C	N	O	S	0	0
			988	621	171	183	13		

- Molecule 26 is a protein called Peptidyl-prolyl isomerase CWC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	150	Total	C	N	O	S	0	0
			1224	789	206	223	6		

- Molecule 27 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	415	Total	C	N	O	S	0	0
			2803	1741	518	537	7		

- Molecule 28 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	875	Total	C	N	O	S	0	0
			6970	4467	1196	1265	42		

- Molecule 29 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	545	Total	C	N	O	S	0	0
			3558	2212	671	667	8		

- Molecule 30 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 31 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	566	Total	C	N	O	S	0	0
			3047	1871	576	599	1		

- Molecule 32 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	149	Total	C	N	O	S	0	0
			947	617	154	174	2		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	124	Total	C	N	O	S	0	0
			819	518	132	167	2		
34	p	128	Total	C	N	O	S	0	0
			843	533	136	172	2		
34	q	381	Total	C	N	O	S	0	0
			2315	1456	396	455	8		
34	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	155	Total	C	N	O	S	0	0
			921	582	159	179	1		

- Molecule 36 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	n	23	Total	C	N	O	0	0
			195	122	41	32		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

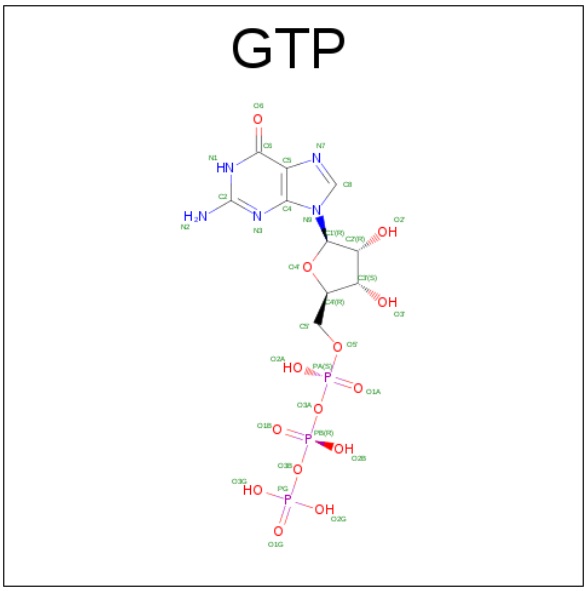
- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
44	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

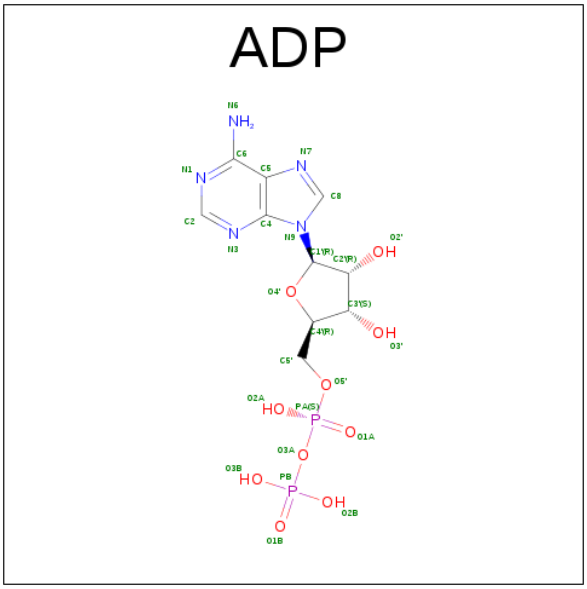
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	Y	1	Total	Mg	0
			1	1	
45	E	4	Total	Mg	0
			4	4	

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	J	3	Total	Zn	0
			3	3	
46	Q	2	Total	Zn	0
			2	2	
46	I	1	Total	Zn	0
			1	1	
46	a	3	Total	Zn	0
			3	3	
46	T	3	Total	Zn	0
			3	3	
46	R	1	Total	Zn	0
			1	1	

- Molecule 47 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



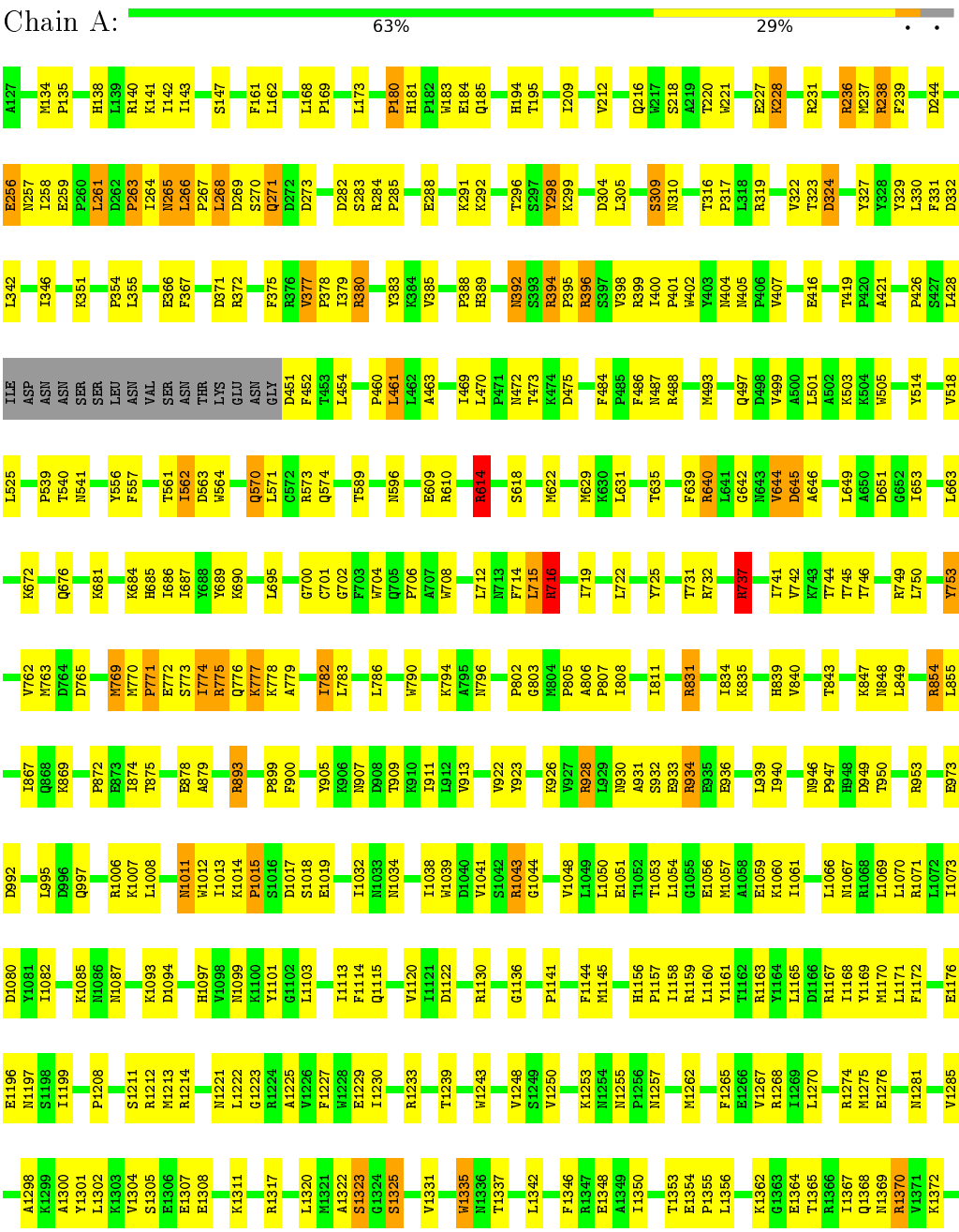
Mol	Chain	Residues	Atoms					AltConf
47	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

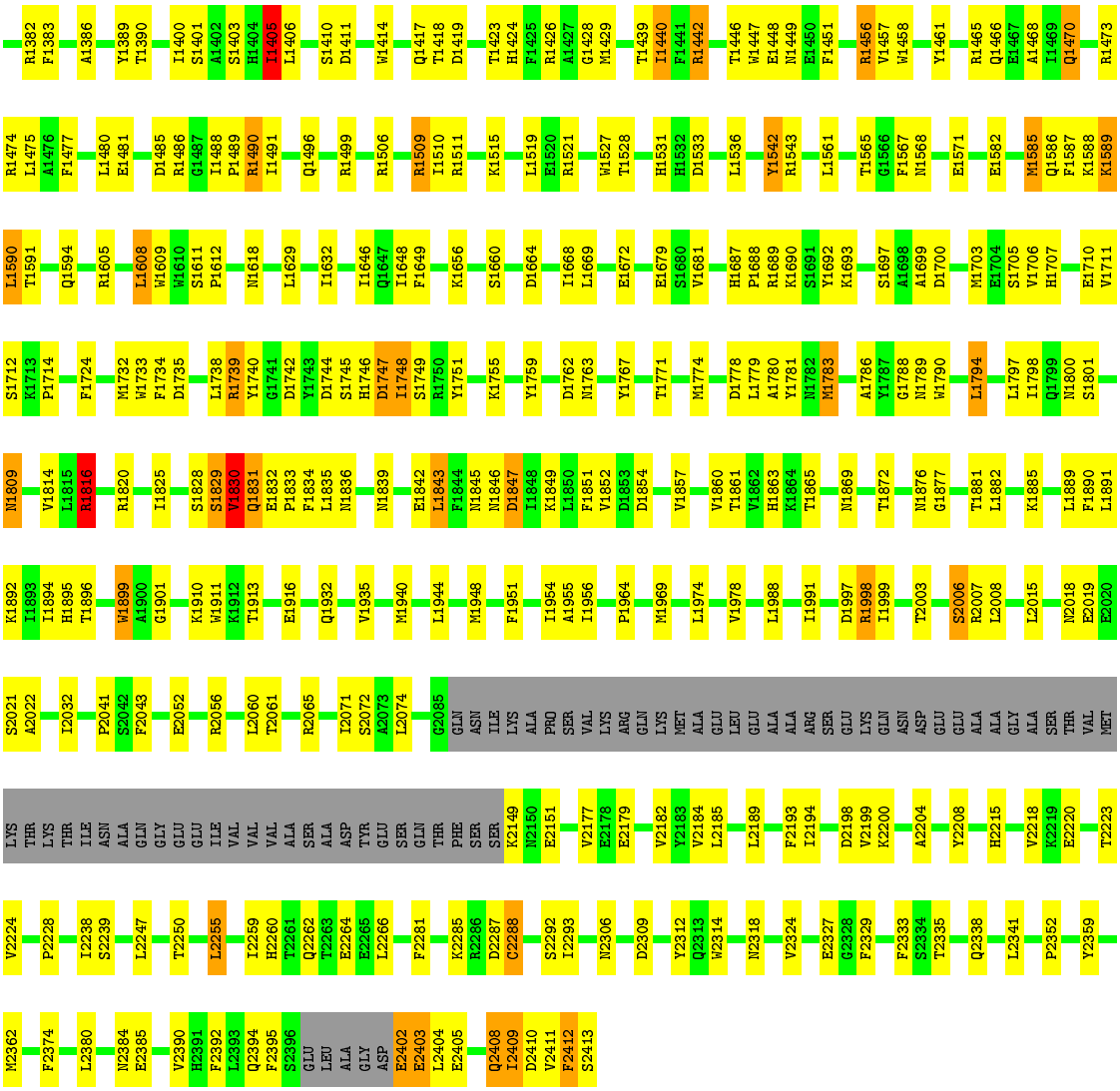
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Pre-mRNA-splicing factor 8

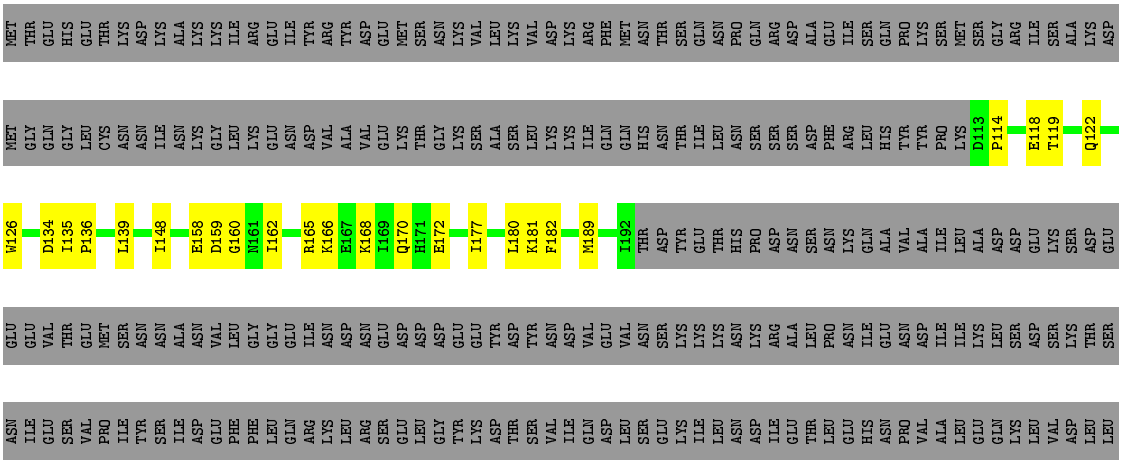
Chain A:

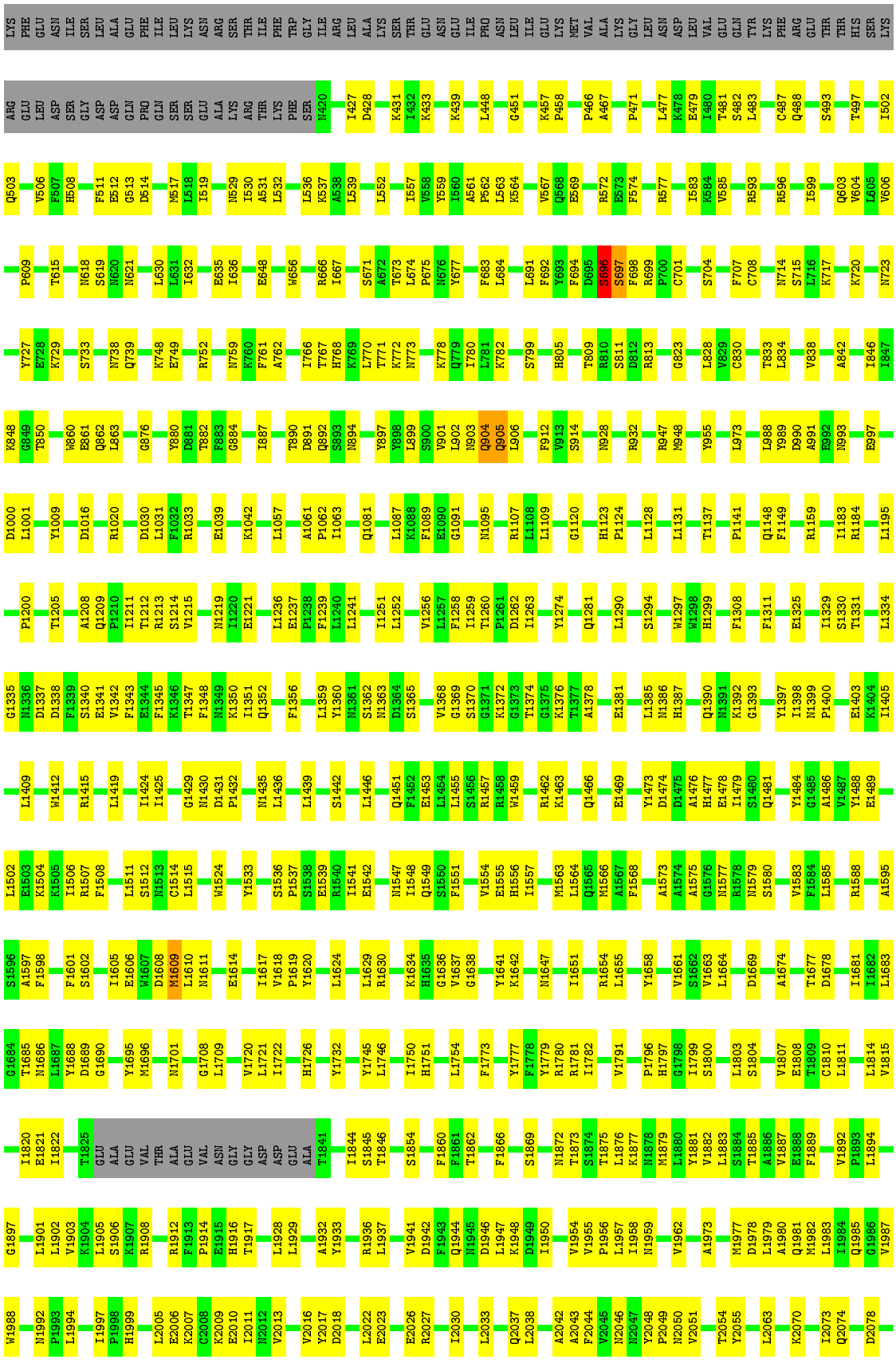




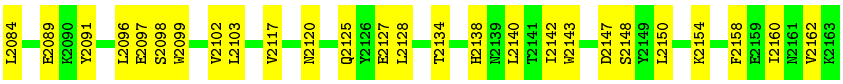
• Molecule 2: Pre-mRNA-splicing helicase BRR2

Chain B:



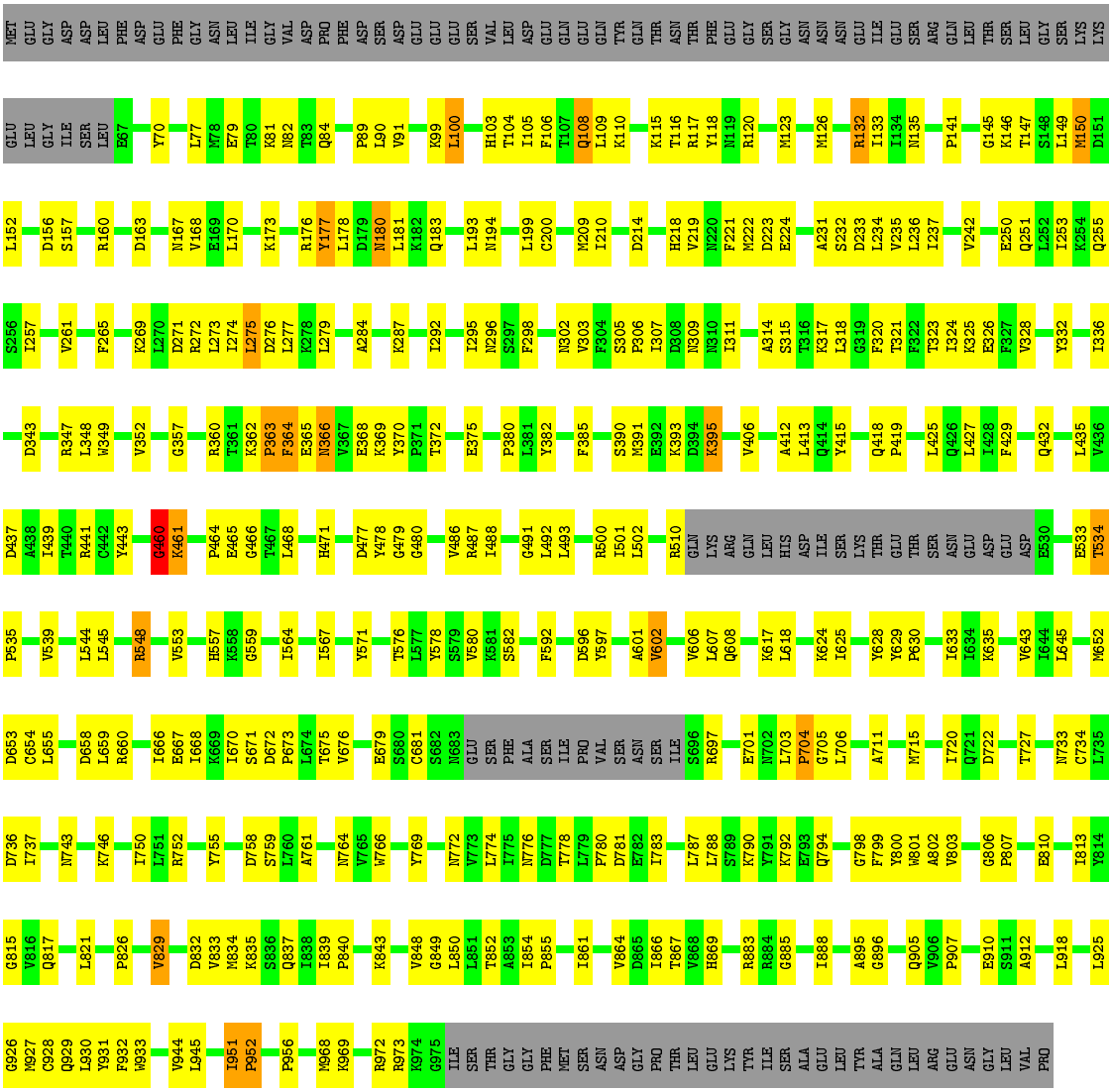


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



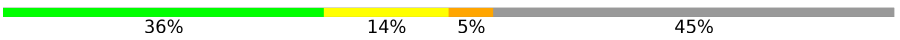
• Molecule 3: Pre-mRNA-splicing factor SNU114

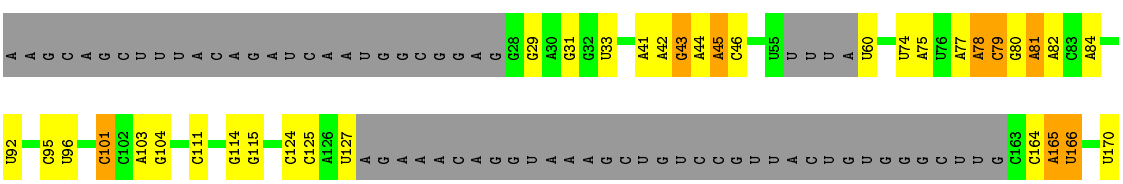
Chain C:



• Molecule 4: Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence

Chain D:

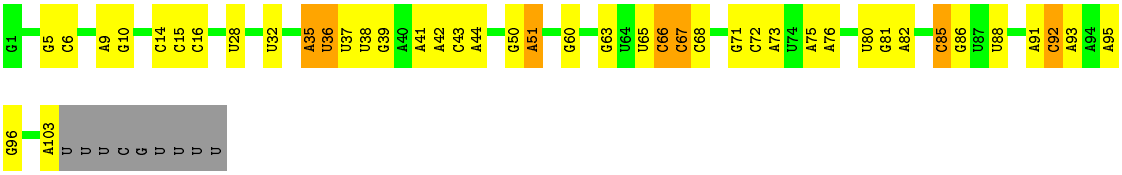




WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

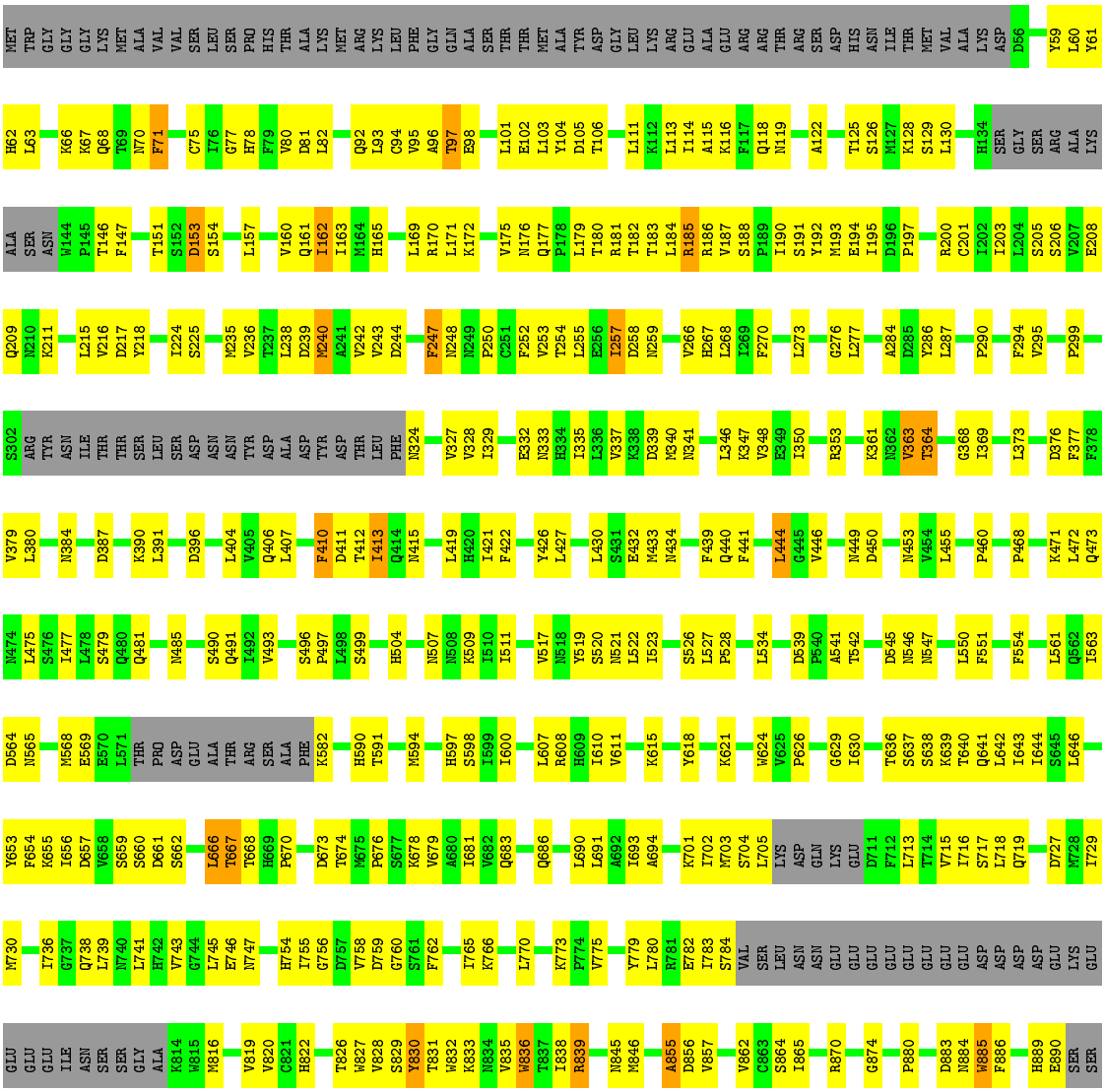
• Molecule 5: Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence

Chain E:

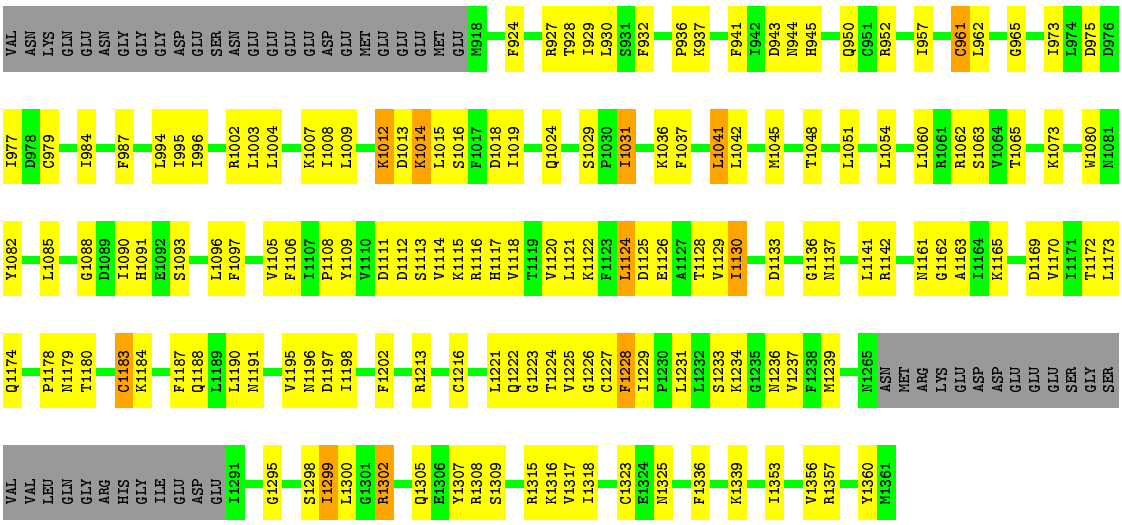


• Molecule 6: Pre-mRNA-splicing factor RSE1

Chain F:

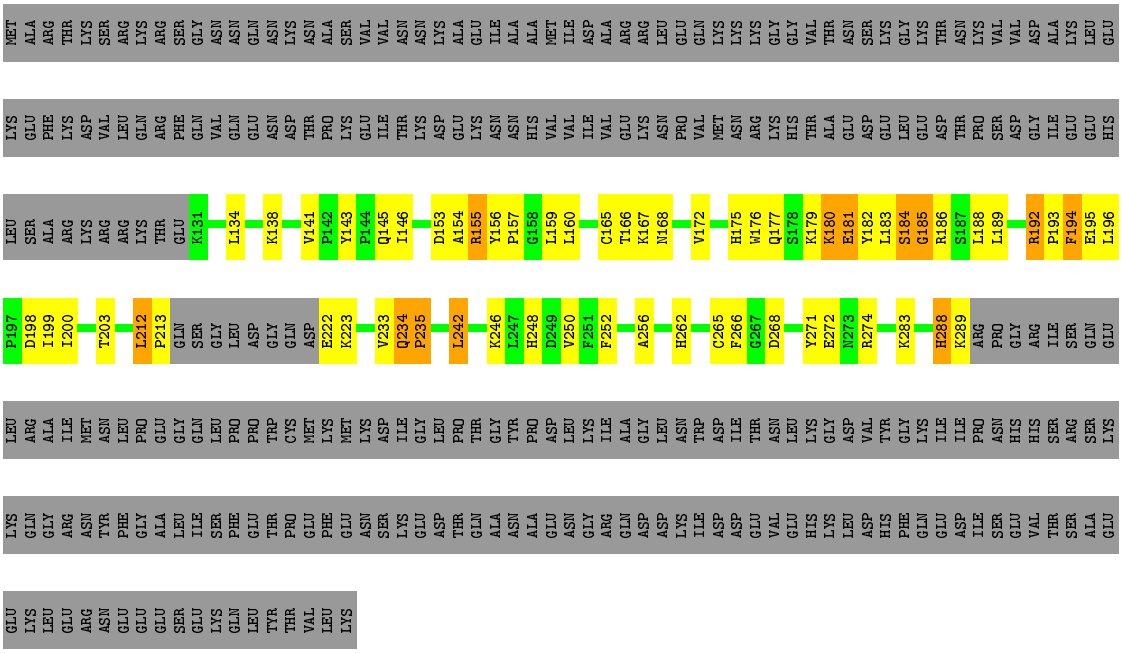


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



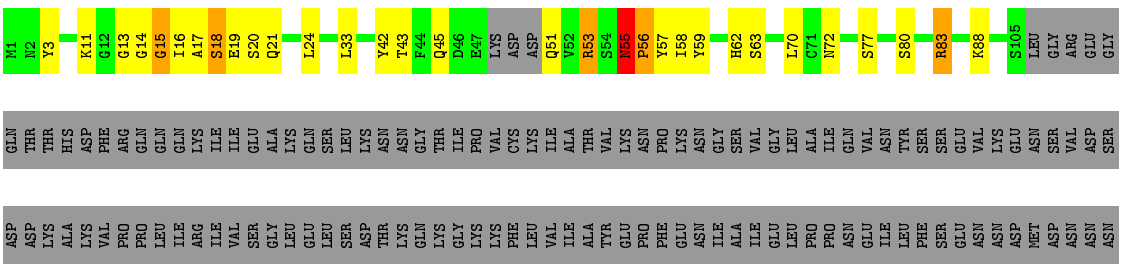
• Molecule 7: Cold sensitive U2 snRNA suppressor 1

Chain H:



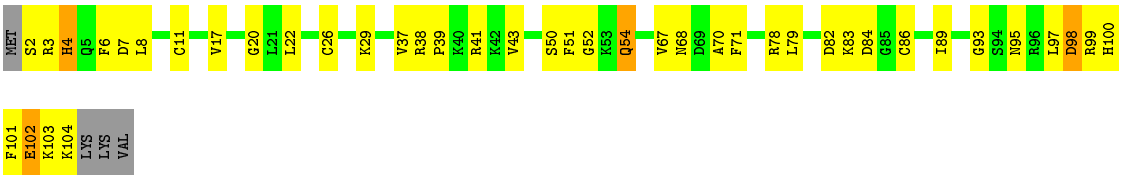
• Molecule 8: Pre-mRNA-splicing factor PRP11

Chain I:



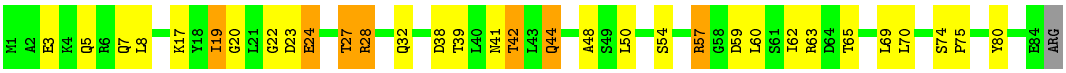
- Molecule 9: Pre-mRNA-splicing factor RDS3

Chain J:



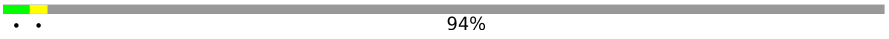
- Molecule 10: RDS3 complex subunit 10

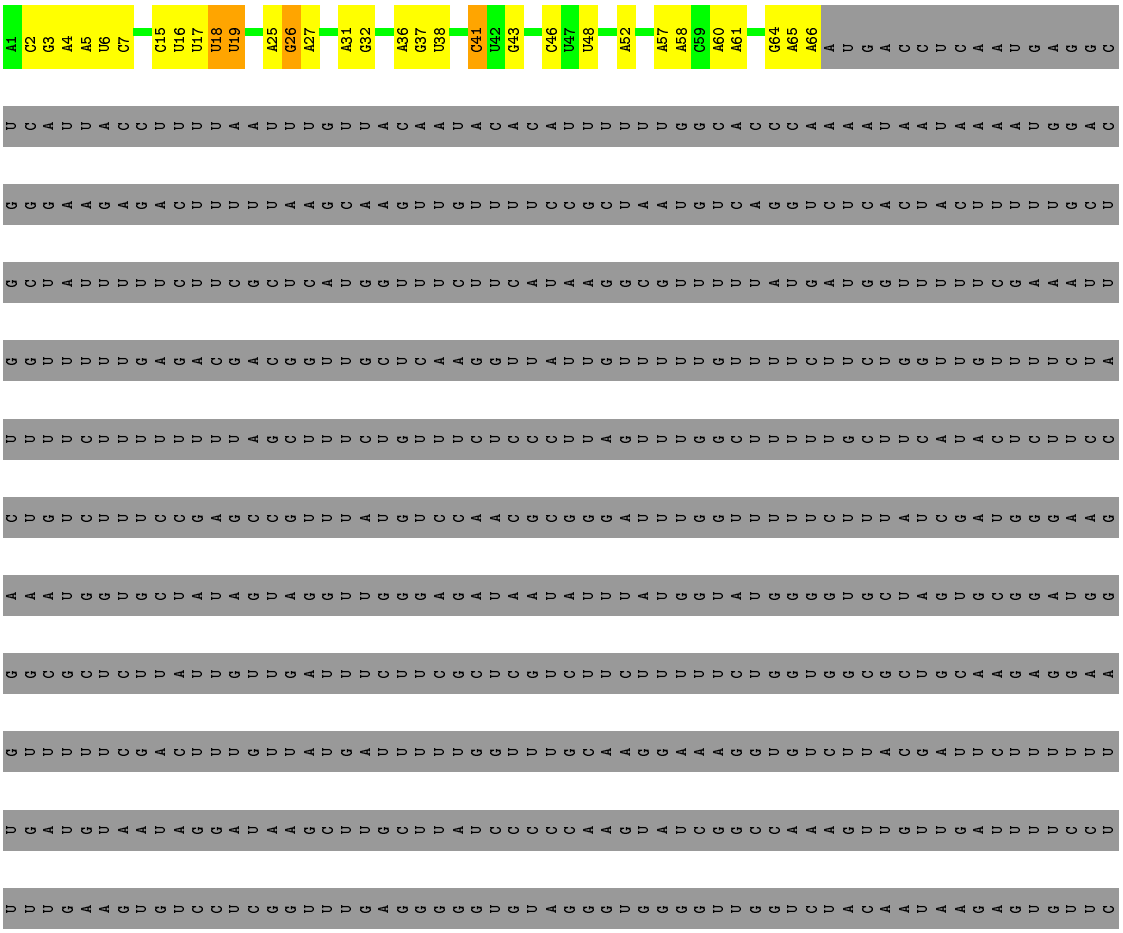
Chain K:

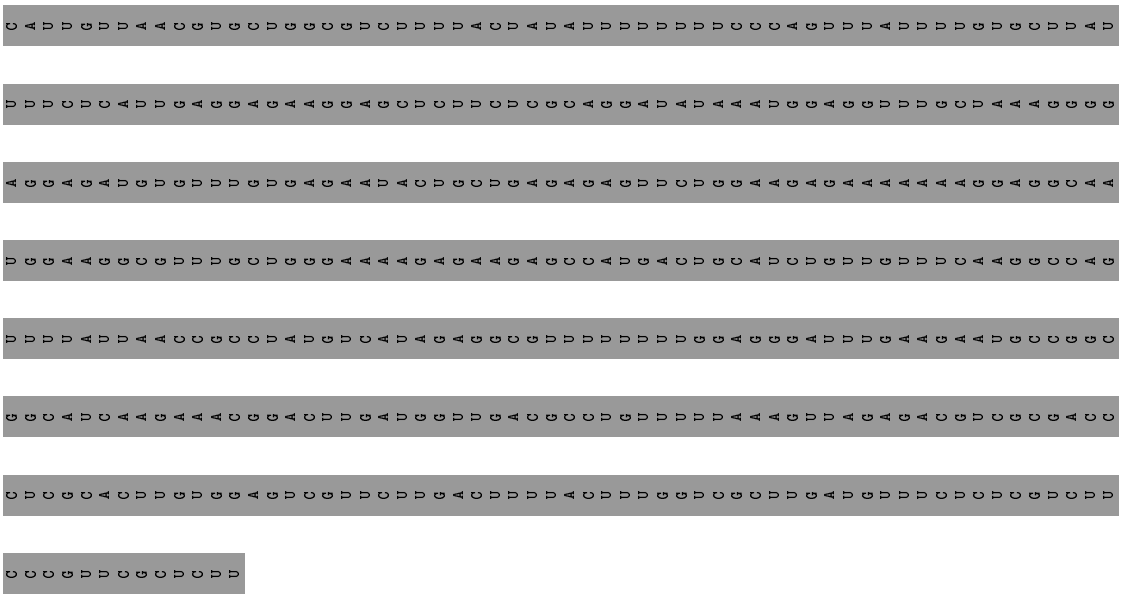


- Molecule 11: U2 snRNA

Chain L:





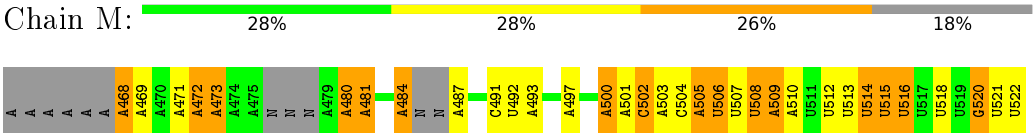


- Molecule 12: Pre-mRNA

Chain N:

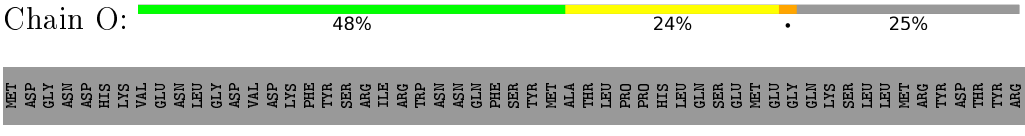
- Molecule 13: Pre-mRNA

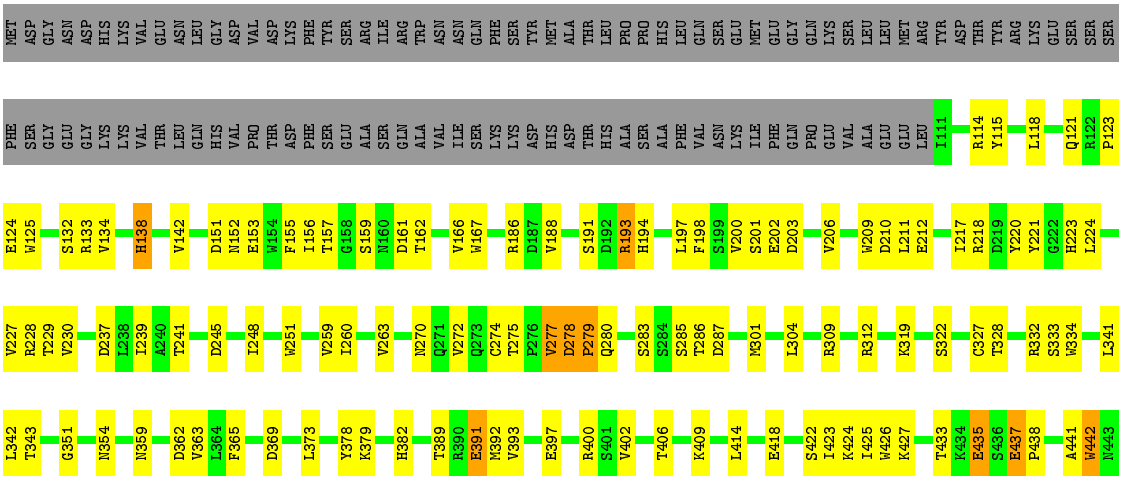
Chain M:

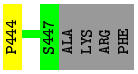


- Molecule 14: Pre-mRNA-splicing factor PRP46

Chain O:

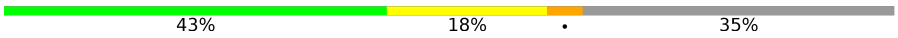


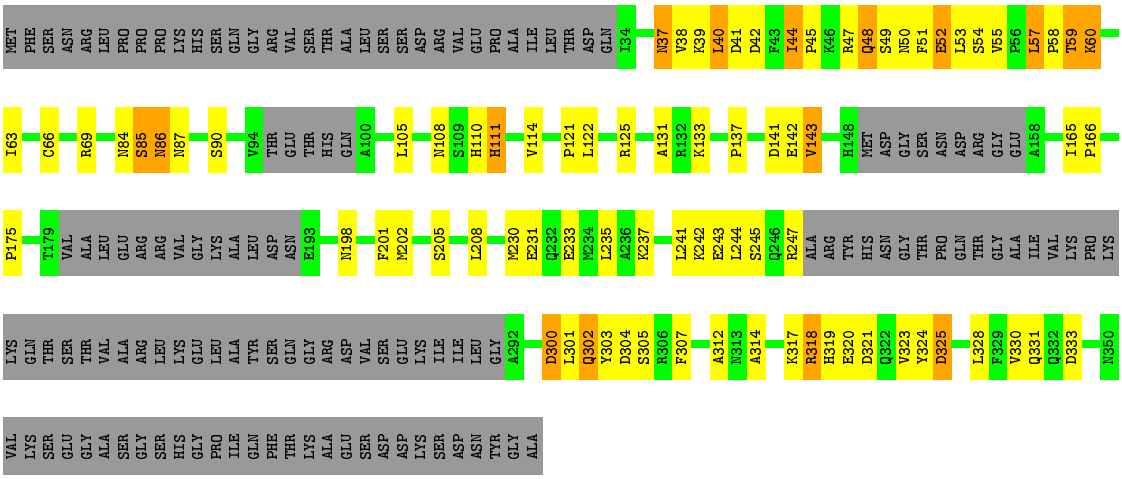




• Molecule 15: Pre-mRNA-processing protein 45

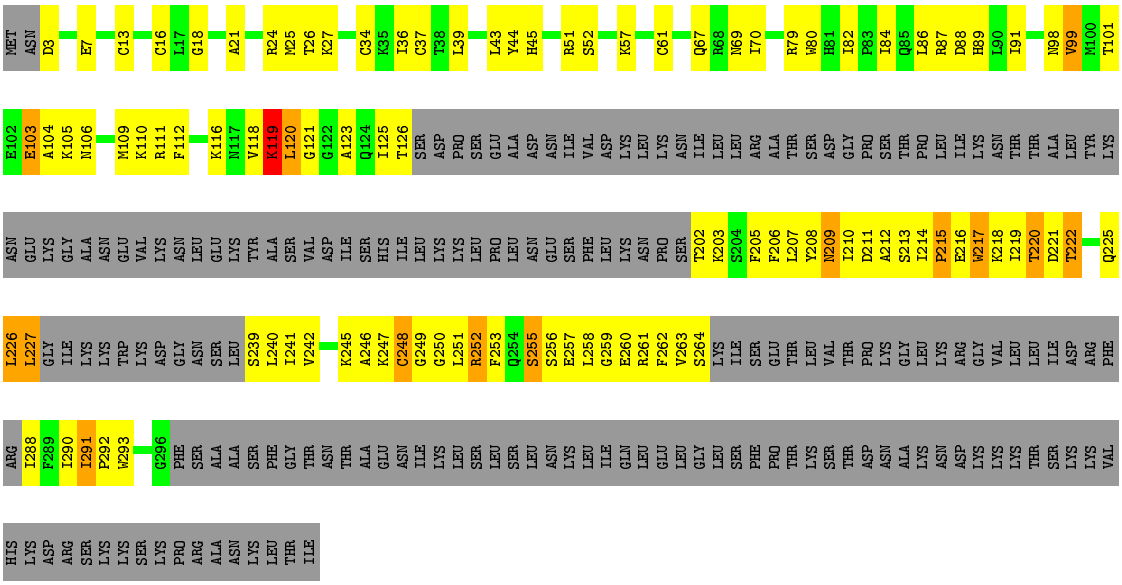
Chain P:





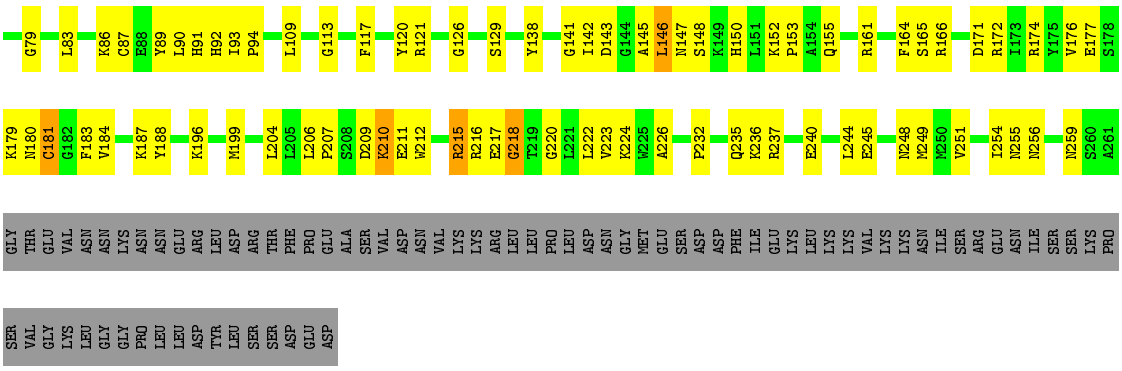
• Molecule 16: Pre-mRNA-splicing factor SLT11

Chain Q:



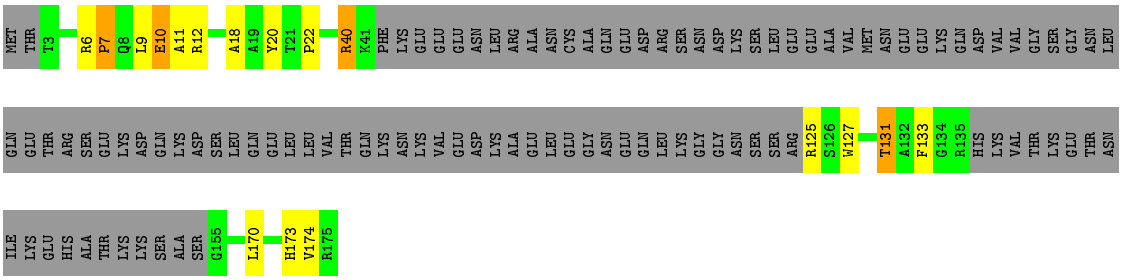
• Molecule 17: Pre-mRNA-splicing factor CWC2

Chain R:



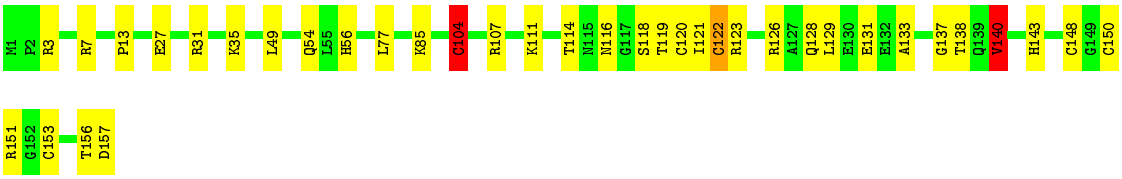
• Molecule 18: Pre-mRNA-splicing factor CWC15

Chain S:



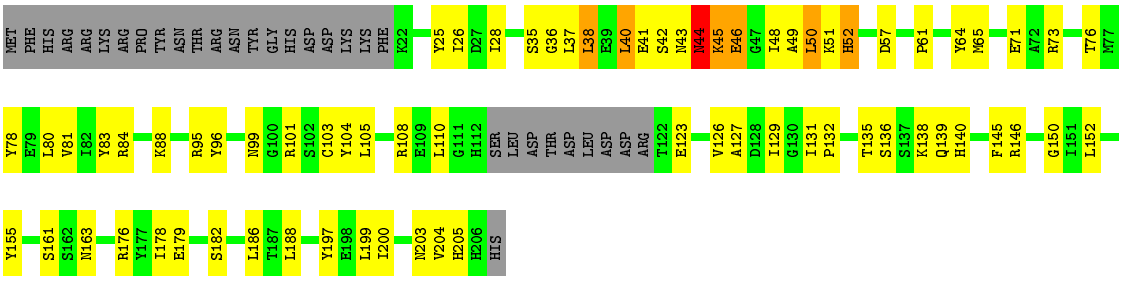
• Molecule 19: Pre-mRNA-splicing factor BUD31

Chain T:



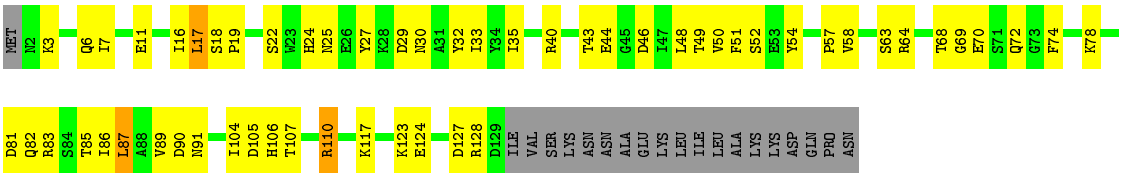
• Molecule 20: Pre-mRNA leakage protein 1

Chain U:



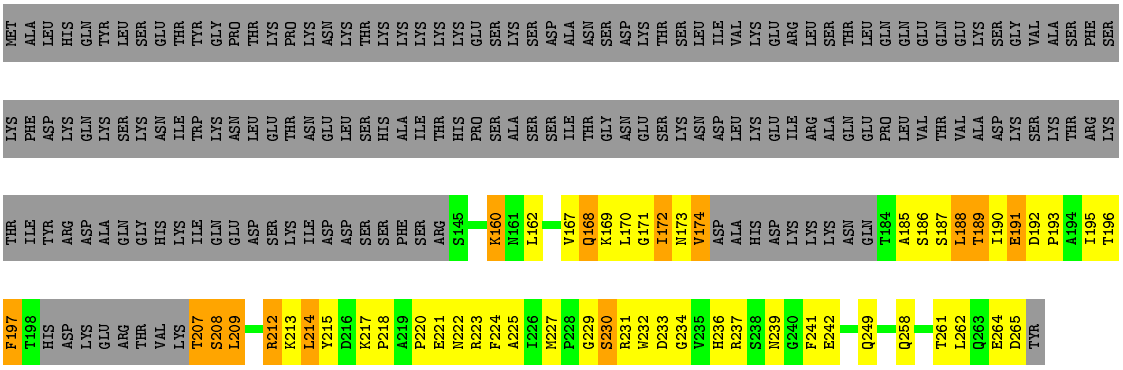
• Molecule 21: U2 snRNP component IST3

Chain V:



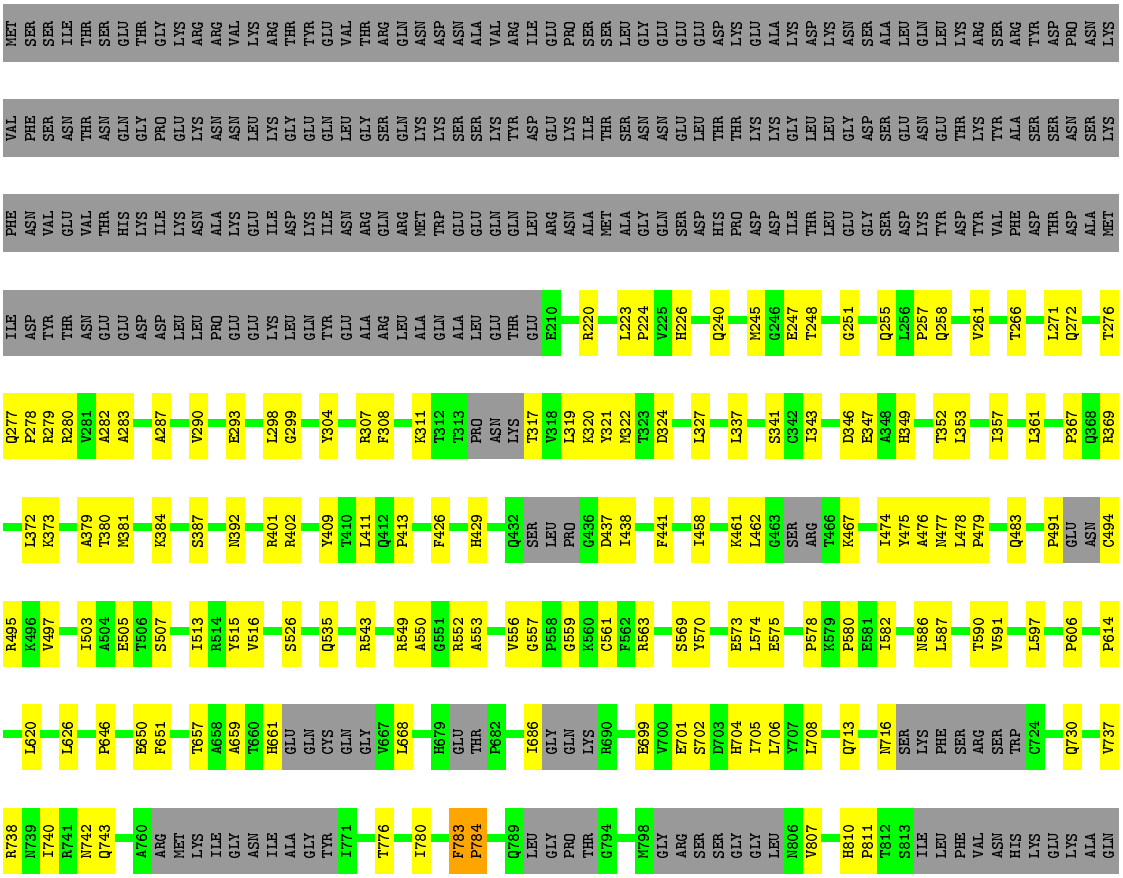
• Molecule 22: Pre-mRNA-splicing factor CWC26

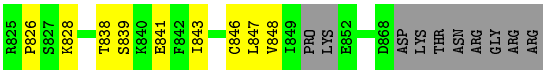
Chain W:



• Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2

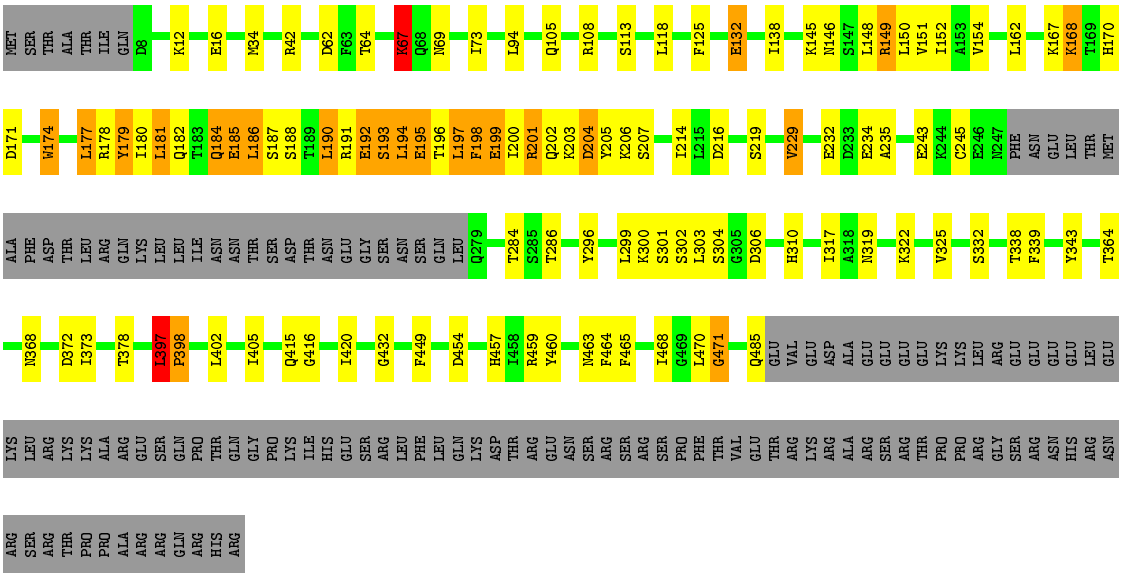
Chain Y:





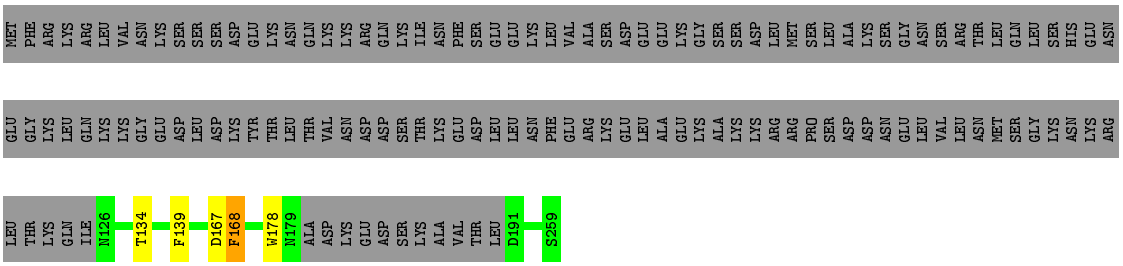
- Molecule 24: Pre-mRNA-splicing factor CWC22

Chain Z:



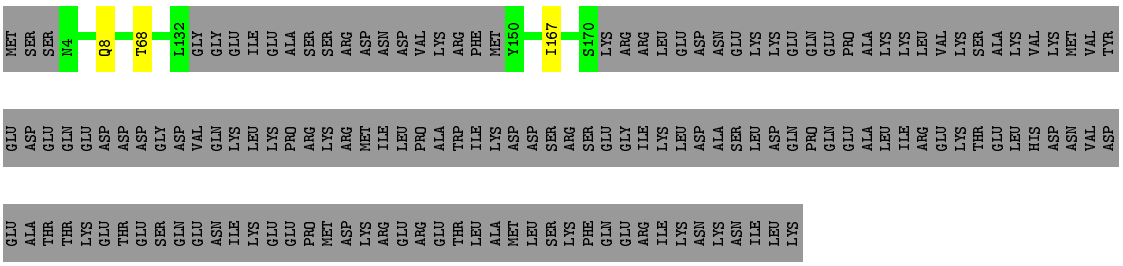
- Molecule 25: Pre-mRNA-splicing factor CWC24

Chain a:



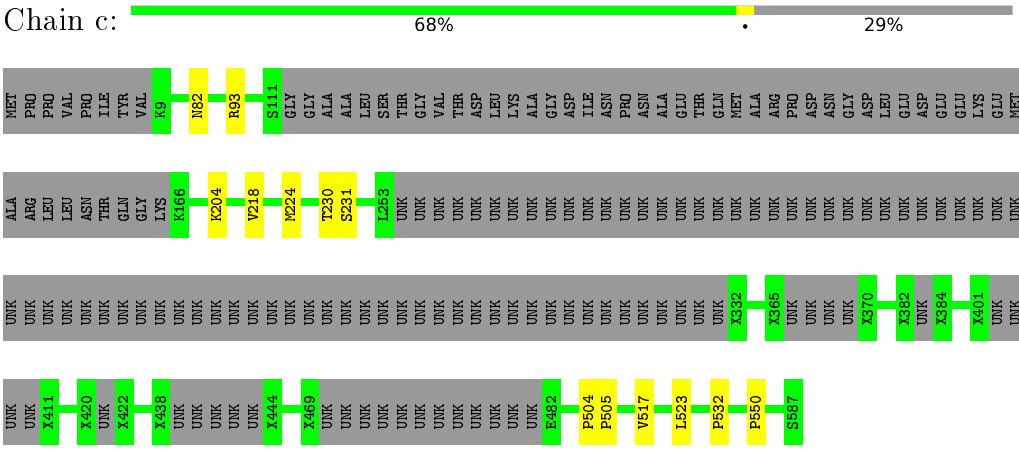
- Molecule 26: Peptidyl-prolyl isomerase CWC27

Chain b:



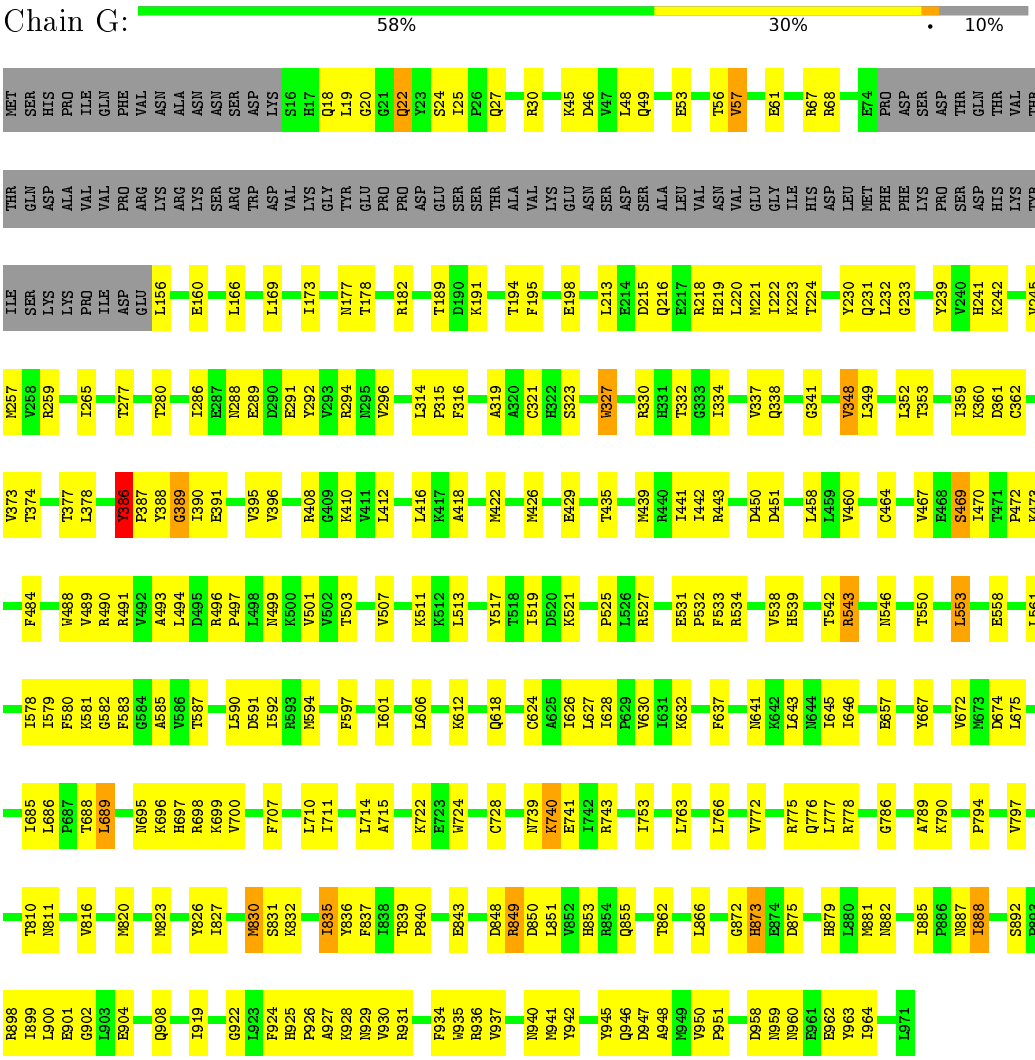
- Molecule 27: Pre-mRNA-splicing factor CEF1

Chain c:



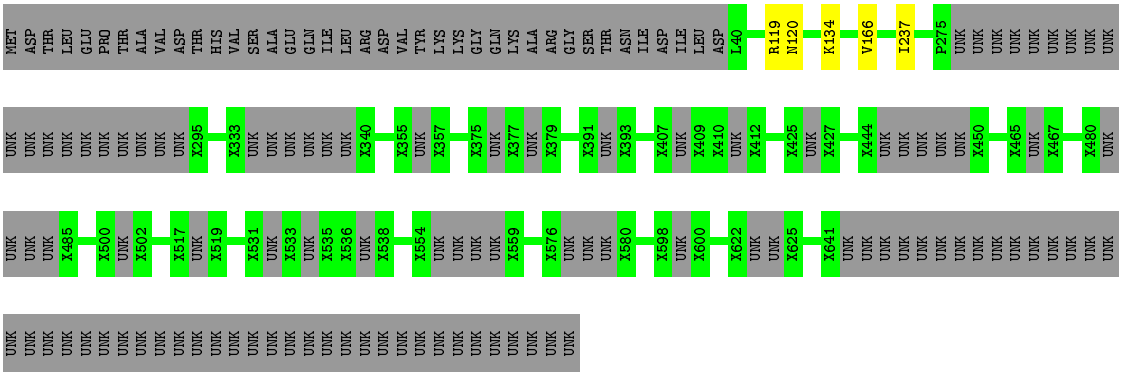
• Molecule 28: U2 snRNP component HSH155

Chain G:



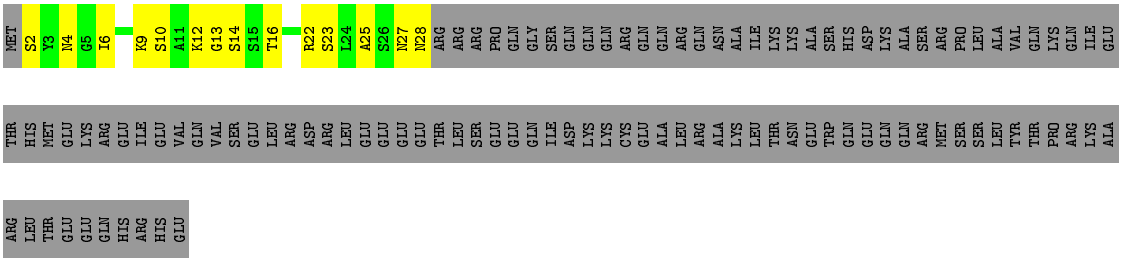
• Molecule 29: Pre-mRNA-splicing factor CLF1

Chain d:



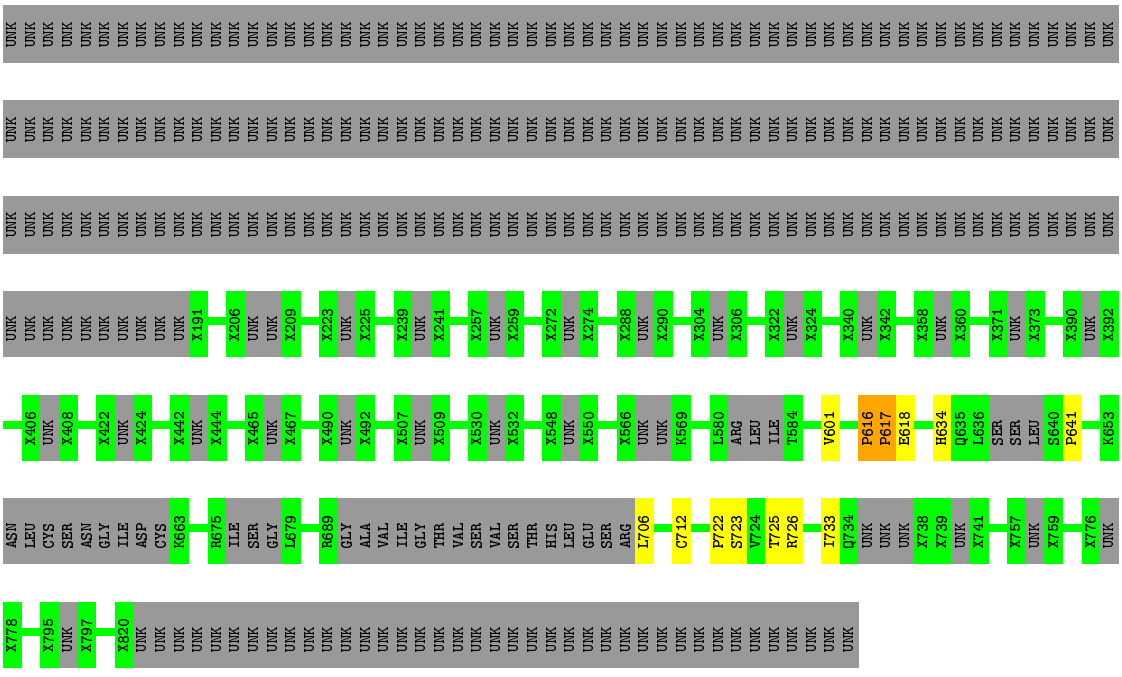
• Molecule 30: Pre-mRNA-splicing factor CWC21

Chain X:



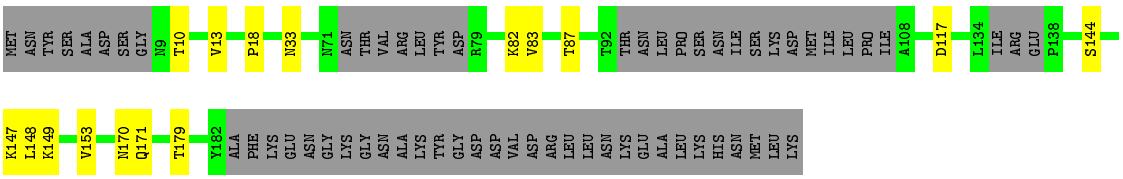
• Molecule 31: Pre-mRNA-splicing factor SYF1

Chain v:



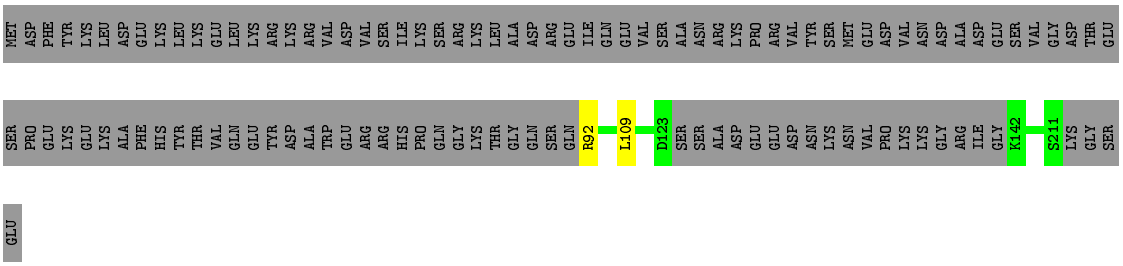
• Molecule 32: Protein HSH49

Chain e:



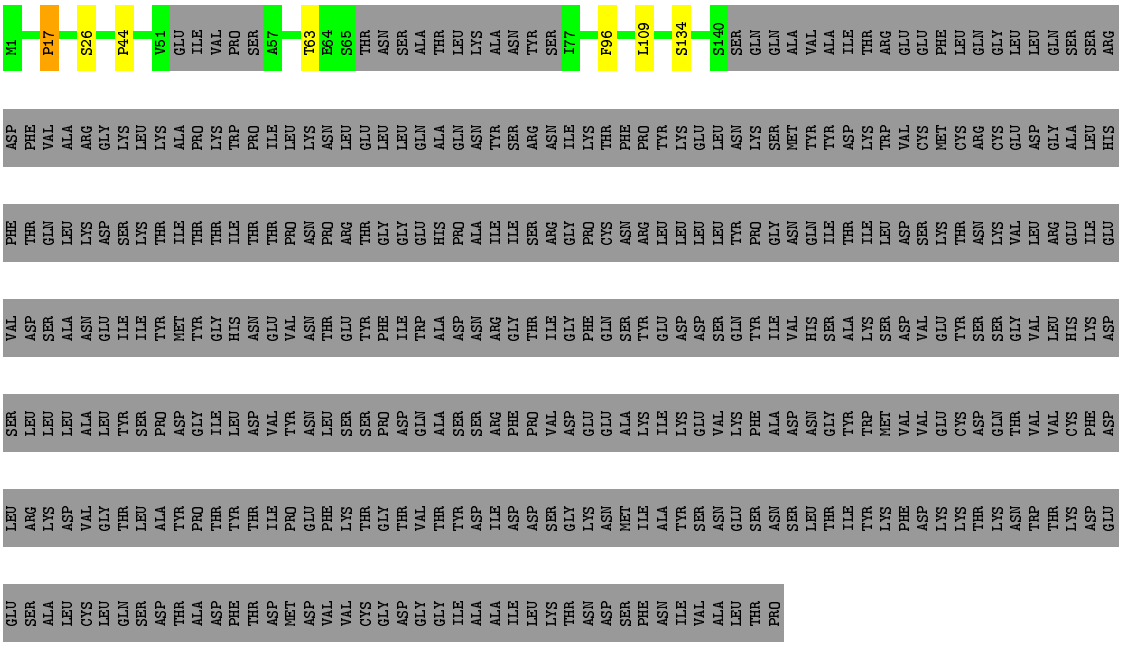
- Molecule 33: Pre-mRNA-splicing factor SYF2

Chain f:



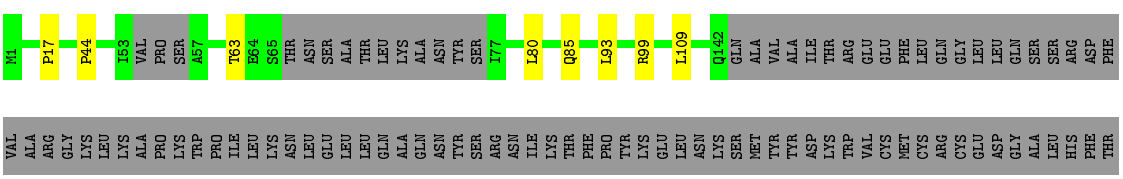
- Molecule 34: Pre-mRNA-processing factor 19

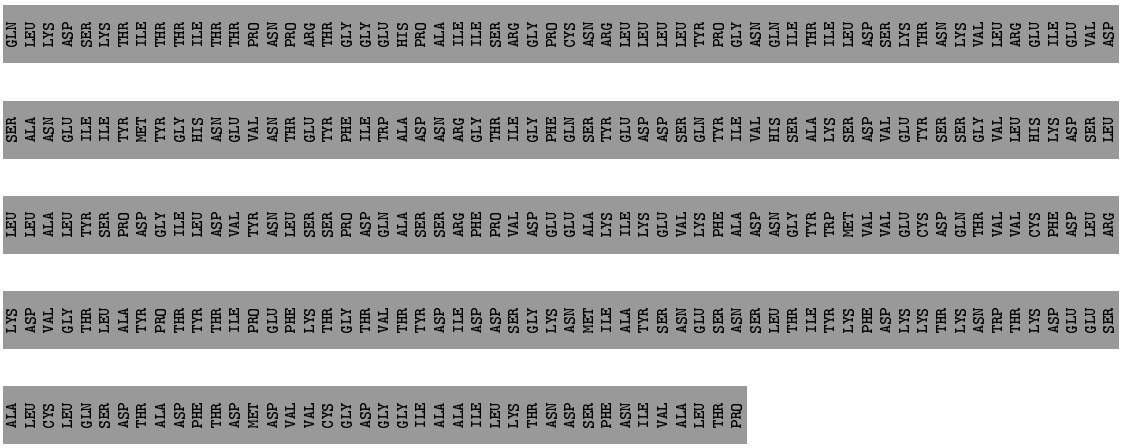
Chain o:



- Molecule 34: Pre-mRNA-processing factor 19

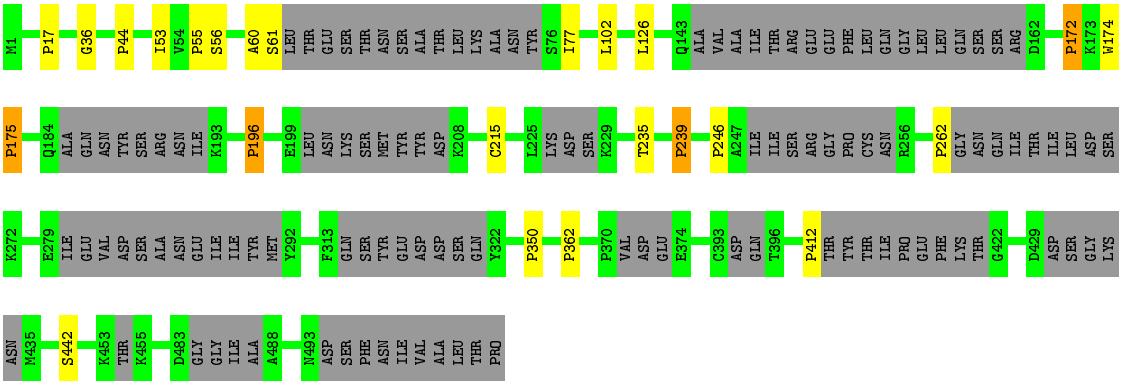
Chain p:





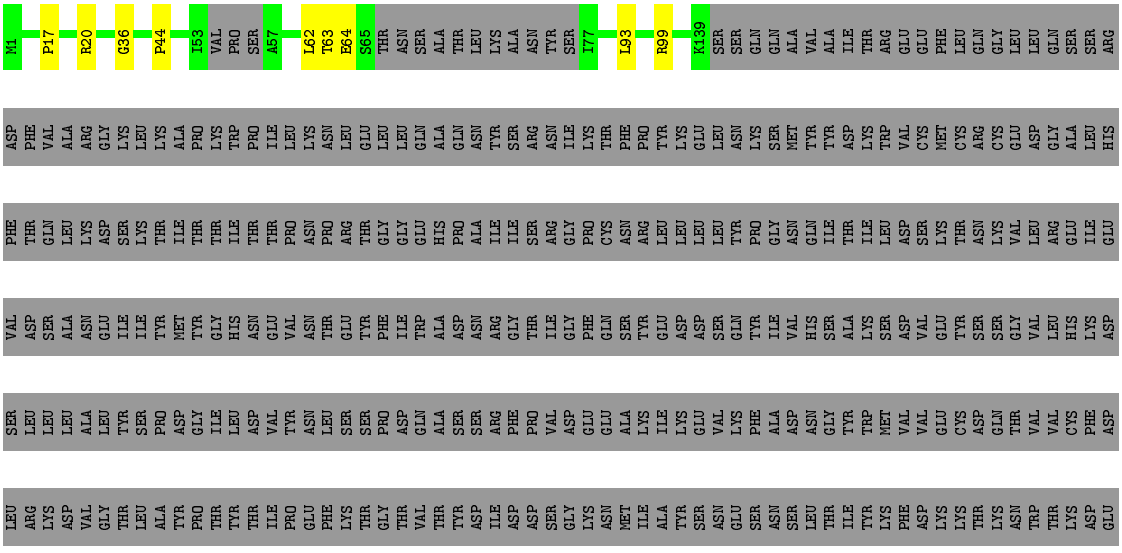
- Molecule 34: Pre-mRNA-processing factor 19

Chain q:



- Molecule 34: Pre-mRNA-processing factor 19

Chain r:

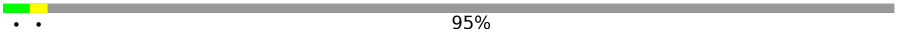


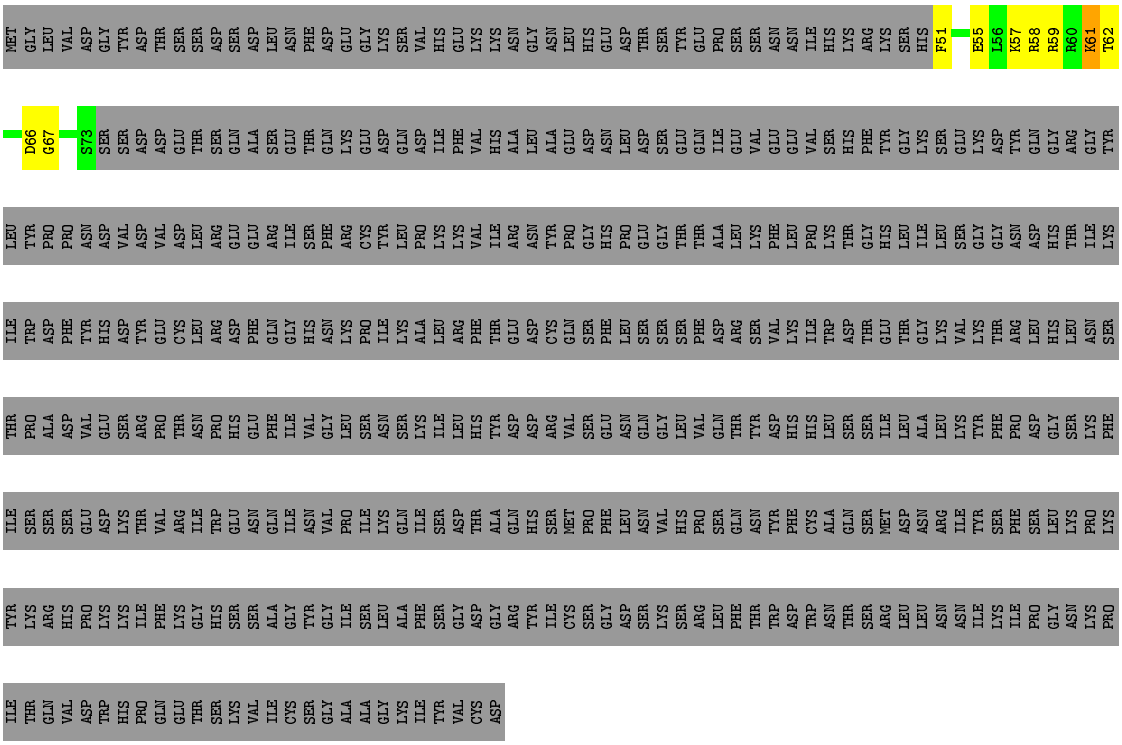
- Molecule 35: Pre-mRNA-splicing factor SNT309

Chain t:

- Molecule 36: Pre-mRNA-processing factor 17

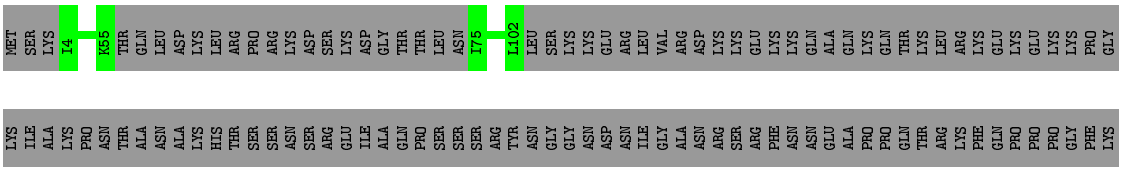
Chain n:





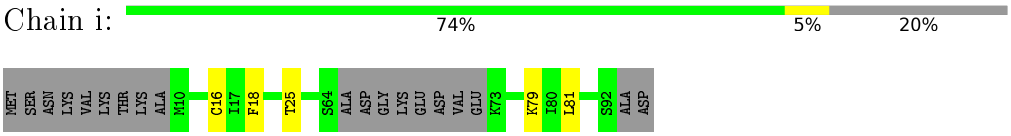
- Molecule 37: Small nuclear ribonucleoprotein-associated protein B

Chain k:



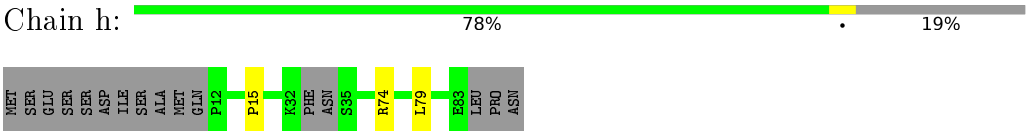
- Molecule 38: Small nuclear ribonucleoprotein E

Chain i:



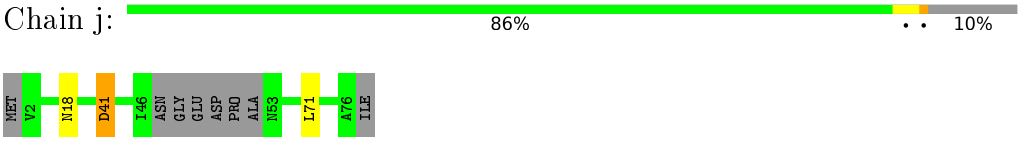
• Molecule 39: Small nuclear ribonucleoprotein F

Chain h:



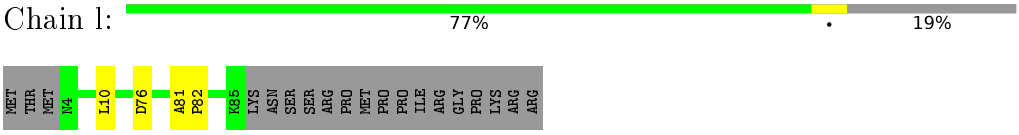
• Molecule 40: Small nuclear ribonucleoprotein G

Chain j:



• Molecule 41: Small nuclear ribonucleoprotein Sm D3

Chain l:

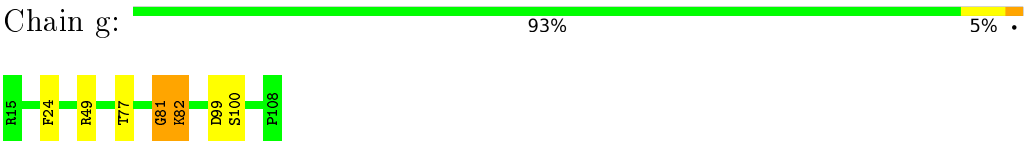


• Molecule 42: Small nuclear ribonucleoprotein Sm D1

Chain m:

• Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain g:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	77312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.77	7/18560 (0.0%)	0.79	16/25158 (0.1%)
10	K	0.81	0/702	0.85	0/939
11	L	0.59	0/1547	0.78	0/2404
12	N	0.55	0/579	0.82	0/897
13	M	0.62	2/1183 (0.2%)	0.93	2/1833 (0.1%)
14	O	0.72	0/2704	0.77	1/3676 (0.0%)
15	P	0.52	0/2008	0.66	1/2703 (0.0%)
16	Q	0.45	1/1496 (0.1%)	0.63	0/2014
17	R	0.50	0/2135	0.63	2/2871 (0.1%)
18	S	0.42	0/592	0.60	0/790
19	T	0.63	1/1315 (0.1%)	0.73	1/1759 (0.1%)
2	B	0.35	0/14812	0.48	0/20077
20	U	0.32	0/1424	0.52	0/1922
21	V	0.66	0/1071	0.73	1/1445 (0.1%)
22	W	0.61	0/856	0.73	1/1149 (0.1%)
23	Y	0.34	0/4085	0.50	1/5499 (0.0%)
24	Z	0.59	0/3712	0.76	4/5004 (0.1%)
25	a	0.60	0/1010	0.68	0/1351
26	b	0.38	0/1252	0.54	0/1692
27	c	0.54	0/2237	0.63	1/2995 (0.0%)
28	G	0.72	0/7104	0.81	3/9632 (0.0%)
29	d	0.42	0/2075	0.55	1/2808 (0.0%)
3	C	0.51	0/7162	0.65	2/9698 (0.0%)
30	X	0.57	0/191	0.75	0/254
31	v	0.41	0/899	0.54	0/1206
32	e	0.47	0/954	0.74	0/1285
33	f	0.43	0/826	0.59	1/1097 (0.1%)
34	o	0.40	0/824	0.52	0/1111
34	p	0.40	0/848	0.55	0/1143
34	q	0.44	0/2312	0.65	0/3097
34	r	0.39	0/828	0.54	1/1117 (0.1%)
35	t	0.42	0/919	0.56	2/1237 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
36	n	0.48	0/200	0.71	0/264
37	k	0.37	0/636	0.61	0/856
38	i	0.42	0/585	0.62	0/795
39	h	0.44	0/564	0.65	1/761 (0.1%)
4	D	0.63	0/2747	0.76	0/4267
40	j	0.37	0/532	0.60	0/715
41	l	0.40	0/634	0.70	0/859
42	m	0.41	0/649	0.61	0/880
43	g	0.45	0/753	0.69	2/1013 (0.2%)
5	E	0.63	0/2452	0.78	0/3817
6	F	0.76	5/9564 (0.1%)	0.84	7/12963 (0.1%)
7	H	0.72	0/1281	0.84	0/1727
8	I	0.77	0/812	0.92	3/1081 (0.3%)
9	J	0.81	0/827	0.85	0/1105
All	All	0.60	16/110458 (0.0%)	0.70	54/150966 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
14	O	0	6
15	P	0	1
16	Q	0	2
19	T	0	2
2	B	0	2
20	U	0	2
24	Z	0	4
28	G	0	3
29	d	0	1
3	C	0	5
33	f	0	1
36	n	0	2
40	j	0	1
41	l	0	2
43	g	0	2
6	F	0	13
7	H	0	6
8	I	0	3
All	All	0	64

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	468	A	N9-C4	-7.77	1.33	1.37
13	M	468	A	C3'-O3'	6.84	1.51	1.42
1	A	1265	PHE	CG-CD1	-6.29	1.29	1.38
6	F	830	TYR	CG-CD2	-6.15	1.31	1.39
1	A	753	TYR	CE1-CZ	-6.00	1.30	1.38
1	A	1335	TRP	CG-CD1	5.94	1.45	1.36
6	F	71	PHE	CG-CD1	-5.93	1.29	1.38
19	T	148	CYS	CB-SG	-5.92	1.72	1.81
1	A	1609	TRP	CB-CG	-5.78	1.39	1.50
6	F	836	TRP	CB-CG	-5.65	1.40	1.50
1	A	298	TYR	CG-CD2	-5.48	1.32	1.39
6	F	1226	GLY	CA-C	-5.46	1.43	1.51
16	Q	215	PRO	N-CD	5.35	1.55	1.47
1	A	708	TRP	CG-CD1	-5.07	1.29	1.36
1	A	1542	TYR	CG-CD2	-5.06	1.32	1.39
6	F	1228	PHE	CG-CD1	-5.05	1.31	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	55	ASN	C-N-CD	-15.28	86.99	120.60
13	M	468	A	C2'-C3'-O3'	9.32	130.00	109.50
13	M	468	A	C4'-C3'-O3'	-9.29	89.89	109.40
1	A	737	ARG	NE-CZ-NH2	-7.86	116.37	120.30
24	Z	397	LEU	C-N-CD	-7.43	104.25	120.60
1	A	1405	ILE	CG1-CB-CG2	-6.74	96.58	111.40
6	F	1124	LEU	CB-CG-CD1	6.63	122.27	111.00
17	R	218	GLY	N-CA-C	6.41	129.12	113.10
28	G	680	PRO	C-N-CD	-6.34	106.64	120.60
24	Z	42	ARG	NE-CZ-NH2	6.09	123.34	120.30
28	G	689	LEU	CB-CG-CD2	-6.08	100.66	111.00
27	c	93	ARG	NE-CZ-NH2	-6.04	117.28	120.30
6	F	179	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	399	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	1317	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	1159	ARG	NE-CZ-NH2	-5.77	117.41	120.30
35	t	105	PRO	CA-CB-CG	5.76	115.75	104.80
3	C	461	LYS	N-CA-CB	5.76	120.96	110.60
6	F	839	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	1440	ILE	CG1-CB-CG2	-5.71	98.84	111.40
14	O	193	ARG	NE-CZ-NH2	-5.63	117.49	120.30
6	F	1130	ILE	CG1-CB-CG2	-5.59	99.11	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	888	ILE	CG1-CB-CG2	-5.57	99.15	111.40
43	g	81	GLY	CA-C-N	-5.55	104.98	117.20
15	P	318	ARG	NE-CZ-NH1	5.55	123.07	120.30
22	W	197	PHE	CB-CG-CD1	-5.54	116.93	120.80
1	A	1816	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1816	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	C	464	PRO	N-CA-CB	5.49	109.89	103.30
1	A	716	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	V	87	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	A	614	ARG	NE-CZ-NH1	5.46	123.03	120.30
19	T	123	ARG	NE-CZ-NH2	-5.41	117.60	120.30
35	t	77	PRO	CA-CB-CG	5.34	114.94	104.80
24	Z	62	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	716	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	831	ARG	NE-CZ-NH1	5.26	122.93	120.30
34	r	62	LEU	CA-CB-CG	-5.23	103.26	115.30
1	A	1825	ILE	CG1-CB-CG2	-5.19	99.97	111.40
6	F	1357	ARG	NE-CZ-NH1	-5.19	117.70	120.30
23	Y	411	LEU	CA-CB-CG	-5.16	103.44	115.30
8	I	15	GLY	N-CA-C	5.15	125.98	113.10
6	F	1041	LEU	CB-CG-CD1	-5.13	102.27	111.00
39	h	74	ARG	NE-CZ-NH1	5.13	122.86	120.30
6	F	240	MET	CA-CB-CG	5.12	122.00	113.30
24	Z	108	ARG	NE-CZ-NH2	5.12	122.86	120.30
17	R	217	GLU	N-CA-C	5.11	124.79	111.00
1	A	1342	LEU	CB-CG-CD2	-5.09	102.35	111.00
43	g	82	LYS	N-CA-C	5.08	124.71	111.00
8	I	33	LEU	CB-CG-CD1	-5.04	102.44	111.00
33	f	109	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	A	1382	ARG	NE-CZ-NH2	-5.01	117.80	120.30
29	d	119	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	1426	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1418	THR	Peptide
1	A	239	PHE	Mainchain,Peptide
1	A	539	PRO	Peptide
1	A	772	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	696	SER	Peptide
2	B	904	GLN	Peptide
3	C	460	GLY	Mainchain,Peptide
3	C	534	THR	Peptide
3	C	70	TYR	Peptide
3	C	951	ILE	Peptide
6	F	1012	LYS	Mainchain,Peptide
6	F	1014	LYS	Mainchain,Peptide
6	F	1183	CYS	Mainchain,Peptide
6	F	185	ARG	Peptide
6	F	206	SER	Peptide
6	F	666	LEU	Peptide
6	F	667	THR	Mainchain,Peptide
6	F	855	ALA	Mainchain,Peptide
28	G	389	GLY	Peptide
28	G	680	PRO	Mainchain,Peptide
7	H	184	SER	Peptide
7	H	185	GLY	Peptide
7	H	212	LEU	Mainchain,Peptide
7	H	234	GLN	Mainchain,Peptide
8	I	13	GLY	Peptide
8	I	14	GLY	Peptide
8	I	15	GLY	Peptide
14	O	123	PRO	Peptide
14	O	278	ASP	Peptide
14	O	351	GLY	Mainchain,Peptide
14	O	437	GLU	Peptide
14	O	441	ALA	Peptide
15	P	85	SER	Peptide
16	Q	103	GLU	Peptide
16	Q	291	ILE	Peptide
19	T	104	CYS	Peptide
19	T	140	VAL	Peptide
20	U	44	ASN	Peptide
20	U	71	GLU	Peptide
24	Z	219	SER	Peptide
24	Z	232	GLU	Peptide
24	Z	397	LEU	Mainchain,Peptide
29	d	237	ILE	Peptide
33	f	92	ARG	Peptide
43	g	81	GLY	Mainchain,Peptide
40	j	41	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
41	l	81	ALA	Mainchain,Peptide
36	n	67	GLY	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18101	0	18027	759	0
2	B	14504	0	14508	407	0
3	C	7014	0	7189	280	0
4	D	2465	0	1251	36	0
5	E	2192	0	1106	40	0
6	F	9380	0	9482	430	0
7	H	1248	0	1263	88	0
8	I	800	0	802	43	0
9	J	814	0	809	50	0
10	K	693	0	705	43	0
11	L	1388	0	701	33	0
12	N	521	0	260	25	0
13	M	1057	0	537	50	0
14	O	2646	0	2639	92	0
15	P	1978	0	1981	112	0
16	Q	1472	0	1485	166	0
17	R	2089	0	2053	168	0
18	S	578	0	565	35	0
19	T	1291	0	1312	32	0
20	U	1401	0	1362	76	0
21	V	1051	0	1015	74	0
22	W	842	0	818	105	0
23	Y	4047	0	3394	122	0
24	Z	3651	0	3707	149	0
25	a	988	0	954	0	0
26	b	1224	0	1217	0	0
27	c	2803	0	2169	0	0
28	G	6970	0	7181	290	0
29	d	3558	0	2329	0	0
30	X	190	0	186	16	0
31	v	3047	0	1177	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	e	947	0	703	0	0
33	f	822	0	845	0	0
34	o	819	0	657	0	0
34	p	843	0	672	0	0
34	q	2315	0	1626	0	0
34	r	823	0	654	0	0
35	t	921	0	605	0	0
36	n	195	0	198	0	0
37	k	631	0	670	0	0
38	i	575	0	597	0	0
39	h	554	0	556	0	0
40	j	529	0	557	0	0
41	l	625	0	647	0	0
42	m	644	0	686	0	0
43	g	741	0	778	0	0
44	C	32	0	12	4	0
45	E	4	0	0	0	0
45	Y	1	0	0	0	0
46	I	1	0	0	0	0
46	J	3	0	0	0	0
46	Q	2	0	0	0	0
46	R	1	0	0	0	0
46	T	3	0	0	0	0
46	a	3	0	0	0	0
47	Y	27	0	12	2	0
All	All	112064	0	102659	3326	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 18.

All (3326) 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)
7:H:262:HIS:CD2	7:H:283:LYS:HZ1	1.31	1.46
23:Y:699:GLU:HB3	23:Y:702:SER:CB	1.49	1.41
22:W:207:THR:O	22:W:214:LEU:CD1	1.68	1.40
16:Q:212:ALA:HB1	17:R:237:ARG:NH2	1.35	1.39
21:V:63:SER:CB	21:V:74:PHE:CE1	2.06	1.38
3:C:116:THR:CG2	3:C:118:TYR:CE1	2.08	1.36
24:Z:192:GLU:CA	24:Z:195:GLU:OE2	1.74	1.34
16:Q:212:ALA:CB	17:R:237:ARG:HH21	1.38	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:PHE:HE2	3:C:295:ILE:CG2	1.42	1.33
7:H:262:HIS:CD2	7:H:283:LYS:NZ	1.90	1.32
17:R:48:VAL:CG2	17:R:216:ARG:O	1.77	1.30
24:Z:192:GLU:HA	24:Z:195:GLU:OE2	1.12	1.29
3:C:116:THR:HG21	3:C:118:TYR:CE1	1.63	1.28
1:A:1748:ILE:HD11	1:A:1783:MET:CB	1.64	1.25
1:A:769:MET:HE1	1:A:811:ILE:CD1	1.66	1.25
1:A:1618:ASN:HB2	1:A:1744:ASP:OD2	1.37	1.23
24:Z:170:HIS:CE1	24:Z:174:TRP:CZ3	2.26	1.22
15:P:57:LEU:CD2	15:P:58:PRO:HD2	1.67	1.22
24:Z:459:ARG:O	24:Z:463:ASN:ND2	1.72	1.21
1:A:1748:ILE:CD1	1:A:1783:MET:HB3	1.70	1.20
3:C:391:MET:CE	3:C:395:LYS:HE2	1.73	1.18
16:Q:215:PRO:HB3	17:R:171:ASP:OD1	1.00	1.17
2:B:880:TYR:O	6:F:686:GLN:NE2	1.77	1.17
1:A:2405:GLU:OE1	2:B:833:THR:OG1	1.59	1.16
3:C:265:PHE:CE2	3:C:295:ILE:HG21	1.81	1.16
1:A:769:MET:CE	1:A:811:ILE:CD1	2.24	1.15
1:A:330:LEU:O	1:A:335:SER:OG	1.63	1.15
16:Q:101:THR:CG2	16:Q:120:LEU:HD21	1.77	1.15
16:Q:79:ARG:CD	16:Q:126:THR:HG23	1.77	1.15
16:Q:215:PRO:CB	17:R:171:ASP:OD1	1.94	1.14
1:A:769:MET:CE	1:A:811:ILE:HD11	1.76	1.14
23:Y:699:GLU:CB	23:Y:702:SER:CB	2.25	1.14
3:C:265:PHE:CE2	3:C:295:ILE:CG2	2.29	1.13
16:Q:101:THR:HG21	16:Q:120:LEU:HD21	1.26	1.13
7:H:262:HIS:HD2	7:H:283:LYS:NZ	1.31	1.13
15:P:57:LEU:HD23	15:P:58:PRO:HD2	1.27	1.13
1:A:1130:ARG:HH11	1:A:1156:HIS:HB3	0.98	1.12
24:Z:170:HIS:CE1	24:Z:174:TRP:HZ3	1.65	1.12
1:A:1130:ARG:NH1	1:A:1156:HIS:HB3	1.66	1.11
3:C:391:MET:HE1	3:C:395:LYS:HE2	1.30	1.11
17:R:48:VAL:HG21	17:R:216:ARG:O	1.49	1.10
16:Q:91:ILE:HG21	16:Q:125:ILE:HD12	1.25	1.09
1:A:769:MET:HE1	1:A:811:ILE:HD12	1.30	1.09
1:A:1509:ARG:NH1	1:A:1533:ASP:OD2	1.86	1.08
3:C:116:THR:CG2	3:C:118:TYR:CD1	2.37	1.08
16:Q:79:ARG:HD3	16:Q:126:THR:HG23	1.13	1.07
16:Q:217:TRP:CH2	17:R:187:LYS:HD3	1.89	1.07
1:A:931:ALA:HA	1:A:934:ARG:NH1	1.68	1.06
16:Q:217:TRP:CZ2	17:R:187:LYS:HD3	1.88	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:197:PHE:CE2	24:Z:463:ASN:HB3	1.89	1.06
24:Z:177:LEU:HD22	24:Z:194:LEU:HD21	1.35	1.06
22:W:189:THR:O	22:W:195:ILE:HG13	1.53	1.06
1:A:1428:GLY:O	30:X:16:THR:HG22	1.55	1.06
21:V:63:SER:HB2	21:V:74:PHE:CE1	1.78	1.05
20:U:45:LYS:HG2	20:U:126:VAL:HG13	1.07	1.05
1:A:1589:LYS:O	8:I:16:ILE:HG13	1.55	1.05
8:I:57:TYR:CE1	8:I:70:LEU:CD1	2.40	1.05
1:A:1122:ASP:OD1	1:A:1161:TYR:OH	1.75	1.04
24:Z:177:LEU:CD2	24:Z:194:LEU:HD21	1.85	1.04
16:Q:79:ARG:HD3	16:Q:126:THR:CG2	1.88	1.04
24:Z:170:HIS:CE1	24:Z:174:TRP:CE3	2.45	1.04
3:C:274:ILE:HG12	3:C:382:TYR:CE1	1.92	1.04
13:M:514:U:H4'	13:M:515:U:H5'	1.38	1.04
24:Z:178:ARG:HG3	24:Z:198:PHE:CE2	1.93	1.03
15:P:319:HIS:HE1	22:W:264:GLU:OE1	1.41	1.03
1:A:1325:SER:O	1:A:1331:VAL:CG2	2.07	1.03
4:D:165:A:H4'	4:D:166:U:C5'	1.89	1.02
1:A:1842:GLU:O	1:A:1845:ASN:ND2	1.91	1.02
1:A:931:ALA:HA	1:A:934:ARG:HH12	1.15	1.02
7:H:288:HIS:O	7:H:289:LYS:HG3	1.60	1.01
1:A:2018:ASN:OD1	1:A:2021:SER:OG	1.77	1.00
16:Q:39:LEU:HD11	16:Q:111:ARG:HG3	1.44	1.00
21:V:48:LEU:O	22:W:231:ARG:NH1	1.95	1.00
24:Z:181:LEU:HG	24:Z:194:LEU:HD13	1.41	1.00
1:A:997:GLN:NE2	1:A:1511:ARG:NH2	2.10	1.00
1:A:563:ASP:OD2	1:A:640:ARG:NH2	1.93	1.00
3:C:150:MET:SD	3:C:178:LEU:HD11	2.01	1.00
28:G:578:ILE:HG23	28:G:579:ILE:HD12	1.41	1.00
16:Q:226:LEU:CD1	16:Q:227:LEU:HD23	1.91	1.00
24:Z:178:ARG:CB	24:Z:198:PHE:HZ	1.74	1.00
17:R:146:LEU:CD2	17:R:211:GLU:OE1	2.09	1.00
15:P:57:LEU:HD23	15:P:58:PRO:CD	1.91	0.99
1:A:1325:SER:O	1:A:1331:VAL:HG23	1.63	0.99
1:A:893:ARG:HG3	1:A:893:ARG:HH11	1.27	0.99
20:U:45:LYS:HG2	20:U:126:VAL:CG1	1.92	0.99
21:V:63:SER:HB3	21:V:74:PHE:CE1	1.99	0.98
4:D:165:A:C4'	4:D:166:U:H5'	1.91	0.98
16:Q:216:GLU:OE2	16:Q:240:LEU:HG	1.64	0.98
1:A:143:ILE:CD1	1:A:570:GLN:HG3	1.94	0.97
16:Q:101:THR:HB	16:Q:120:LEU:HD11	1.44	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:37:ASN:OD1	15:P:143:VAL:HG11	1.63	0.97
17:R:48:VAL:HG22	17:R:216:ARG:O	1.64	0.97
3:C:116:THR:HG21	3:C:118:TYR:CZ	1.97	0.97
16:Q:226:LEU:HD21	16:Q:262:PHE:CD1	2.00	0.97
10:K:57:ARG:NH1	10:K:59:ASP:OD2	1.97	0.96
22:W:208:SER:HB2	22:W:212:ARG:O	1.65	0.96
18:S:9:LEU:HD21	18:S:11:ALA:HB3	1.45	0.96
16:Q:91:ILE:HG21	16:Q:125:ILE:CD1	1.96	0.96
1:A:1012:TRP:NE1	1:A:1122:ASP:OD2	2.00	0.95
15:P:57:LEU:HD22	15:P:58:PRO:HD2	1.46	0.95
19:T:104:CYS:SG	19:T:150:CYS:HB2	2.06	0.95
24:Z:170:HIS:HE1	24:Z:174:TRP:CZ3	1.75	0.95
6:F:1113:SER:O	7:H:168:ASN:ND2	1.99	0.95
22:W:207:THR:O	22:W:214:LEU:HD13	0.78	0.95
16:Q:226:LEU:CG	16:Q:227:LEU:HD23	1.97	0.95
3:C:126:MET:SD	3:C:132:ARG:NH1	2.39	0.94
16:Q:226:LEU:HD11	16:Q:227:LEU:HD23	1.49	0.94
22:W:197:PHE:CZ	24:Z:463:ASN:HB3	2.01	0.94
3:C:116:THR:HG23	3:C:118:TYR:CE1	2.01	0.94
6:F:363:VAL:HG12	6:F:364:THR:H	1.32	0.94
8:I:57:TYR:CE1	8:I:70:LEU:HD13	2.02	0.94
15:P:319:HIS:CE1	22:W:264:GLU:OE1	2.21	0.94
1:A:769:MET:HE1	1:A:811:ILE:HD11	1.41	0.94
3:C:177:TYR:CE1	3:C:548:ARG:HD3	2.03	0.94
15:P:53:LEU:HD23	15:P:54:SER:N	1.83	0.94
20:U:45:LYS:CG	20:U:126:VAL:HG13	1.97	0.93
10:K:38:ASP:O	10:K:42:THR:HG23	1.67	0.93
16:Q:79:ARG:CD	16:Q:126:THR:CG2	2.45	0.93
20:U:50:LEU:HA	20:U:139:GLN:HE22	1.32	0.93
1:A:143:ILE:HD13	1:A:570:GLN:HG3	1.49	0.93
3:C:116:THR:HG22	3:C:118:TYR:CD1	2.01	0.93
1:A:774:ILE:HD12	1:A:775:ARG:N	1.84	0.93
24:Z:199:GLU:O	24:Z:202:GLN:HG2	1.68	0.93
21:V:63:SER:HB2	21:V:74:PHE:HE1	1.24	0.93
24:Z:174:TRP:CZ2	24:Z:197:LEU:HD11	2.04	0.92
4:D:165:A:H4'	4:D:166:U:H5'	0.95	0.92
1:A:351:LYS:NZ	12:N:91:A:OP1	2.02	0.92
17:R:206:LEU:HG	17:R:207:PRO:HD2	1.51	0.92
22:W:213:LYS:HB3	22:W:230:SER:OG	1.70	0.92
16:Q:255:SER:OG	16:Q:257:GLU:HG2	1.70	0.91
6:F:656:ILE:HA	6:F:662:SER:O	1.69	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1111:ASP:OD2	7:H:167:LYS:NZ	2.02	0.91
23:Y:505:GLU:O	23:Y:552:ARG:NH2	2.04	0.91
7:H:262:HIS:CD2	7:H:283:LYS:HZ2	1.87	0.91
8:I:53:ARG:HB3	8:I:53:ARG:NH1	1.85	0.91
16:Q:214:ILE:HD11	16:Q:218:LYS:CG	1.99	0.91
1:A:1364:GLU:OE1	1:A:1403:SER:CB	2.19	0.90
6:F:690:LEU:HA	6:F:703:MET:O	1.71	0.90
1:A:1130:ARG:HH11	1:A:1156:HIS:CB	1.82	0.90
3:C:117:ARG:NH1	3:C:156:ASP:O	2.05	0.90
1:A:143:ILE:CD1	1:A:570:GLN:CG	2.49	0.90
1:A:777:LYS:CE	1:A:777:LYS:HA	2.00	0.90
23:Y:626:LEU:CD1	23:Y:650:GLU:HA	2.02	0.90
19:T:120:CYS:HB2	19:T:122:CYS:HB3	1.54	0.90
24:Z:178:ARG:CG	24:Z:198:PHE:CZ	2.54	0.90
15:P:53:LEU:HD23	15:P:54:SER:H	1.36	0.89
15:P:60:LYS:HE3	15:P:63:ILE:HD11	1.51	0.89
1:A:997:GLN:HE22	1:A:1511:ARG:NH2	1.69	0.89
1:A:1816:ARG:HH11	1:A:1816:ARG:HG2	1.37	0.89
1:A:1122:ASP:OD1	1:A:1161:TYR:CZ	2.25	0.89
17:R:3:SER:O	17:R:7:LYS:HD3	1.73	0.89
1:A:1836:ASN:ND2	1:A:2006:SER:OG	2.04	0.89
1:A:273:ASP:HA	1:A:310:ASN:HD21	1.38	0.89
3:C:219:VAL:HG11	3:C:931:TYR:HB3	1.53	0.89
22:W:207:THR:C	22:W:214:LEU:HD13	1.93	0.89
22:W:214:LEU:HD21	22:W:227:MET:HB2	1.54	0.89
28:G:675:LEU:HD11	28:G:714:LEU:HB3	1.54	0.89
1:A:322:VAL:HG21	1:A:327:TYR:CE2	2.08	0.88
13:M:514:U:O2'	13:M:515:U:OP2	1.89	0.88
21:V:63:SER:OG	21:V:74:PHE:CE1	2.26	0.88
16:Q:212:ALA:HB3	17:R:237:ARG:HH21	1.36	0.88
21:V:63:SER:OG	21:V:74:PHE:CZ	2.26	0.88
1:A:928:ARG:HD2	1:A:1582:GLU:OE2	1.70	0.88
6:F:161:GLN:HG2	6:F:163:ILE:CG2	2.03	0.88
28:G:830:MET:O	28:G:832:LYS:N	2.06	0.88
1:A:1364:GLU:OE1	1:A:1403:SER:OG	1.91	0.88
1:A:342:LEU:HD13	1:A:392:ASN:HD21	1.36	0.88
8:I:57:TYR:CD1	8:I:70:LEU:HD13	2.09	0.88
23:Y:491:PRO:O	23:Y:494:CYS:CB	2.22	0.88
1:A:1488:ILE:HG22	1:A:1489:PRO:HD3	1.55	0.88
1:A:614:ARG:HG2	1:A:614:ARG:HH11	1.39	0.88
11:L:41:C:H5"	11:L:41:C:H6	1.39	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:188:LEU:HD21	24:Z:415:GLN:HG2	1.53	0.88
20:U:38:LEU:HD22	21:V:46:ASP:OD1	1.74	0.87
16:Q:212:ALA:CB	17:R:237:ARG:NH2	2.12	0.87
1:A:1571:GLU:HB3	15:P:331:GLN:OE1	1.75	0.87
6:F:1116:ARG:HH22	6:F:1141:LEU:HD21	1.37	0.87
3:C:265:PHE:HE2	3:C:295:ILE:HG23	1.38	0.87
22:W:188:LEU:HG	24:Z:378:THR:CG2	2.04	0.87
1:A:1056:GLU:HB3	1:A:1059:GLU:HB2	1.56	0.87
5:E:38:U:O2	17:R:196:LYS:NZ	2.08	0.87
28:G:578:ILE:HG23	28:G:579:ILE:CD1	2.05	0.87
15:P:44:ILE:HD13	15:P:45:PRO:O	1.74	0.87
1:A:1295:GLN:HE21	24:Z:432:GLY:HA3	1.40	0.86
1:A:2412:PHE:O	1:A:2413:SER:OG	1.93	0.86
17:R:138:TYR:CE1	17:R:181:CYS:HB3	2.10	0.86
9:J:3:ARG:NH1	28:G:901:GLU:OE2	2.09	0.86
22:W:190:ILE:O	22:W:192:ASP:N	2.07	0.86
1:A:1458:TRP:CD2	28:G:25:ILE:HG22	2.11	0.86
24:Z:192:GLU:HA	24:Z:195:GLU:CD	1.94	0.86
1:A:854:ARG:HH21	1:A:854:ARG:HG2	1.41	0.86
28:G:213:LEU:HD13	28:G:218:ARG:HB2	1.58	0.85
1:A:1608:LEU:HD11	1:A:1648:ILE:HD11	1.59	0.85
16:Q:91:ILE:CG2	16:Q:125:ILE:HD12	2.04	0.85
1:A:299:LYS:HA	1:A:493:MET:HG3	1.58	0.85
1:A:610:ARG:NH2	12:N:101:U:OP2	2.10	0.84
3:C:274:ILE:HD13	3:C:385:PHE:CE2	2.11	0.84
1:A:2403:GLU:N	1:A:2403:GLU:OE2	2.09	0.84
1:A:978:ILE:HG22	18:S:174:VAL:HA	1.58	0.84
23:Y:626:LEU:HD13	23:Y:650:GLU:HA	1.57	0.84
24:Z:178:ARG:HG3	24:Z:198:PHE:HE2	1.38	0.84
2:B:2084:LEU:HD11	2:B:2120:ASN:HA	1.57	0.84
6:F:257:ILE:HD11	10:K:74:SER:HB2	1.60	0.84
1:A:856:TRP:CD1	18:S:174:VAL:HG11	2.13	0.84
1:A:1876:ASN:OD1	1:A:1895:HIS:HD2	1.61	0.83
14:O:354:ASN:ND2	14:O:369:ASP:OD1	2.11	0.83
3:C:265:PHE:CE2	3:C:295:ILE:HG23	2.12	0.83
13:M:505:A:O4'	13:M:505:A:OP1	1.96	0.83
16:Q:209:ASN:ND2	16:Q:288:ILE:O	2.12	0.83
3:C:265:PHE:HE2	3:C:295:ILE:HG21	1.17	0.83
17:R:146:LEU:HD21	17:R:211:GLU:OE1	1.76	0.83
17:R:22:ILE:HG22	17:R:30:PHE:CZ	2.13	0.83
24:Z:149:ARG:NH1	24:Z:193:SER:HB3	1.94	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:217:TRP:CE2	17:R:187:LYS:HD3	2.14	0.82
10:K:22:GLY:HA3	28:G:935:TRP:CZ3	2.14	0.82
23:Y:526:SER:O	23:Y:535:GLN:CG	2.26	0.82
1:A:997:GLN:NE2	1:A:1511:ARG:HH22	1.77	0.82
6:F:185:ARG:HD3	28:G:946:GLN:OE1	1.80	0.82
1:A:777:LYS:HA	1:A:777:LYS:HZ2	1.44	0.82
15:P:37:ASN:OD1	15:P:143:VAL:CG1	2.27	0.82
12:N:110:U:O2'	17:R:141:GLY:HA2	1.78	0.82
17:R:55:PRO:HB3	17:R:93:ILE:HD11	1.59	0.82
1:A:796:ASN:ND2	1:A:861:GLN:OE1	2.12	0.82
7:H:180:LYS:HA	7:H:180:LYS:CE	2.10	0.82
2:B:508:HIS:ND1	2:B:512:GLU:OE1	2.10	0.82
16:Q:226:LEU:HG	16:Q:227:LEU:HD23	1.59	0.82
1:A:1364:GLU:OE1	1:A:1403:SER:HB3	1.80	0.82
1:A:1742:ASP:H	1:A:1745:SER:HB3	1.45	0.82
1:A:769:MET:HE2	1:A:811:ILE:CD1	2.09	0.82
24:Z:180:ILE:HG22	24:Z:186:LEU:HD21	1.62	0.82
1:A:775:ARG:O	1:A:779:ALA:N	2.12	0.82
5:E:50:G:O2'	5:E:51:A:N7	2.12	0.81
28:G:881:MET:HG2	28:G:885:ILE:HD11	1.62	0.81
3:C:395:LYS:HB2	3:C:395:LYS:NZ	1.95	0.81
16:Q:209:ASN:ND2	16:Q:288:ILE:HG22	1.95	0.81
8:I:55:ASN:HD22	8:I:56:PRO:N	1.78	0.81
22:W:209:LEU:HD12	22:W:209:LEU:O	1.81	0.81
1:A:931:ALA:CA	1:A:934:ARG:HH12	1.92	0.81
2:B:433:LYS:HE2	2:B:914:SER:HA	1.62	0.81
2:B:696:SER:O	2:B:698:PHE:N	2.13	0.81
2:B:773:ASN:ND2	6:F:754:HIS:CE1	2.49	0.81
28:G:835:ILE:O	28:G:837:PHE:N	2.14	0.81
24:Z:192:GLU:N	24:Z:192:GLU:OE1	2.14	0.81
3:C:274:ILE:CG1	3:C:382:TYR:CE1	2.63	0.81
16:Q:256:SER:O	16:Q:259:GLY:N	2.14	0.81
20:U:40:LEU:HG	20:U:49:ALA:HB2	1.63	0.81
23:Y:702:SER:O	23:Y:706:LEU:N	2.14	0.81
16:Q:215:PRO:HG3	16:Q:217:TRP:CZ3	2.16	0.81
22:W:188:LEU:CD2	24:Z:415:GLN:HG2	2.10	0.81
24:Z:459:ARG:O	24:Z:463:ASN:CG	2.18	0.81
1:A:194:HIS:CD2	15:P:122:LEU:HD22	2.16	0.81
1:A:143:ILE:HD12	1:A:570:GLN:HG2	1.62	0.81
15:P:303:TYR:HB3	15:P:307:PHE:HD2	1.45	0.81
1:A:309:SER:OG	1:A:475:ASP:HB3	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:178:ARG:HA	24:Z:198:PHE:CZ	2.15	0.81
13:M:515:U:O2'	28:G:291:GLU:OE2	1.99	0.80
17:R:146:LEU:HD22	17:R:211:GLU:OE1	1.79	0.80
17:R:210:LYS:NZ	17:R:210:LYS:HA	1.96	0.80
3:C:219:VAL:O	3:C:222:MET:HG2	1.80	0.80
28:G:435:THR:HG21	28:G:467:VAL:HG21	1.62	0.80
15:P:41:ASP:O	15:P:44:ILE:HG22	1.81	0.80
24:Z:178:ARG:CB	24:Z:198:PHE:CZ	2.64	0.80
2:B:762:ALA:HA	2:B:766:ILE:HD11	1.64	0.80
8:I:57:TYR:CE1	8:I:70:LEU:HD11	2.15	0.80
15:P:241:LEU:O	15:P:245:SER:CB	2.30	0.80
16:Q:207:LEU:HB2	16:Q:249:GLY:O	1.81	0.80
1:A:342:LEU:HD13	1:A:392:ASN:ND2	1.95	0.80
16:Q:222:THR:HA	16:Q:225:GLN:NE2	1.96	0.80
2:B:2102:VAL:HB	2:B:2143:TRP:HB2	1.62	0.80
6:F:886:PHE:HE2	6:F:1225:VAL:HG21	1.46	0.80
16:Q:209:ASN:O	16:Q:209:ASN:ND2	2.15	0.80
16:Q:217:TRP:CH2	17:R:187:LYS:CD	2.64	0.80
1:A:1846:ASN:O	1:A:1847:ASP:O	1.99	0.80
16:Q:214:ILE:HD11	16:Q:218:LYS:HG2	1.62	0.79
6:F:590:HIS:HE1	6:F:637:SER:HB3	1.47	0.79
28:G:338:GLN:HG3	28:G:377:THR:HG22	1.63	0.79
1:A:1668:ILE:HD13	1:A:1801:SER:HB2	1.62	0.79
1:A:253:GLN:O	1:A:257:ASN:ND2	2.15	0.79
6:F:441:PHE:HB3	6:F:475:LEU:HD23	1.63	0.79
22:W:189:THR:HG22	22:W:195:ILE:HD11	1.63	0.79
1:A:777:LYS:HA	1:A:777:LYS:NZ	1.96	0.79
6:F:1125:ASP:HB3	6:F:1128:THR:HG22	1.64	0.79
16:Q:69:ASN:HB2	16:Q:123:ALA:HB1	1.63	0.79
24:Z:152:ILE:CD1	24:Z:194:LEU:HA	2.12	0.79
1:A:2018:ASN:CG	1:A:2021:SER:HG	1.86	0.79
1:A:238:ARG:HH11	1:A:238:ARG:CB	1.96	0.79
19:T:121:ILE:HD11	19:T:129:LEU:HD21	1.65	0.79
20:U:52:HIS:HE1	20:U:103:CYS:SG	2.06	0.79
24:Z:180:ILE:O	24:Z:184:GLN:HB2	1.82	0.79
6:F:364:THR:OG1	6:F:384:ASN:ND2	2.14	0.79
24:Z:460:TYR:HA	24:Z:463:ASN:HD22	1.47	0.79
1:A:147:SER:OG	1:A:573:ARG:NH2	2.15	0.79
8:I:53:ARG:NH2	8:I:58:ILE:O	2.16	0.79
3:C:265:PHE:CD2	3:C:295:ILE:HG21	2.17	0.78
5:E:42:A:N1	17:R:38:SER:O	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:226:LEU:HD21	16:Q:262:PHE:CE1	2.19	0.78
17:R:7:LYS:O	17:R:61:LYS:N	2.14	0.78
20:U:36:GLY:O	20:U:40:LEU:HB2	1.83	0.78
17:R:46:ARG:NH2	17:R:220:GLY:O	2.15	0.78
1:A:1041:VAL:HG11	1:A:1253:LYS:HA	1.66	0.78
13:M:500:A:H5'	13:M:500:A:C8	2.19	0.78
24:Z:152:ILE:HD13	24:Z:194:LEU:HA	1.64	0.78
28:G:904:GLU:CD	28:G:940:ASN:HB3	2.03	0.78
15:P:318:ARG:HA	22:W:261:THR:HG22	1.65	0.78
1:A:1034:ASN:ND2	28:G:20:GLY:HA2	1.98	0.78
1:A:525:LEU:HD12	1:A:686:ILE:CD1	2.14	0.78
16:Q:209:ASN:HD22	16:Q:288:ILE:HG22	1.48	0.78
24:Z:178:ARG:HG3	24:Z:198:PHE:CZ	2.17	0.78
17:R:15:GLU:O	17:R:18:LEU:HD12	1.84	0.77
20:U:51:LYS:HG3	20:U:52:HIS:N	1.99	0.77
1:A:1057:MET:HE2	1:A:1114:PHE:CE1	2.19	0.77
1:A:1485:ASP:O	1:A:1490:ARG:NH2	2.17	0.77
6:F:676:PRO:HB3	6:F:693:ILE:HD11	1.66	0.77
13:M:514:U:H4'	13:M:515:U:C5'	2.13	0.77
24:Z:197:LEU:HD12	24:Z:197:LEU:O	1.84	0.77
10:K:44:GLN:NE2	10:K:70:LEU:HD21	1.98	0.77
16:Q:91:ILE:CG2	16:Q:125:ILE:CD1	2.61	0.77
4:D:41:A:N6	4:D:78:A:H2'	2.00	0.77
13:M:500:A:H8	13:M:500:A:H5'	1.48	0.77
17:R:207:PRO:O	17:R:212:TRP:CE2	2.37	0.77
23:Y:299:GLY:HA3	23:Y:311:LYS:HE3	1.67	0.77
3:C:105:ILE:O	3:C:180:ASN:ND2	2.18	0.77
24:Z:170:HIS:NE2	24:Z:174:TRP:CZ3	2.51	0.77
1:A:614:ARG:NH1	12:N:98:A:H5"	2.00	0.77
24:Z:192:GLU:C	24:Z:195:GLU:OE2	2.22	0.77
2:B:656:TRP:HE1	2:B:928:ASN:HB3	1.46	0.77
1:A:1073:ILE:HG23	1:A:1074:VAL:HG23	1.66	0.77
1:A:525:LEU:HD12	1:A:686:ILE:HD11	1.65	0.77
3:C:607:LEU:HD22	3:C:668:ILE:HD12	1.67	0.77
28:G:464:CYS:O	28:G:470:ILE:HD11	1.84	0.77
6:F:719:GLN:HG2	6:F:762:PHE:HD2	1.50	0.77
7:H:176:TRP:O	7:H:177:GLN:HG2	1.83	0.77
11:L:19:U:O2	15:P:175:PRO:HD2	1.84	0.77
2:B:1820:ILE:HG22	2:B:1846:THR:HG22	1.66	0.77
17:R:3:SER:O	17:R:7:LYS:CD	2.33	0.76
18:S:9:LEU:HD23	18:S:11:ALA:N	1.99	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1561:LEU:CD1	1:A:1608:LEU:HD22	2.16	0.76
28:G:539:HIS:O	28:G:543:ARG:HG3	1.85	0.76
10:K:42:THR:HG21	28:G:950:VAL:HG21	1.67	0.76
17:R:145:ALA:HB2	17:R:204:LEU:HD12	1.65	0.76
6:F:324:ASN:OD1	6:F:341:ASN:ND2	2.19	0.76
1:A:742:VAL:CG1	14:O:224:LEU:HD23	2.16	0.76
23:Y:258:GLN:HE21	23:Y:290:VAL:HG13	1.48	0.76
24:Z:168:LYS:NZ	24:Z:171:ASP:HB2	1.99	0.76
1:A:1403:SER:OG	1:A:1429:MET:SD	2.43	0.76
2:B:1674:ALA:HB3	2:B:1709:LEU:HD13	1.67	0.76
28:G:632:LYS:HD2	28:G:672:VAL:HG13	1.65	0.76
1:A:1093:LYS:NZ	11:L:27:A:OP1	2.19	0.76
28:G:778:ARG:NH1	28:G:811:ASN:OD1	2.18	0.76
17:R:206:LEU:HG	17:R:207:PRO:CD	2.16	0.76
17:R:8:SER:HA	17:R:61:LYS:O	1.85	0.76
24:Z:181:LEU:HG	24:Z:194:LEU:CD1	2.14	0.76
24:Z:192:GLU:CB	24:Z:195:GLU:OE2	2.33	0.76
18:S:9:LEU:CD2	18:S:11:ALA:HB3	2.14	0.76
20:U:52:HIS:CE1	20:U:103:CYS:SG	2.79	0.76
7:H:180:LYS:HA	7:H:180:LYS:HE3	1.67	0.75
9:J:7:ASP:OD1	9:J:8:LEU:HD23	1.86	0.75
16:Q:217:TRP:CZ3	17:R:187:LYS:HD3	2.20	0.75
22:W:215:TYR:CE2	22:W:232:TRP:HE3	2.04	0.75
24:Z:178:ARG:CG	24:Z:198:PHE:CE2	2.67	0.75
6:F:236:VAL:HG13	6:F:257:ILE:HG23	1.65	0.75
10:K:32:GLN:NE2	28:G:960:ASN:HB3	2.02	0.75
16:Q:202:THR:HA	16:Q:252:ARG:HG3	1.68	0.75
22:W:214:LEU:HD21	22:W:227:MET:CB	2.16	0.75
1:A:1325:SER:O	1:A:1331:VAL:HG21	1.86	0.75
1:A:216:GLN:O	1:A:220:THR:HG23	1.86	0.75
1:A:782:ILE:O	1:A:782:ILE:HD12	1.87	0.75
1:A:525:LEU:CD1	1:A:686:ILE:HD12	2.17	0.75
6:F:703:MET:HE3	6:F:713:LEU:HB2	1.69	0.75
23:Y:626:LEU:HD11	23:Y:650:GLU:CB	2.17	0.75
2:B:2022:LEU:HB2	2:B:2027:ARG:HE	1.52	0.75
6:F:611:VAL:HG21	6:F:621:LYS:HE2	1.67	0.75
1:A:1335:TRP:CH2	1:A:1364:GLU:HG3	2.21	0.75
2:B:1370:SER:HB3	2:B:1376:LYS:HD3	1.68	0.75
1:A:2408:GLN:HE21	1:A:2408:GLN:HA	1.52	0.74
5:E:67:C:H6	5:E:67:C:H5"	1.51	0.74
6:F:886:PHE:CE2	6:F:1225:VAL:HG21	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:183:LEU:HD22	7:H:188:LEU:HD11	1.68	0.74
16:Q:215:PRO:HG3	16:Q:217:TRP:CH2	2.21	0.74
1:A:1835:LEU:HD11	1:A:1836:ASN:ND2	2.02	0.74
2:B:766:ILE:HG22	2:B:767:THR:H	1.50	0.74
21:V:63:SER:HB3	21:V:74:PHE:CD1	2.22	0.74
22:W:215:TYR:CE2	22:W:232:TRP:CE3	2.75	0.74
1:A:143:ILE:HD12	1:A:570:GLN:CG	2.17	0.74
3:C:219:VAL:HG21	3:C:929:GLN:HB3	1.68	0.74
6:F:641:GLN:HE21	6:F:653:TYR:HE1	1.35	0.74
24:Z:310:HIS:CD2	30:X:23:SER:HA	2.22	0.74
6:F:957:ILE:HG22	6:F:962:LEU:HD11	1.69	0.74
1:A:1034:ASN:HD22	28:G:20:GLY:H	1.34	0.74
2:B:901:VAL:HG22	2:B:906:LEU:HD22	1.68	0.74
1:A:936:GLU:HG2	1:A:986:PRO:HB3	1.69	0.74
17:R:22:ILE:HG22	17:R:30:PHE:CE2	2.22	0.74
24:Z:178:ARG:CA	24:Z:198:PHE:HZ	1.99	0.74
1:A:431:ILE:HG23	24:Z:182:GLN:HG2	1.70	0.74
17:R:87:CYS:HB3	17:R:91:HIS:HE1	1.53	0.74
1:A:1034:ASN:HD22	28:G:20:GLY:N	1.84	0.74
1:A:1286:TRP:NE1	1:A:1348:GLU:OE1	2.21	0.74
6:F:161:GLN:HG2	6:F:163:ILE:HG22	1.70	0.74
22:W:188:LEU:HG	24:Z:378:THR:HG22	1.70	0.74
1:A:2287:ASP:O	1:A:2288:CYS:O	2.05	0.73
23:Y:247:GLU:OE1	23:Y:402:ARG:CG	2.36	0.73
17:R:14:LYS:HE3	17:R:14:LYS:N	2.03	0.73
2:B:636:ILE:HG22	2:B:671:SER:HB2	1.68	0.73
3:C:177:TYR:CE1	3:C:548:ARG:CD	2.71	0.73
1:A:930:ASN:O	1:A:934:ARG:NH1	2.22	0.73
2:B:1387:HIS:NE2	2:B:1393:GLY:O	2.20	0.73
6:F:78:HIS:NE2	6:F:81:ASP:OD1	2.21	0.73
1:A:1836:ASN:ND2	1:A:2006:SER:HG	1.86	0.73
15:P:241:LEU:O	15:P:245:SER:HB2	1.88	0.73
1:A:268:LEU:HD23	1:A:268:LEU:O	1.88	0.73
7:H:198:ASP:OD1	7:H:199:ILE:N	2.21	0.73
20:U:25:TYR:HB3	21:V:117:LYS:HG2	1.71	0.73
21:V:63:SER:CB	21:V:74:PHE:HE1	1.82	0.73
22:W:190:ILE:C	22:W:192:ASP:H	1.92	0.73
13:M:513:U:OP2	28:G:259:ARG:NH1	2.21	0.73
6:F:276:GLY:O	28:G:388:TYR:O	2.07	0.73
1:A:1163:ARG:HH11	1:A:1163:ARG:HG2	1.53	0.73
24:Z:174:TRP:CH2	24:Z:197:LEU:HD11	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:ASP:HB2	6:F:114:ILE:HD11	1.71	0.72
6:F:547:ASN:HA	6:F:563:ILE:O	1.90	0.72
1:A:1034:ASN:HD22	28:G:20:GLY:CA	2.02	0.72
2:B:514:ASP:OD1	2:B:537:LYS:NZ	2.20	0.72
6:F:1124:LEU:HB2	6:F:1130:ILE:HD11	1.69	0.72
6:F:1222:GLN:NE2	10:K:48:ALA:CA	2.51	0.72
16:Q:101:THR:CG2	16:Q:120:LEU:CD2	2.65	0.72
16:Q:207:LEU:O	16:Q:248:CYS:HA	1.89	0.72
6:F:379:VAL:HG22	6:F:391:LEU:HB2	1.70	0.72
1:A:854:ARG:NE	11:L:25:A:OP1	2.22	0.72
1:A:2408:GLN:CA	1:A:2408:GLN:HE21	2.03	0.72
12:N:111:U:H4'	12:N:112:U:OP2	1.89	0.72
1:A:1305:SER:OG	1:A:1307:GLU:OE1	2.06	0.72
3:C:348:LEU:HD12	3:C:372:THR:HG22	1.71	0.72
28:G:222:ILE:HG23	28:G:265:ILE:HD11	1.71	0.72
2:B:1236:LEU:HD11	2:B:1258:PHE:HB3	1.71	0.72
6:F:396:ASP:HB2	6:F:404:LEU:HG	1.71	0.72
6:F:961:CYS:O	6:F:962:LEU:HD12	1.89	0.72
6:F:186:ARG:NH2	10:K:38:ASP:OD1	2.22	0.72
14:O:210:ASP:HB2	14:O:217:ILE:HG13	1.69	0.72
1:A:1509:ARG:HH12	1:A:1533:ASP:CG	1.93	0.72
6:F:335:ILE:HD12	6:F:407:LEU:HD11	1.72	0.72
15:P:241:LEU:O	15:P:245:SER:N	2.21	0.72
24:Z:186:LEU:N	24:Z:186:LEU:HD12	2.05	0.72
24:Z:454:ASP:HB3	24:Z:457:HIS:HD2	1.53	0.72
28:G:587:THR:HB	28:G:630:VAL:HG21	1.70	0.72
23:Y:467:LYS:CB	23:Y:494:CYS:HA	2.19	0.72
1:A:269:ASP:OD1	1:A:271:GLN:N	2.22	0.71
2:B:699:ARG:NH1	2:B:701:CYS:O	2.22	0.71
2:B:1620:TYR:HD1	2:B:1651:ILE:HG23	1.55	0.71
1:A:1122:ASP:OD1	1:A:1161:TYR:CE2	2.43	0.71
1:A:238:ARG:HH11	1:A:238:ARG:HB3	1.56	0.71
14:O:259:VAL:HG12	14:O:260:ILE:HG13	1.72	0.71
17:R:23:PRO:O	17:R:37:TRP:NE1	2.23	0.71
24:Z:178:ARG:CA	24:Z:198:PHE:CZ	2.73	0.71
1:A:377:VAL:HG12	1:A:378:PRO:HD2	1.73	0.71
6:F:1222:GLN:HE22	10:K:48:ALA:HB2	1.55	0.71
6:F:180:THR:HG21	6:F:188:SER:HB2	1.72	0.71
1:A:570:GLN:O	1:A:574:GLN:HG2	1.89	0.71
3:C:265:PHE:CD2	3:C:295:ILE:HD13	2.26	0.71
6:F:104:TYR:OH	6:F:481:GLN:NE2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:63:SER:CB	21:V:74:PHE:CD1	2.70	0.71
23:Y:699:GLU:CG	23:Y:702:SER:CB	2.69	0.71
1:A:2018:ASN:CG	1:A:2021:SER:OG	2.29	0.71
1:A:2052:GLU:O	1:A:2056:ARG:HB2	1.91	0.71
1:A:324:ASP:OD1	1:A:324:ASP:N	2.23	0.71
24:Z:181:LEU:HD21	24:Z:191:ARG:HG3	1.71	0.71
16:Q:221:ASP:C	16:Q:225:GLN:HE21	1.93	0.71
4:D:174:G:OP1	4:D:174:G:H4'	1.90	0.71
6:F:927:ARG:HG3	6:F:928:THR:HG23	1.72	0.71
6:F:932:PHE:HA	6:F:984:ILE:HD11	1.73	0.71
7:H:199:ILE:HG22	7:H:250:VAL:HG13	1.72	0.71
2:B:1583:VAL:HG22	2:B:1681:ILE:HB	1.72	0.71
17:R:210:LYS:HZ3	17:R:210:LYS:HA	1.52	0.71
21:V:48:LEU:O	22:W:231:ARG:CZ	2.39	0.71
23:Y:307:ARG:HE	23:Y:646:PRO:HB2	1.56	0.71
24:Z:170:HIS:CE1	24:Z:174:TRP:HE3	2.08	0.71
7:H:192:ARG:HB3	7:H:192:ARG:CZ	2.19	0.70
1:A:168:LEU:HB3	1:A:622:MET:HE2	1.71	0.70
1:A:790:TRP:HE1	1:A:794:LYS:HE3	1.56	0.70
3:C:232:SER:OG	3:C:234:LEU:O	2.09	0.70
16:Q:259:GLY:O	16:Q:263:VAL:HG23	1.90	0.70
22:W:170:LEU:O	22:W:172:ILE:HG12	1.90	0.70
16:Q:69:ASN:CB	16:Q:123:ALA:HB1	2.20	0.70
1:A:1405:ILE:HG22	1:A:1406:LEU:H	1.56	0.70
1:A:183:TRP:CZ2	1:A:216:GLN:OE1	2.45	0.70
19:T:120:CYS:CB	19:T:122:CYS:HB3	2.21	0.70
20:U:35:SER:OG	21:V:46:ASP:OD2	2.08	0.70
2:B:1605:ILE:HG22	2:B:1606:GLU:H	1.57	0.70
28:G:851:LEU:HD21	28:G:895:ALA:HB2	1.73	0.70
7:H:288:HIS:C	7:H:289:LYS:HG3	2.10	0.70
1:A:774:ILE:HG13	1:A:778:LYS:HD2	1.72	0.70
3:C:133:ILE:HG22	3:C:209:MET:HB3	1.73	0.70
3:C:602:VAL:HG21	3:C:932:PHE:CE2	2.27	0.70
6:F:427:LEU:N	6:F:439:PHE:O	2.22	0.70
23:Y:220:ARG:O	23:Y:226:HIS:NE2	2.25	0.70
24:Z:191:ARG:NH1	24:Z:192:GLU:OE2	2.24	0.70
1:A:518:VAL:HG11	1:A:689:TYR:HD2	1.56	0.70
16:Q:226:LEU:CD2	16:Q:262:PHE:CE1	2.75	0.70
1:A:1846:ASN:O	1:A:1847:ASP:C	2.30	0.70
20:U:40:LEU:O	20:U:43:ASN:O	2.09	0.70
1:A:1362:LYS:NZ	30:X:13:GLY:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:550:THR:HG23	28:G:553:LEU:CD2	2.22	0.70
9:J:102:GLU:OE1	9:J:103:LYS:N	2.25	0.70
1:A:1130:ARG:HD3	1:A:1156:HIS:CD2	2.27	0.70
5:E:67:C:C2	5:E:82:A:C2	2.80	0.70
24:Z:310:HIS:HD2	30:X:23:SER:HA	1.54	0.70
1:A:1054:LEU:HD21	1:A:1168:ILE:HD11	1.72	0.69
1:A:1337:THR:HG21	15:P:321:ASP:HB3	1.73	0.69
2:B:673:THR:OG1	2:B:904:GLN:NE2	2.24	0.69
3:C:152:LEU:HD13	3:C:432:GLN:HE22	1.56	0.69
6:F:1170:VAL:HG12	6:F:1184:LYS:HD2	1.72	0.69
10:K:44:GLN:HE21	10:K:70:LEU:HD21	1.57	0.69
11:L:19:U:O4'	11:L:19:U:OP2	2.09	0.69
17:R:207:PRO:O	17:R:212:TRP:CD2	2.43	0.69
2:B:882:THR:HG23	6:F:686:GLN:HE22	1.57	0.69
4:D:173:U:H4'	4:D:174:G:OP1	1.91	0.69
23:Y:280:ARG:NH2	23:Y:476:ALA:O	2.23	0.69
1:A:237:MET:HE1	1:A:635:THR:HG22	1.73	0.69
3:C:780:PRO:HA	3:C:783:ILE:HB	1.74	0.69
7:H:141:VAL:CG1	7:H:165:CYS:SG	2.80	0.69
15:P:319:HIS:HE1	22:W:264:GLU:CD	1.96	0.69
6:F:384:ASN:O	6:F:415:ASN:ND2	2.18	0.69
20:U:50:LEU:CA	20:U:139:GLN:HE22	2.03	0.69
2:B:1362:SER:O	2:B:1507:ARG:NH1	2.25	0.69
3:C:602:VAL:HG21	3:C:932:PHE:CD2	2.28	0.69
6:F:1073:LYS:HD2	6:F:1090:ILE:HD11	1.74	0.69
7:H:186:ARG:NH2	8:I:70:LEU:O	2.25	0.69
24:Z:174:TRP:CZ2	24:Z:197:LEU:CD1	2.75	0.69
24:Z:178:ARG:CG	24:Z:198:PHE:HZ	2.01	0.69
3:C:132:ARG:HH11	3:C:132:ARG:HG3	1.57	0.69
28:G:386:TYR:CG	28:G:387:PRO:HD3	2.27	0.69
7:H:180:LYS:HD3	7:H:184:SER:OG	1.92	0.69
20:U:43:ASN:O	20:U:44:ASN:ND2	2.20	0.69
23:Y:553:ALA:HB1	23:Y:559:GLY:HA3	1.75	0.69
2:B:1473:TYR:O	2:B:1511:LEU:N	2.25	0.69
7:H:167:LYS:HD2	7:H:167:LYS:O	1.93	0.69
11:L:41:C:C5'	11:L:41:C:H6	2.05	0.69
14:O:263:VAL:HG13	18:S:11:ALA:HB2	1.74	0.69
15:P:301:LEU:HD11	15:P:303:TYR:CE1	2.27	0.69
17:R:14:LYS:CA	17:R:14:LYS:HE3	2.23	0.69
10:K:3:GLU:OE2	10:K:7:GLN:OE1	2.10	0.69
16:Q:209:ASN:ND2	16:Q:288:ILE:CG2	2.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:142:ILE:HG21	17:R:180:ASN:ND2	2.07	0.69
22:W:171:GLY:C	22:W:172:ILE:HG12	2.13	0.69
1:A:1057:MET:HG3	1:A:1239:THR:HG21	1.74	0.69
1:A:1843:LEU:N	1:A:1843:LEU:HD23	2.08	0.69
2:B:667:ILE:HG21	2:B:684:LEU:HD22	1.74	0.69
16:Q:34:CYS:SG	16:Q:61:CYS:N	2.65	0.69
18:S:9:LEU:HD21	18:S:11:ALA:CB	2.20	0.69
1:A:1281:ASN:HD21	1:A:1285:VAL:HB	1.57	0.69
2:B:585:VAL:HG12	2:B:604:VAL:HB	1.74	0.69
6:F:97:THR:OG1	6:F:97:THR:O	2.07	0.69
1:A:396:ARG:HG3	1:A:396:ARG:HH11	1.57	0.68
1:A:893:ARG:HG3	1:A:893:ARG:NH1	2.03	0.68
2:B:1681:ILE:HG12	2:B:1721:LEU:HB3	1.75	0.68
2:B:552:LEU:HB3	2:B:603:GLN:HE21	1.56	0.68
3:C:236:LEU:HD21	3:C:435:LEU:HD11	1.75	0.68
14:O:433:THR:OG1	14:O:435:GLU:OE1	2.10	0.68
2:B:1689:ASP:HB2	2:B:1696:MET:HG2	1.76	0.68
3:C:219:VAL:CG1	3:C:931:TYR:HB3	2.22	0.68
9:J:51:PHE:HD2	9:J:52:GLY:H	1.40	0.68
6:F:187:VAL:HG21	10:K:17:LYS:O	1.93	0.68
23:Y:626:LEU:HD11	23:Y:650:GLU:CA	2.24	0.68
1:A:1015:PRO:HG2	1:A:1510:ILE:HG12	1.76	0.68
2:B:1551:PHE:HE2	2:B:1563:MET:HA	1.57	0.68
28:G:61:GLU:OE2	28:G:68:ARG:NH2	2.21	0.68
24:Z:177:LEU:HD21	24:Z:194:LEU:HD21	1.75	0.68
1:A:1053:THR:HG22	1:A:1167:ARG:HD2	1.75	0.68
6:F:1222:GLN:NE2	10:K:48:ALA:HA	2.09	0.68
1:A:1935:VAL:HG11	1:A:1940:MET:HB2	1.75	0.68
28:G:22:GLN:HA	28:G:22:GLN:OE1	1.92	0.68
28:G:348:VAL:HG13	28:G:349:LEU:H	1.58	0.68
1:A:1056:GLU:OE2	1:A:1059:GLU:OE1	2.12	0.68
2:B:990:ASP:OD2	2:B:993:ASN:ND2	2.26	0.68
3:C:412:ALA:HA	3:C:415:TYR:CE2	2.29	0.68
16:Q:69:ASN:ND2	16:Q:126:THR:HB	2.08	0.68
16:Q:34:CYS:HB3	16:Q:36:ILE:H	1.58	0.68
1:A:1561:LEU:HD11	1:A:1608:LEU:HD22	1.74	0.68
3:C:100:LEU:HD21	3:C:479:GLY:C	2.14	0.68
6:F:1096:LEU:HD13	6:F:1187:PHE:HZ	1.58	0.68
6:F:600:ILE:HD13	6:F:642:LEU:HD13	1.75	0.68
7:H:185:GLY:HA3	8:I:72:ASN:HD21	1.59	0.68
1:A:1286:TRP:CD1	1:A:1448:GLU:HG3	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:ASN:CB	1:A:1744:ASP:OD2	2.30	0.68
1:A:763:MET:HE2	1:A:779:ALA:HB1	1.76	0.68
28:G:464:CYS:O	28:G:470:ILE:CD1	2.41	0.68
16:Q:210:ILE:HG22	16:Q:211:ASP:O	1.93	0.68
20:U:38:LEU:HD23	21:V:49:THR:HG21	1.75	0.68
24:Z:190:LEU:HD23	24:Z:191:ARG:N	2.09	0.68
1:A:1829:SER:O	1:A:1830:VAL:HG22	1.94	0.68
2:B:1822:ILE:HG12	2:B:1844:ILE:HG12	1.75	0.68
6:F:363:VAL:O	6:F:364:THR:HG23	1.94	0.68
14:O:217:ILE:HG22	14:O:218:ARG:HG3	1.75	0.68
1:A:2262:GLN:HG2	1:A:2264:GLU:H	1.60	0.67
1:A:518:VAL:HG12	1:A:685:HIS:HB3	1.76	0.67
2:B:1638:GLY:HA3	2:B:1664:LEU:HD12	1.75	0.67
9:J:41:ARG:NH1	9:J:82:ASP:OD2	2.26	0.67
15:P:84:ASN:O	15:P:125:ARG:NH1	2.27	0.67
5:E:28:U:H1'	16:Q:51:ARG:NH2	2.10	0.67
1:A:237:MET:CE	1:A:635:THR:HG22	2.24	0.67
5:E:85:C:O4'	5:E:85:C:OP1	2.12	0.67
6:F:783:ILE:HG13	6:F:784:SER:H	1.58	0.67
7:H:188:LEU:HD13	28:G:849:ARG:HB2	1.74	0.67
1:A:1861:THR:HG1	1:A:1863:HIS:HE2	1.40	0.67
8:I:53:ARG:HH11	8:I:53:ARG:HB3	1.58	0.67
16:Q:79:ARG:HD2	16:Q:126:THR:HG23	1.73	0.67
2:B:1057:LEU:HD21	2:B:1089:PHE:HE1	1.59	0.67
6:F:594:MET:O	6:F:598:SER:OG	2.13	0.67
6:F:884:ASN:OD1	6:F:885:TRP:N	2.26	0.67
12:N:114:U:OP1	17:R:174:ARG:NH2	2.27	0.67
1:A:769:MET:CE	1:A:811:ILE:HD12	2.05	0.67
3:C:343:ASP:O	3:C:347:ARG:HG2	1.93	0.67
24:Z:364:THR:O	24:Z:368:ASN:ND2	2.26	0.67
1:A:1034:ASN:HD22	28:G:20:GLY:HA2	1.59	0.67
1:A:1843:LEU:HA	1:A:1849:LYS:NZ	2.10	0.67
6:F:1116:ARG:NH2	6:F:1141:LEU:HD21	2.10	0.67
14:O:230:VAL:HG22	14:O:241:THR:HG22	1.75	0.67
16:Q:69:ASN:HD21	16:Q:126:THR:HG21	1.59	0.67
17:R:172:ARG:HH22	17:R:237:ARG:NH1	1.92	0.67
1:A:1335:TRP:CZ2	1:A:1364:GLU:HG3	2.30	0.67
2:B:1455:LEU:O	2:B:1462:ARG:NH1	2.28	0.67
2:B:487:CYS:HB2	2:B:536:LEU:HD13	1.76	0.67
20:U:108:ARG:NH1	20:U:136:SER:O	2.28	0.67
2:B:1141:PRO:O	2:B:1299:HIS:NE2	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:752:ARG:HD3	3:C:759:SER:HA	1.76	0.67
1:A:1322:ALA:O	1:A:1323:SER:CB	2.41	0.67
3:C:100:LEU:HD21	3:C:480:GLY:N	2.10	0.67
6:F:639:LYS:HB3	6:F:686:GLN:HA	1.77	0.67
7:H:185:GLY:O	7:H:188:LEU:N	2.28	0.67
23:Y:626:LEU:CD1	23:Y:650:GLU:CA	2.72	0.67
1:A:525:LEU:CD1	1:A:686:ILE:CD1	2.73	0.67
3:C:100:LEU:HD13	3:C:108:GLN:OE1	1.95	0.67
3:C:135:ASN:ND2	3:C:559:GLY:O	2.26	0.67
11:L:57:A:OP1	28:G:928:LYS:HB3	1.95	0.67
16:Q:214:ILE:CD1	16:Q:218:LYS:HG2	2.25	0.67
6:F:180:THR:O	9:J:83:LYS:HD2	1.94	0.66
3:C:79:GLU:HG3	15:P:202:MET:SD	48.51	0.66
1:A:1197:ASN:ND2	1:A:1221:ASN:OD1	2.27	0.66
1:A:763:MET:CE	1:A:779:ALA:HB1	2.26	0.66
3:C:251:GLN:HE21	3:C:255:GLN:HE21	1.43	0.66
19:T:133:ALA:O	19:T:137:GLY:N	2.29	0.66
24:Z:178:ARG:HB2	24:Z:198:PHE:HZ	1.60	0.66
2:B:1466:GLN:HB2	2:B:1502:LEU:HD11	1.76	0.66
3:C:365:GLU:HG3	3:C:366:ASN:H	1.60	0.66
17:R:54:GLN:H	17:R:58:HIS:HD2	1.40	0.66
17:R:9:ALA:HB1	17:R:58:HIS:O	1.96	0.66
1:A:978:ILE:CG2	18:S:174:VAL:HA	2.26	0.66
20:U:83:TYR:HB3	20:U:88:LYS:HG2	1.77	0.66
1:A:854:ARG:HH21	1:A:854:ARG:CG	2.09	0.66
13:M:506:U:OP2	28:G:698:ARG:HD3	1.94	0.66
16:Q:101:THR:CB	16:Q:120:LEU:HD11	2.22	0.66
6:F:387:ASP:HA	6:F:412:THR:HG22	1.76	0.66
28:G:359:ILE:HG21	28:G:378:LEU:HD21	1.78	0.66
16:Q:226:LEU:C	16:Q:226:LEU:HD12	2.15	0.66
1:A:1050:LEU:HD23	1:A:1248:VAL:HG22	1.77	0.66
21:V:57:PRO:HG2	22:W:231:ARG:HH21	1.61	0.66
3:C:803:VAL:HG13	3:C:813:ILE:HB	1.76	0.66
4:D:60:U:O2	4:D:60:U:H3'	1.95	0.66
14:O:134:VAL:HG22	14:O:424:LYS:HG2	1.78	0.66
16:Q:226:LEU:HD21	16:Q:262:PHE:HD1	1.57	0.66
17:R:146:LEU:HD23	17:R:147:ASN:N	2.10	0.66
17:R:210:LYS:CE	17:R:210:LYS:HA	2.25	0.66
2:B:1541:ILE:HG13	2:B:1542:GLU:HG3	1.78	0.66
6:F:184:LEU:O	28:G:947:ASP:OD2	2.13	0.66
6:F:71:PHE:HE2	6:F:481:GLN:HE22	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:319:HIS:CD2	15:P:320:GLU:H	2.13	0.66
23:Y:251:GLY:HA2	47:Y:902:ADP:H5'2	1.78	0.66
1:A:1172:PHE:HZ	1:A:1230:ILE:HD11	1.60	0.66
1:A:1365:THR:O	1:A:1369:ASN:ND2	2.29	0.66
2:B:2050:ASN:ND2	2:B:2078:ASP:OD1	2.29	0.66
5:E:67:C:C5'	5:E:67:C:H6	2.07	0.66
24:Z:168:LYS:HZ3	24:Z:171:ASP:HB2	1.61	0.66
1:A:1067:ASN:O	1:A:1071:ARG:HG2	1.96	0.65
1:A:978:ILE:HG22	18:S:173:HIS:O	1.97	0.65
2:B:988:LEU:HB2	2:B:997:GLU:HB3	1.78	0.65
3:C:274:ILE:HD13	3:C:385:PHE:HE2	1.60	0.65
6:F:161:GLN:O	6:F:163:ILE:HG23	1.96	0.65
6:F:165:HIS:HB3	6:F:170:ARG:HD3	1.78	0.65
6:F:943:ASP:HB2	6:F:952:ARG:HG2	1.76	0.65
16:Q:69:ASN:HD21	16:Q:126:THR:CG2	2.08	0.65
1:A:769:MET:HE2	1:A:811:ILE:HD11	1.69	0.65
3:C:465:GLU:CD	3:C:466:GLY:H	1.99	0.65
6:F:290:PRO:HB2	10:K:80:TYR:CE1	2.31	0.65
20:U:43:ASN:C	20:U:44:ASN:HD22	1.99	0.65
23:Y:438:ILE:HA	23:Y:515:TYR:HB2	1.78	0.65
1:A:299:LYS:HA	1:A:493:MET:CG	2.26	0.65
3:C:500:ARG:NH1	3:C:534:THR:OG1	2.29	0.65
6:F:446:VAL:HG21	6:F:453:ASN:HD21	1.61	0.65
8:I:62:HIS:NE2	28:G:848:ASP:OD1	2.28	0.65
1:A:859:ASN:ND2	18:S:170:LEU:HD12	2.11	0.65
6:F:154:SER:HA	6:F:182:THR:HG22	1.76	0.65
6:F:75:CYS:HB2	6:F:129:SER:OG	1.96	0.65
19:T:27:GLU:OE2	19:T:31:ARG:NE	2.30	0.65
1:A:1053:THR:HG22	1:A:1167:ARG:CD	2.26	0.65
1:A:228:LYS:HG2	1:A:695:LEU:HD13	1.79	0.65
1:A:831:ARG:HD3	1:A:848:ASN:HD21	1.60	0.65
6:F:590:HIS:CE1	6:F:637:SER:HB3	2.32	0.65
28:G:288:ASN:OD1	28:G:289:GLU:N	2.30	0.65
1:A:745:THR:HG21	14:O:203:ASP:HB2	1.77	0.65
6:F:411:ASP:OD2	6:F:472:LEU:HG	1.95	0.65
16:Q:70:ILE:HG21	16:Q:84:ILE:HD11	1.79	0.65
23:Y:349:HIS:CE1	23:Y:379:ALA:H	2.13	0.65
23:Y:570:TYR:HA	23:Y:574:LEU:HD12	1.77	0.65
2:B:1609:MET:HB3	2:B:1611:ASN:H	1.62	0.65
1:A:777:LYS:HA	1:A:777:LYS:HE3	1.78	0.65
6:F:626:PRO:HB3	6:F:630:ILE:HB	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:57:TYR:O	8:I:59:TYR:CD1	2.50	0.65
15:P:325:ASP:N	15:P:325:ASP:OD1	2.23	0.65
21:V:72:GLN:HA	21:V:72:GLN:OE1	1.97	0.65
24:Z:149:ARG:NH1	24:Z:193:SER:CB	2.60	0.65
24:Z:190:LEU:HD23	24:Z:190:LEU:C	2.18	0.65
1:A:2255:LEU:O	1:A:2285:LYS:NZ	2.30	0.65
6:F:1112:ASP:OD1	6:F:1113:SER:N	2.30	0.65
28:G:334:ILE:HD11	28:G:362:CYS:HB3	1.79	0.65
17:R:172:ARG:HH22	17:R:237:ARG:HH11	1.45	0.65
1:A:2412:PHE:HD1	1:A:2413:SER:N	1.95	0.65
5:E:15:C:H2'	5:E:16:C:C6	2.31	0.65
7:H:141:VAL:HG13	7:H:165:CYS:SG	2.37	0.65
3:C:218:HIS:HB3	3:C:221:PHE:HD2	1.61	0.64
19:T:150:CYS:SG	19:T:151:ARG:N	2.70	0.64
1:A:322:VAL:HG11	1:A:327:TYR:CD2	2.32	0.64
2:B:180:LEU:HD21	28:G:592:ILE:HD13	1.79	0.64
23:Y:272:GLN:NE2	23:Y:317:THR:OG1	2.30	0.64
23:Y:626:LEU:HD11	23:Y:650:GLU:HB3	1.79	0.64
24:Z:402:LEU:HG	24:Z:405:ILE:HD12	1.79	0.64
18:S:125:ARG:O	18:S:125:ARG:HG2	1.97	0.64
23:Y:474:ILE:HA	23:Y:478:LEU:HD11	1.78	0.64
23:Y:738:ARG:O	23:Y:742:ASN:CG	2.35	0.64
24:Z:192:GLU:O	24:Z:195:GLU:OE2	2.15	0.64
28:G:904:GLU:OE1	28:G:940:ASN:HB3	1.96	0.64
17:R:31:ASN:ND2	17:R:38:SER:OG	2.22	0.64
23:Y:838:THR:HG23	23:Y:839:SER:H	1.61	0.64
1:A:227:GLU:OE2	1:A:231:ARG:NH1	2.30	0.64
2:B:675:PRO:HD3	2:B:905:GLN:H	1.62	0.64
6:F:1093:SER:OG	6:F:1114:VAL:O	2.12	0.64
2:B:503:GLN:NE2	2:B:529:ASN:HB2	2.13	0.64
1:A:372:ARG:O	3:C:973:ARG:NH2	2.31	0.64
20:U:45:LYS:O	20:U:48:ILE:N	2.30	0.64
2:B:1205:THR:HB	2:B:1221:GLU:HB2	1.80	0.64
6:F:924:PHE:HD2	6:F:952:ARG:HD2	1.63	0.64
28:G:645:ILE:HD11	28:G:679:GLN:HG2	1.78	0.64
3:C:360:ARG:HG2	3:C:362:LYS:HB2	1.79	0.64
23:Y:505:GLU:OE2	23:Y:549:ARG:NE	2.25	0.64
1:A:775:ARG:HG2	1:A:776:GLN:N	2.12	0.64
2:B:882:THR:HG23	6:F:686:GLN:NE2	2.12	0.64
28:G:542:THR:O	28:G:546:ASN:ND2	2.30	0.64
13:M:480:A:O2'	13:M:481:A:H8	1.81	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:101:THR:HG22	16:Q:120:LEU:HD21	1.74	0.64
16:Q:207:LEU:N	16:Q:249:GLY:O	2.31	0.64
23:Y:659:ALA:HB1	23:Y:668:LEU:CB	2.27	0.64
1:A:777:LYS:CA	1:A:777:LYS:HZ2	2.10	0.64
2:B:749:GLU:OE1	2:B:752:ARG:NH1	2.30	0.64
1:A:404:ASN:HD21	3:C:927:MET:HE3	1.63	0.64
10:K:20:GLY:O	28:G:942:TYR:CE2	2.51	0.64
24:Z:184:GLN:HE21	24:Z:184:GLN:CA	2.11	0.64
1:A:1156:HIS:CE1	18:S:127:TRP:HB2	2.33	0.63
1:A:375:PHE:HE2	1:A:1414:TRP:CZ2	2.16	0.63
1:A:330:LEU:O	1:A:335:SER:CB	2.46	0.63
3:C:104:THR:HG22	3:C:181:LEU:HD12	1.81	0.63
23:Y:686:ILE:HD11	23:Y:730:GLN:HB2	1.81	0.63
23:Y:704:HIS:HD2	23:Y:847:LEU:CG	2.11	0.63
24:Z:194:LEU:O	24:Z:194:LEU:HD22	1.98	0.63
28:G:569:PHE:HE1	28:G:580:PHE:HE1	1.46	0.63
24:Z:200:ILE:O	24:Z:204:ASP:N	2.28	0.63
9:J:51:PHE:CZ	9:J:54:GLN:HB2	2.33	0.63
12:N:95:U:O2'	12:N:96:U:H5"	1.98	0.63
1:A:1739:ARG:HD2	1:A:1778:ASP:OD1	1.98	0.63
2:B:596:ARG:HA	2:B:599:ILE:HD12	1.81	0.63
3:C:829:VAL:HA	3:C:832:ASP:HB2	1.81	0.63
17:R:212:TRP:O	17:R:215:ARG:HB3	1.98	0.63
2:B:1432:PRO:HA	2:B:1435:ASN:HD22	1.62	0.63
20:U:45:LYS:HE3	20:U:46:GLU:H	1.63	0.63
21:V:52:SER:HB3	22:W:231:ARG:CZ	2.29	0.63
1:A:1061:ILE:HD12	1:A:1103:LEU:HB2	1.81	0.63
2:B:158:GLU:HG3	2:B:159:ASP:H	1.63	0.63
15:P:317:LYS:HB3	22:W:258:GLN:OE1	1.99	0.63
1:A:1876:ASN:OD1	1:A:1895:HIS:CD2	2.49	0.63
2:B:1459:TRP:HA	2:B:1462:ARG:HB2	1.79	0.63
2:B:427:ILE:HD11	2:B:973:LEU:HD23	1.80	0.63
3:C:580:VAL:HG22	3:C:582:SER:H	1.62	0.63
6:F:102:GLU:OE2	6:F:116:LYS:NZ	2.32	0.63
28:G:390:ILE:HD12	28:G:426:MET:HA	1.81	0.63
1:A:609:GLU:OE2	5:E:43:C:O2'	2.09	0.63
2:B:2013:VAL:HG13	2:B:2018:ASP:HB3	1.80	0.63
3:C:108:GLN:O	3:C:109:LEU:HD12	1.99	0.63
6:F:1060:LEU:HD11	6:F:1062:ARG:HH21	1.64	0.63
1:A:1458:TRP:CE2	28:G:25:ILE:HG22	2.34	0.63
13:M:468:A:H3'	13:M:469:A:C8	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1430:ASN:ND2	2:B:2091:TYR:OH	2.32	0.62
22:W:189:THR:HG22	22:W:195:ILE:CD1	2.29	0.62
1:A:1424:HIS:CD2	30:X:6:ILE:HD13	2.34	0.62
3:C:193:LEU:HD23	3:C:224:GLU:HB3	1.81	0.62
6:F:201:CYS:HB3	6:F:215:LEU:HD12	1.82	0.62
16:Q:87:ARG:HH22	16:Q:123:ALA:HA	1.63	0.62
1:A:1831:GLN:O	1:A:1834:PHE:N	2.29	0.62
3:C:510:ARG:NH1	3:C:533:GLU:OE1	2.33	0.62
6:F:1178:PRO:HG2	7:H:146:ILE:HD11	1.81	0.62
1:A:1044:GLY:HA3	1:A:1176:GLU:HG3	1.81	0.62
1:A:1286:TRP:HA	1:A:1448:GLU:OE2	1.99	0.62
1:A:1829:SER:C	1:A:1830:VAL:HG13	2.20	0.62
6:F:597:HIS:ND1	6:F:597:HIS:O	2.32	0.62
28:G:531:GLU:OE1	28:G:534:ARG:NH2	2.33	0.62
28:G:925:HIS:O	28:G:931:ARG:NH2	2.32	0.62
6:F:259:ASN:O	10:K:75:PRO:HD3	1.99	0.62
16:Q:217:TRP:CZ2	17:R:187:LYS:CD	2.77	0.62
17:R:66:ASN:N	17:R:66:ASN:OD1	2.32	0.62
23:Y:282:ALA:HB2	23:Y:507:SER:HB3	1.82	0.62
20:U:135:THR:O	20:U:163:ASN:ND2	2.32	0.62
2:B:1031:LEU:HD22	2:B:1128:LEU:HD21	1.82	0.62
3:C:231:ALA:O	3:C:487:ARG:NH1	2.33	0.62
3:C:697:ARG:NH1	3:C:852:THR:OG1	2.33	0.62
6:F:551:PHE:HD2	6:F:591:THR:HG21	1.63	0.62
6:F:736:ILE:HG23	6:F:738:GLN:H	1.63	0.62
28:G:550:THR:HG23	28:G:553:LEU:HD22	1.81	0.62
6:F:1222:GLN:HE22	10:K:48:ALA:CA	2.11	0.62
14:O:285:SER:OG	14:O:287:ASP:OD1	2.14	0.62
23:Y:278:PRO:HB3	23:Y:352:THR:HG21	1.82	0.62
1:A:1846:ASN:OD1	1:A:1847:ASP:N	2.33	0.62
1:A:771:PRO:O	14:O:309:ARG:NH2	2.32	0.62
6:F:412:THR:O	6:F:413:ILE:HG23	1.99	0.62
9:J:103:LYS:O	9:J:104:LYS:HB2	1.99	0.62
16:Q:255:SER:HG	16:Q:257:GLU:HG2	1.65	0.62
2:B:1598:PHE:O	2:B:1602:SER:N	2.33	0.62
7:H:262:HIS:HD2	7:H:283:LYS:HZ1	0.70	0.62
13:M:472:A:O2'	13:M:473:A:H8	1.81	0.62
23:Y:626:LEU:HD11	23:Y:650:GLU:HA	1.81	0.62
1:A:1843:LEU:HD13	1:A:1851:PHE:HZ	1.64	0.62
1:A:319:ARG:HD3	1:A:486:PHE:HE2	1.64	0.62
6:F:71:PHE:HA	6:F:97:THR:HG22	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:HD23	3:C:336:ILE:HG21	1.81	0.61
2:B:126:TRP:HH2	2:B:177:ILE:HD11	1.65	0.61
21:V:11:GLU:HG2	21:V:16:ILE:HG21	1.82	0.61
24:Z:195:GLU:HG2	24:Z:196:THR:N	2.15	0.61
1:A:1275:MET:O	1:A:1276:GLU:HG2	2.00	0.61
6:F:153:ASP:O	6:F:154:SER:OG	2.14	0.61
13:M:468:A:H3'	13:M:469:A:H8	1.64	0.61
16:Q:215:PRO:HB2	16:Q:217:TRP:CE3	2.36	0.61
16:Q:226:LEU:HG	16:Q:227:LEU:CD2	2.29	0.61
22:W:186:SER:C	22:W:190:ILE:HD12	2.20	0.61
1:A:396:ARG:HG3	1:A:396:ARG:NH1	2.13	0.61
2:B:1159:ARG:NH1	2:B:1183:ILE:O	2.30	0.61
2:B:1479:ILE:HB	2:B:1489:GLU:HB2	1.83	0.61
6:F:766:LYS:HD3	6:F:836:TRP:NE1	2.14	0.61
17:R:4:TRP:CD1	17:R:92:HIS:HB3	2.34	0.61
24:Z:148:LEU:HD12	24:Z:190:LEU:HD11	1.80	0.61
1:A:1163:ARG:NH1	1:A:1163:ARG:HG2	2.15	0.61
1:A:394:ARG:CG	1:A:394:ARG:HH11	2.13	0.61
28:G:443:ARG:NE	28:G:478:GLU:OE2	2.33	0.61
7:H:248:HIS:CE1	7:H:252:PHE:HD2	2.18	0.61
3:C:932:PHE:O	3:C:933:TRP:CD1	2.53	0.61
6:F:1197:ASP:OD2	6:F:1224:THR:OG1	2.10	0.61
28:G:675:LEU:HD13	28:G:715:ALA:HB2	1.81	0.61
8:I:16:ILE:O	8:I:17:ALA:HB3	2.00	0.61
1:A:395:PRO:HB2	1:A:398:VAL:HG21	1.82	0.61
1:A:911:ILE:HG23	1:A:997:GLN:HB3	1.83	0.61
2:B:593:ARG:NH1	2:B:621:ASN:OD1	2.22	0.61
1:A:725:TYR:CD1	5:E:72:C:H1'	2.36	0.61
18:S:9:LEU:HD23	18:S:11:ALA:H	1.63	0.61
21:V:82:GLN:H	22:W:168:GLN:HE21	1.48	0.61
5:E:35:A:O2'	5:E:36:U:O5'	2.18	0.61
6:F:93:LEU:HD23	6:F:422:PHE:HZ	1.64	0.61
22:W:160:LYS:HB2	22:W:160:LYS:NZ	2.14	0.61
1:A:271:GLN:O	1:A:271:GLN:NE2	2.34	0.61
2:B:880:TYR:O	6:F:686:GLN:CD	2.38	0.61
6:F:332:GLU:OE1	6:F:332:GLU:N	2.30	0.61
28:G:360:LYS:HD2	28:G:395:VAL:HG12	1.83	0.61
15:P:53:LEU:CD2	15:P:54:SER:N	2.60	0.61
23:Y:337:LEU:O	23:Y:369:ARG:NH1	2.31	0.61
1:A:143:ILE:CD1	1:A:570:GLN:HG2	2.22	0.61
1:A:1474:ARG:NH1	15:P:304:ASP:OD1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PHE:CE2	1:A:1414:TRP:CZ2	2.89	0.61
2:B:134:ASP:CG	2:B:752:ARG:HH22	2.04	0.61
3:C:701:GLU:HG2	3:C:703:LEU:H	1.65	0.61
7:H:141:VAL:HG12	7:H:143:TYR:H	1.64	0.61
1:A:1672:GLU:HG3	1:A:1797:LEU:HD11	1.81	0.61
1:A:183:TRP:CE2	1:A:216:GLN:OE1	2.53	0.61
3:C:697:ARG:NH1	3:C:848:VAL:O	2.34	0.61
14:O:322:SER:OG	14:O:378:TYR:OH	2.13	0.61
20:U:51:LYS:O	20:U:52:HIS:HB3	1.99	0.61
1:A:273:ASP:HA	1:A:310:ASN:ND2	2.14	0.60
1:A:379:ILE:HG22	1:A:379:ILE:O	2.00	0.60
3:C:223:ASP:HB3	3:C:630:PRO:HG2	1.84	0.60
9:J:51:PHE:CE2	9:J:54:GLN:HB2	2.36	0.60
15:P:241:LEU:HD13	20:U:204:VAL:HA	1.81	0.60
2:B:439:LYS:HE2	2:B:862:GLN:HB2	1.83	0.60
2:B:536:LEU:HD23	2:B:539:LEU:HD12	1.82	0.60
3:C:233:ASP:OD1	3:C:487:ARG:NH2	2.32	0.60
4:D:78:A:H4'	4:D:79:C:OP1	2.00	0.60
6:F:190:ILE:O	6:F:191:SER:OG	2.15	0.60
7:H:262:HIS:CD2	7:H:283:LYS:CE	2.84	0.60
13:M:514:U:H5"	13:M:515:U:H5"	1.82	0.60
16:Q:226:LEU:HD11	16:Q:227:LEU:CD2	2.29	0.60
17:R:210:LYS:HD3	17:R:211:GLU:N	2.16	0.60
22:W:208:SER:HA	22:W:214:LEU:CD1	2.31	0.60
24:Z:317:ILE:HD13	24:Z:325:VAL:HG21	1.82	0.60
6:F:128:LYS:NZ	6:F:193:MET:O	2.30	0.60
28:G:450:ASP:OD1	28:G:451:ASP:N	2.34	0.60
28:G:739:ASN:OD1	28:G:740:LYS:N	2.33	0.60
21:V:89:VAL:HG22	21:V:104:ILE:HG22	1.83	0.60
1:A:1130:ARG:HD3	1:A:1156:HIS:CG	2.36	0.60
1:A:194:HIS:NE2	15:P:122:LEU:HD22	2.15	0.60
2:B:1212:THR:HG22	2:B:1213:ARG:H	1.66	0.60
2:B:2006:GLU:O	2:B:2010:GLU:N	2.21	0.60
6:F:432:GLU:O	6:F:485:ASN:ND2	2.35	0.60
15:P:110:HIS:CE1	16:Q:18:GLY:O	2.54	0.60
17:R:138:TYR:HE1	17:R:181:CYS:HB3	1.66	0.60
24:Z:170:HIS:HE1	24:Z:174:TRP:HZ3	1.15	0.60
1:A:2392:PHE:HE1	2:B:1062:PRO:HB2	1.67	0.60
1:A:849:LEU:HD12	1:A:973:GLU:HB3	1.84	0.60
7:H:198:ASP:OD1	7:H:199:ILE:HG12	2.02	0.60
13:M:505:A:C4'	13:M:505:A:OP1	2.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:64:GLY:O	17:R:68:GLY:N	2.35	0.60
24:Z:170:HIS:NE2	24:Z:174:TRP:CE3	2.69	0.60
24:Z:184:GLN:HE21	24:Z:185:GLU:H	1.48	0.60
1:A:268:LEU:O	1:A:269:ASP:HB3	2.01	0.60
1:A:631:LEU:HD21	1:A:663:LEU:HD13	1.84	0.60
22:W:229:GLY:O	22:W:231:ARG:N	2.35	0.60
24:Z:184:GLN:HE21	24:Z:184:GLN:HA	1.66	0.60
24:Z:149:ARG:HH11	24:Z:193:SER:CB	2.14	0.60
1:A:1835:LEU:HD12	1:A:1836:ASN:N	2.17	0.60
1:A:514:TYR:HB3	1:A:518:VAL:CG2	2.32	0.60
3:C:147:THR:HG23	3:C:178:LEU:HB2	1.84	0.60
3:C:806:GLY:H	3:C:810:GLU:HA	1.66	0.60
6:F:1065:THR:HG22	6:F:1105:VAL:HG23	1.84	0.60
7:H:235:PRO:O	28:G:722:LYS:NZ	2.35	0.60
9:J:4:HIS:CD2	13:M:502:C:H4'	2.37	0.60
14:O:115:TYR:OH	14:O:444:PRO:O	2.19	0.60
15:P:41:ASP:OD1	15:P:42:ASP:N	2.34	0.60
23:Y:248:THR:OG1	23:Y:552:ARG:NH2	2.32	0.60
1:A:1843:LEU:HA	1:A:1849:LYS:HZ2	1.67	0.60
6:F:1222:GLN:HE22	10:K:48:ALA:CB	2.14	0.60
13:M:468:A:H5"	13:M:469:A:OP2	2.02	0.60
21:V:123:LYS:O	21:V:127:ASP:N	2.34	0.60
24:Z:188:SER:O	24:Z:192:GLU:HG2	2.01	0.60
24:Z:470:LEU:HD12	24:Z:471:GLY:H	1.66	0.60
6:F:347:LYS:HD2	6:F:460:PRO:HB2	1.84	0.60
30:X:27:ASN:OD1	30:X:28:ASN:N	2.31	0.60
24:Z:470:LEU:HD12	24:Z:471:GLY:N	2.17	0.60
2:B:1016:ASP:OD2	2:B:1020:ARG:NH1	2.34	0.60
7:H:183:LEU:HD23	7:H:272:GLU:HG3	1.83	0.60
16:Q:67:GLN:NE2	16:Q:116:LYS:O	2.34	0.60
17:R:244:LEU:O	17:R:248:ASN:ND2	2.35	0.60
20:U:78:TYR:H	20:U:99:ASN:HD21	1.49	0.60
24:Z:178:ARG:HD3	24:Z:182:GLN:HE22	1.67	0.60
1:A:1051:GLU:HB3	1:A:1167:ARG:HH21	1.67	0.59
1:A:1739:ARG:CD	1:A:1778:ASP:OD1	2.50	0.59
2:B:1381:GLU:OE2	2:B:1412:TRP:NE1	2.35	0.59
3:C:234:LEU:HD23	3:C:443:TYR:HB2	1.84	0.59
16:Q:79:ARG:HD2	16:Q:126:THR:CG2	2.28	0.59
1:A:744:THR:O	1:A:749:ARG:NH2	2.35	0.59
1:A:933:GLU:N	1:A:933:GLU:OE1	2.34	0.59
2:B:148:ILE:HG23	2:B:189:MET:HE1	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ILE:HD11	6:F:759:ASP:HB3	1.84	0.59
1:A:2392:PHE:CE1	2:B:1062:PRO:HB2	2.36	0.59
2:B:1690:GLY:HA3	2:B:1894:LEU:HB2	1.82	0.59
6:F:105:ASP:OD1	6:F:106:THR:N	2.36	0.59
6:F:1179:ASN:OD1	6:F:1180:THR:N	2.35	0.59
6:F:299:PRO:HD2	6:F:377:PHE:CE1	2.37	0.59
6:F:433:MET:O	6:F:485:ASN:HB3	2.03	0.59
9:J:100:HIS:CE1	28:G:257:MET:HG3	2.37	0.59
23:Y:828:LYS:HB2	28:G:429:GLU:OE2	2.03	0.59
17:R:69:GLN:HE21	17:R:71:PHE:HD2	1.49	0.59
22:W:264:GLU:HG3	22:W:265:ASP:H	1.68	0.59
23:Y:409:TYR:OH	23:Y:563:ARG:NH1	2.36	0.59
2:B:1325:GLU:HA	2:B:1350:LYS:HE3	1.84	0.59
6:F:1222:GLN:NE2	10:K:48:ALA:N	2.51	0.59
28:G:538:VAL:O	28:G:542:THR:HG23	2.01	0.59
7:H:181:GLU:O	7:H:182:TYR:HB3	2.02	0.59
12:N:110:U:HO2'	17:R:141:GLY:HA2	1.66	0.59
20:U:110:LEU:N	20:U:123:GLU:OE1	2.30	0.59
1:A:610:ARG:HE	1:A:614:ARG:HH21	1.48	0.59
2:B:1369:GLY:N	2:B:1533:TYR:O	2.29	0.59
5:E:28:U:C1'	19:T:121:ILE:HD13	2.31	0.59
6:F:1007:LYS:HE3	6:F:1009:LEU:HD21	1.82	0.59
28:G:919:ILE:CD1	28:G:937:VAL:HG11	2.32	0.59
10:K:50:LEU:HD22	10:K:62:ILE:HG23	1.84	0.59
15:P:301:LEU:H	15:P:301:LEU:CD2	2.16	0.59
16:Q:98:ASN:O	16:Q:99:VAL:HG12	2.01	0.59
1:A:1056:GLU:HB2	1:A:1060:LYS:HG3	1.85	0.59
1:A:1054:LEU:HD21	1:A:1168:ILE:CD1	2.31	0.59
1:A:1829:SER:O	1:A:1830:VAL:HG13	2.01	0.59
2:B:134:ASP:OD2	2:B:752:ARG:NH2	2.35	0.59
22:W:173:ASN:O	22:W:174:VAL:HG12	2.02	0.59
3:C:106:PHE:CE1	3:C:548:ARG:O	2.56	0.59
3:C:117:ARG:HG2	3:C:157:SER:O	2.03	0.59
7:H:182:TYR:O	7:H:272:GLU:CD	2.40	0.59
15:P:110:HIS:O	15:P:111:HIS:HB2	2.01	0.59
21:V:40:ARG:NH1	21:V:72:GLN:O	2.36	0.59
1:A:676:GLN:HG2	1:A:714:PHE:HB2	1.83	0.59
3:C:116:THR:HG23	3:C:118:TYR:HE1	1.64	0.59
3:C:826:PRO:HB2	3:C:832:ASP:HB3	1.83	0.59
6:F:266:VAL:HG12	6:F:290:PRO:HA	1.84	0.59
6:F:607:LEU:HB2	6:F:624:TRP:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:121:GLN:NE2	15:P:49:SER:O	2.36	0.59
14:O:194:HIS:NE2	14:O:237:ASP:OD1	2.32	0.59
24:Z:187:SER:OG	24:Z:190:LEU:HB3	2.03	0.59
17:R:211:GLU:O	17:R:211:GLU:HG2	2.03	0.59
20:U:45:LYS:CE	20:U:45:LYS:HA	2.31	0.59
24:Z:167:LYS:NZ	24:Z:171:ASP:OD2	2.26	0.59
1:A:1410:SER:HB3	1:A:1423:THR:H	1.67	0.59
1:A:1899:TRP:CE3	1:A:1899:TRP:HA	2.38	0.59
2:B:506:VAL:HG12	2:B:692:PHE:CD2	2.38	0.59
6:F:411:ASP:OD1	6:F:472:LEU:HA	2.03	0.59
28:G:922:GLY:HA3	28:G:934:PHE:CD2	2.37	0.59
17:R:164:PHE:CD2	17:R:184:VAL:HG21	2.38	0.59
6:F:1097:PHE:HE1	6:F:1108:PRO:HB3	1.68	0.58
14:O:277:VAL:HG13	15:P:63:ILE:HG22	1.85	0.58
15:P:323:VAL:HG23	15:P:324:TYR:CG	2.38	0.58
1:A:1295:GLN:NE2	24:Z:432:GLY:HA3	2.15	0.58
1:A:218:SER:O	1:A:221:TRP:HB3	2.02	0.58
2:B:1209:GLN:OE1	2:B:1219:ASN:ND2	2.36	0.58
6:F:96:ALA:HB2	6:F:101:LEU:HD13	1.84	0.58
8:I:53:ARG:CZ	8:I:53:ARG:HB3	2.32	0.58
1:A:774:ILE:HD12	1:A:774:ILE:C	2.22	0.58
2:B:2051:VAL:O	2:B:2154:LYS:NZ	2.36	0.58
6:F:545:ASP:OD1	6:F:546:ASN:N	2.36	0.58
6:F:582:LYS:O	6:F:608:ARG:NH2	2.35	0.58
1:A:1229:GLU:OE1	18:S:127:TRP:CH2	2.56	0.58
1:A:2403:GLU:O	1:A:2404:LEU:HB2	2.02	0.58
2:B:2147:ASP:OD1	2:B:2148:SER:N	2.36	0.58
3:C:108:GLN:C	3:C:109:LEU:HD12	2.23	0.58
3:C:250:GLU:OE2	3:C:298:PHE:CZ	2.57	0.58
6:F:1002:ARG:NH2	6:F:1004:LEU:HD11	2.19	0.58
6:F:836:TRP:CZ3	6:F:838:ILE:HG23	2.39	0.58
10:K:57:ARG:HH11	10:K:57:ARG:HB3	1.67	0.58
14:O:156:ILE:CD1	14:O:197:LEU:HD22	2.33	0.58
15:P:59:THR:O	15:P:63:ILE:HG23	2.03	0.58
1:A:1748:ILE:HD11	1:A:1783:MET:HB3	0.73	0.58
28:G:519:ILE:HG21	28:G:561:LEU:HD12	1.85	0.58
14:O:275:THR:OG1	14:O:279:PRO:O	2.22	0.58
1:A:790:TRP:NE1	1:A:794:LYS:HE3	2.18	0.58
6:F:369:ILE:HD11	6:F:380:LEU:HB2	1.84	0.58
28:G:294:ARG:HB3	28:G:332:THR:HG21	1.84	0.58
7:H:159:LEU:HD13	10:K:28:ARG:HG3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:155:PHE:CE2	14:O:167:TRP:HB2	2.39	0.58
19:T:3:ARG:NH2	19:T:85:LYS:O	2.34	0.58
24:Z:149:ARG:CZ	24:Z:193:SER:HB3	2.32	0.58
3:C:302:ASN:OD1	3:C:303:VAL:N	2.36	0.58
6:F:243:VAL:HG12	6:F:244:ASP:O	2.03	0.58
2:B:773:ASN:ND2	6:F:754:HIS:HE1	1.99	0.58
16:Q:70:ILE:HD13	16:Q:84:ILE:HD11	1.84	0.58
1:A:2189:LEU:O	1:A:2193:PHE:CB	2.52	0.58
3:C:418:GLN:HB3	3:C:419:PRO:HD3	1.83	0.58
6:F:163:ILE:HD13	6:F:172:LYS:HD3	1.85	0.58
28:G:386:TYR:HB3	28:G:387:PRO:CD	2.34	0.58
28:G:904:GLU:CD	28:G:940:ASN:CB	2.72	0.58
23:Y:843:ILE:HG22	23:Y:846:CYS:SG	2.44	0.58
1:A:1669:LEU:HD11	1:A:1734:PHE:CE2	2.39	0.58
1:A:1899:TRP:HE3	1:A:1899:TRP:HA	1.68	0.58
2:B:502:ILE:HG23	2:B:694:PHE:HE2	1.69	0.58
6:F:118:GLN:HE21	6:F:1299:ILE:HD13	1.68	0.58
28:G:550:THR:HG21	28:G:590:LEU:HD23	1.84	0.58
11:L:19:U:C2	15:P:175:PRO:HD2	2.39	0.58
6:F:1125:ASP:OD1	6:F:1126:GLU:N	2.30	0.58
20:U:155:TYR:HD1	20:U:179:GLU:HA	1.68	0.58
1:A:618:SER:OG	1:A:725:TYR:HB3	2.04	0.57
1:A:759:ARG:NH2	1:A:783:LEU:HD23	2.19	0.57
6:F:1111:ASP:HB2	6:F:1183:CYS:SG	2.44	0.57
6:F:541:ALA:HB2	6:F:618:TYR:HE1	1.69	0.57
15:P:318:ARG:HH22	15:P:325:ASP:HB3	1.68	0.57
16:Q:25:MET:HB2	16:Q:45:HIS:O	2.04	0.57
21:V:58:VAL:HG12	22:W:212:ARG:CZ	2.35	0.57
3:C:703:LEU:O	3:C:705:GLY:N	2.37	0.57
28:G:216:GLN:HE21	28:G:220:LEU:HD11	1.68	0.57
6:F:186:ARG:HB3	10:K:41:ASN:ND2	2.19	0.57
17:R:152:LYS:HG2	17:R:153:PRO:HD2	1.85	0.57
1:A:309:SER:HG	1:A:475:ASP:HB3	1.68	0.57
1:A:514:TYR:HB3	1:A:518:VAL:HG21	1.85	0.57
3:C:385:PHE:HE1	3:C:425:LEU:HD11	1.70	0.57
15:P:110:HIS:O	16:Q:21:ALA:O	2.23	0.57
5:E:32:U:H5'	16:Q:45:HIS:CE1	2.39	0.57
1:A:1748:ILE:CD1	1:A:1783:MET:C	2.73	0.57
1:A:140:ARG:HH21	1:A:252:GLU:HB3	1.68	0.57
2:B:880:TYR:O	6:F:686:GLN:CG	2.53	0.57
3:C:855:PRO:HG2	3:C:944:VAL:HG21	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:728:CYS:SG	28:G:753:ILE:HG21	2.43	0.57
10:K:19:ILE:HG22	10:K:20:GLY:N	2.18	0.57
1:A:322:VAL:HG11	1:A:327:TYR:CG	2.39	0.57
2:B:1588:ARG:HE	2:B:1942:ASP:CG	2.08	0.57
3:C:391:MET:CE	3:C:395:LYS:CE	2.67	0.57
6:F:1029:SER:OG	6:F:1045:MET:SD	2.57	0.57
8:I:3:TYR:CD2	12:N:99:G:C6	2.92	0.57
9:J:98:ASP:OD2	28:G:223:LYS:NZ	2.33	0.57
12:N:110:U:O2'	17:R:141:GLY:CA	2.51	0.57
14:O:223:HIS:CD2	14:O:227:VAL:HG21	2.39	0.57
1:A:1527:TRP:CE3	1:A:1528:THR:HG23	2.39	0.57
1:A:1762:ASP:OD1	1:A:1763:ASN:N	2.37	0.57
1:A:266:LEU:HG	1:A:267:PRO:HD2	1.85	0.57
1:A:184:GLU:OE2	1:A:283:SER:HA	2.04	0.57
6:F:1142:ARG:HB2	6:F:1190:LEU:HD22	1.87	0.57
6:F:783:ILE:HG13	6:F:784:SER:N	2.19	0.57
7:H:172:VAL:HG23	28:G:934:PHE:CZ	2.40	0.57
9:J:4:HIS:ND1	13:M:500:A:O2'	2.38	0.57
21:V:78:LYS:NZ	22:W:162:LEU:O	2.37	0.57
24:Z:200:ILE:HA	24:Z:203:LYS:HB2	1.86	0.57
1:A:1161:TYR:HD1	1:A:1170:MET:HG2	1.69	0.57
1:A:2409:ILE:HG22	1:A:2411:VAL:HG23	1.86	0.57
2:B:861:GLU:HG2	2:B:862:GLN:H	1.70	0.57
3:C:798:GLY:HA2	3:C:839:ILE:HG23	1.87	0.57
28:G:618:GLN:NE2	28:G:657:GLU:HB2	2.19	0.57
7:H:192:ARG:HH11	7:H:192:ARG:HG2	1.69	0.57
16:Q:240:LEU:HD12	16:Q:241:ILE:N	2.20	0.57
18:S:9:LEU:CD2	18:S:11:ALA:H	2.18	0.57
1:A:1735:ASP:OD2	1:A:1767:TYR:OH	2.22	0.57
1:A:1857:VAL:HG21	1:A:1913:THR:HG21	1.87	0.57
2:B:1866:PHE:HA	2:B:1869:SER:HB2	1.87	0.57
3:C:701:GLU:HB3	3:C:704:PRO:HA	1.86	0.57
3:C:761:ALA:HA	3:C:764:ASN:HB2	1.85	0.57
3:C:788:LEU:HB3	3:C:792:LYS:HE2	1.87	0.57
5:E:67:C:O2	5:E:82:A:C2	2.58	0.57
17:R:48:VAL:HG21	17:R:216:ARG:C	2.24	0.57
23:Y:349:HIS:CD2	23:Y:380:THR:HG23	2.39	0.57
24:Z:460:TYR:HA	24:Z:463:ASN:ND2	2.18	0.57
1:A:1697:SER:HG	1:A:1767:TYR:HH	1.49	0.57
1:A:1892:LYS:NZ	1:A:1916:GLU:OE1	2.38	0.57
2:B:1688:TYR:HA	2:B:1695:TYR:HD1	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:HIS:ND1	4:D:95:C:C2	2.73	0.57
6:F:1174:GLN:CD	6:F:1184:LYS:HD3	2.25	0.57
14:O:138:HIS:NE2	14:O:159:SER:HB2	2.19	0.57
23:Y:279:ARG:HD3	23:Y:503:ILE:HG12	1.87	0.57
4:D:78:A:O2'	4:D:79:C:O5'	2.20	0.57
6:F:504:HIS:HD2	6:F:511:ILE:HD11	1.68	0.57
28:G:239:TYR:HD1	28:G:242:LYS:HD2	1.70	0.57
17:R:93:ILE:HD13	17:R:166:ARG:O	2.05	0.57
20:U:37:LEU:O	20:U:41:GLU:HG2	2.05	0.57
1:A:2072:SER:O	28:G:527:ARG:NH2	2.38	0.56
1:A:472:ASN:HB2	3:C:390:SER:OG	2.05	0.56
2:B:891:ASP:OD1	2:B:892:GLN:N	2.38	0.56
3:C:883:ARG:NH2	3:C:912:ALA:O	2.35	0.56
6:F:520:SER:O	6:F:874:GLY:HA2	2.04	0.56
15:P:230:MET:SD	20:U:73:ARG:HB3	2.45	0.56
1:A:1405:ILE:CD1	1:A:1439:THR:HG21	2.35	0.56
1:A:1458:TRP:HE1	1:A:1489:PRO:HD2	1.70	0.56
1:A:416:GLU:HB3	1:A:419:THR:HG23	1.86	0.56
2:B:1345:PHE:HE1	2:B:1348:PHE:HA	1.69	0.56
2:B:1585:LEU:HD21	2:B:1683:LEU:HD23	1.87	0.56
6:F:924:PHE:CD2	6:F:952:ARG:HD2	2.38	0.56
28:G:61:GLU:CD	28:G:68:ARG:HH21	2.07	0.56
7:H:156:TYR:OH	10:K:27:THR:HG22	2.04	0.56
20:U:131:ILE:HG13	20:U:188:LEU:HD11	1.87	0.56
1:A:1660:SER:HB3	1:A:1809:ASN:OD1	2.05	0.56
1:A:1846:ASN:O	1:A:1885:LYS:NZ	2.32	0.56
1:A:2384:ASN:OD1	1:A:2385:GLU:N	2.38	0.56
3:C:123:MET:HB2	3:C:199:LEU:HD23	1.87	0.56
6:F:642:LEU:HD21	6:F:644:ILE:HG23	1.87	0.56
1:A:893:ARG:NH2	1:A:1136:GLY:O	2.38	0.56
6:F:541:ALA:HB2	6:F:618:TYR:CE1	2.40	0.56
15:P:58:PRO:O	15:P:59:THR:HG23	2.05	0.56
15:P:66:CYS:HA	15:P:69:ARG:HG2	1.86	0.56
17:R:207:PRO:O	17:R:212:TRP:CG	2.58	0.56
22:W:186:SER:O	22:W:190:ILE:HD12	2.04	0.56
23:Y:220:ARG:NH1	23:Y:258:GLN:OE1	2.38	0.56
1:A:1322:ALA:O	1:A:1323:SER:OG	2.21	0.56
1:A:366:GLU:HG3	1:A:372:ARG:HH11	1.69	0.56
3:C:292:ILE:HG12	3:C:311:ILE:HD13	1.88	0.56
3:C:501:ILE:HD13	3:C:567:ILE:HG23	1.87	0.56
6:F:1085:LEU:HB2	6:F:1097:PHE:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1124:LEU:HB2	6:F:1130:ILE:CD1	2.35	0.56
28:G:189:THR:O	28:G:231:GLN:NE2	2.29	0.56
16:Q:215:PRO:CB	16:Q:217:TRP:CE3	2.88	0.56
17:R:9:ALA:CB	17:R:58:HIS:O	2.54	0.56
5:E:28:U:H1'	19:T:121:ILE:HD13	1.86	0.56
21:V:27:TYR:HD2	21:V:30:ASN:HD22	1.51	0.56
1:A:1816:ARG:CG	1:A:1816:ARG:HH11	2.14	0.56
1:A:2189:LEU:O	1:A:2193:PHE:HB2	2.06	0.56
1:A:805:PRO:HG2	1:A:808:ILE:HD12	1.87	0.56
7:H:166:THR:HG22	7:H:167:LYS:N	2.21	0.56
15:P:231:GLU:O	15:P:235:LEU:N	2.38	0.56
15:P:303:TYR:HB3	15:P:307:PHE:CD2	2.34	0.56
23:Y:776:THR:O	23:Y:780:ILE:N	2.37	0.56
1:A:2306:ASN:HB2	1:A:2335:THR:HB	1.86	0.56
3:C:769:TYR:OH	3:C:774:LEU:HB2	2.05	0.56
3:C:706:LEU:HD21	3:C:833:VAL:HG22	1.87	0.56
28:G:827:ILE:O	28:G:827:ILE:HG13	2.04	0.56
21:V:49:THR:HG23	22:W:233:ASP:HB2	1.87	0.56
23:Y:223:LEU:HD11	47:Y:902:ADP:H4'	1.86	0.56
3:C:167:ASN:ND2	3:C:173:LYS:HG3	2.21	0.56
3:C:235:VAL:HG13	3:C:261:VAL:HG11	1.88	0.56
6:F:1161:ASN:OD1	6:F:1162:GLY:N	2.39	0.56
6:F:182:THR:O	6:F:183:THR:HG23	2.06	0.56
6:F:493:VAL:HA	6:F:937:LYS:HG2	1.87	0.56
6:F:701:LYS:HG2	6:F:718:LEU:HD23	1.86	0.56
9:J:8:LEU:HD21	9:J:93:GLY:HA3	1.87	0.56
17:R:13:VAL:CG1	17:R:17:GLU:HB3	2.35	0.56
22:W:170:LEU:HD22	22:W:170:LEU:N	2.20	0.56
1:A:1007:LYS:HD3	1:A:1141:PRO:HG3	1.88	0.56
2:B:1474:ASP:HA	2:B:1511:LEU:HB2	1.86	0.56
2:B:901:VAL:HA	2:B:906:LEU:HB2	1.88	0.56
6:F:527:LEU:HD12	6:F:528:PRO:HD2	1.87	0.56
28:G:579:ILE:N	28:G:579:ILE:HD12	2.21	0.56
28:G:904:GLU:OE2	28:G:940:ASN:CB	2.54	0.56
15:P:300:ASP:OD1	15:P:300:ASP:N	2.38	0.56
24:Z:152:ILE:HD11	24:Z:194:LEU:HA	1.87	0.56
2:B:448:LEU:HD21	2:B:899:LEU:HD21	1.86	0.56
1:A:454:LEU:N	3:C:357:GLY:O	2.37	0.56
6:F:200:ARG:HH11	6:F:250:PRO:HD3	1.70	0.56
6:F:944:ASN:HD21	6:F:979:CYS:H	1.54	0.56
15:P:301:LEU:N	15:P:301:LEU:HD23	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:226:LEU:HD12	16:Q:226:LEU:O	2.05	0.56
17:R:142:ILE:CG2	17:R:180:ASN:ND2	2.69	0.56
1:A:934:ARG:NH2	1:A:1587:PHE:CZ	2.73	0.56
1:A:228:LYS:HD3	1:A:700:GLY:HA3	1.86	0.56
2:B:1811:LEU:HD23	2:B:1814:LEU:HD12	1.88	0.56
6:F:534:LEU:HD21	6:F:550:LEU:HD11	1.88	0.56
6:F:181:ARG:NH1	9:J:84:ASP:OD1	2.39	0.56
10:K:23:ASP:OD1	10:K:24:GLU:N	2.35	0.56
11:L:19:U:O2'	15:P:175:PRO:HG2	2.06	0.56
11:L:43:G:N2	13:M:492:U:O2	2.39	0.56
3:C:90:LEU:HD22	14:O:211:LEU:HD22	1.87	0.56
1:A:1367:ILE:O	1:A:1370:ARG:HB3	2.07	0.55
1:A:380:ARG:HG2	1:A:380:ARG:HH11	1.69	0.55
1:A:687:ILE:HD11	1:A:706:PRO:HG2	1.88	0.55
2:B:2042:ALA:O	2:B:2046:ASN:ND2	2.39	0.55
6:F:104:TYR:HD1	6:F:113:LEU:HA	1.70	0.55
6:F:363:VAL:HG12	6:F:364:THR:N	2.13	0.55
6:F:855:ALA:HA	6:F:856:ASP:C	2.26	0.55
1:A:1145:MET:HB3	28:G:19:LEU:HB2	1.87	0.55
28:G:386:TYR:CG	28:G:387:PRO:CD	2.88	0.55
11:L:19:U:C6	11:L:19:U:OP2	2.58	0.55
1:A:1094:ASP:OD1	11:L:25:A:N3	2.39	0.55
21:V:48:LEU:C	22:W:231:ARG:NH1	2.59	0.55
1:A:541:ASN:HD21	4:D:79:C:H5	1.52	0.55
1:A:930:ASN:HB3	1:A:933:GLU:OE1	2.06	0.55
2:B:532:LEU:HD13	2:B:577:ARG:HD2	1.88	0.55
3:C:106:PHE:CZ	3:C:548:ARG:O	2.59	0.55
3:C:576:THR:HG22	3:C:592:PHE:HD2	1.71	0.55
6:F:161:GLN:HG2	6:F:163:ILE:HG23	1.87	0.55
6:F:608:ARG:HD3	6:F:610:ILE:HD11	1.87	0.55
6:F:638:SER:HB3	6:F:641:GLN:HB3	1.88	0.55
1:A:1233:ARG:CD	18:S:131:THR:HG21	2.36	0.55
22:W:197:PHE:CZ	24:Z:463:ASN:CB	2.83	0.55
23:Y:591:VAL:HG11	23:Y:620:LEU:HD23	1.87	0.55
24:Z:184:GLN:HA	24:Z:184:GLN:NE2	2.21	0.55
1:A:2255:LEU:H	1:A:2255:LEU:HD12	1.71	0.55
1:A:2314:TRP:NE1	1:A:2327:GLU:O	2.38	0.55
28:G:587:THR:HG22	28:G:594:MET:HE3	1.88	0.55
7:H:185:GLY:CA	8:I:72:ASN:HD21	2.19	0.55
17:R:150:HIS:HB3	17:R:155:GLN:HB2	1.88	0.55
1:A:1405:ILE:HD13	1:A:1439:THR:HG21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:O	1:A:273:ASP:OD2	2.25	0.55
1:A:332:ASP:O	1:A:333:LYS:C	2.45	0.55
1:A:640:ARG:HG2	1:A:640:ARG:NH1	2.20	0.55
1:A:668:ARG:HD2	12:N:96:U:H4'	1.88	0.55
2:B:1000:ASP:OD1	2:B:1001:LEU:N	2.40	0.55
2:B:1547:ASN:N	2:B:1720:VAL:O	2.39	0.55
2:B:2070:LYS:HD3	2:B:2127:GLU:HB3	1.89	0.55
3:C:715:MET:SD	3:C:772:ASN:HB3	2.46	0.55
6:F:115:ALA:HB2	6:F:169:LEU:HD12	1.88	0.55
28:G:820:MET:HA	28:G:823:MET:HG2	1.88	0.55
9:J:103:LYS:O	9:J:104:LYS:CB	2.55	0.55
17:R:164:PHE:CE1	17:R:199:MET:HG3	2.42	0.55
19:T:111:LYS:HA	19:T:118:SER:HB2	1.88	0.55
20:U:48:ILE:HG22	20:U:49:ALA:N	2.21	0.55
21:V:87:LEU:HD21	22:W:222:ASN:HD21	1.71	0.55
3:C:437:ASP:OD1	3:C:441:ARG:NH2	2.40	0.55
3:C:617:LYS:HD2	3:C:666:ILE:HG23	1.87	0.55
3:C:672:ASP:OD1	3:C:673:PRO:HD2	2.06	0.55
6:F:1216:CYS:SG	6:F:1228:PHE:HB2	2.46	0.55
6:F:177:GLN:OE1	9:J:17:VAL:HG12	2.06	0.55
13:M:506:U:OP2	28:G:698:ARG:NH1	2.40	0.55
7:H:141:VAL:HG11	7:H:165:CYS:SG	2.45	0.55
7:H:192:ARG:HH11	7:H:192:ARG:CG	2.18	0.55
7:H:185:GLY:HA3	8:I:72:ASN:ND2	2.22	0.55
9:J:79:LEU:HD21	28:G:866:LEU:HD21	1.87	0.55
15:P:87:ASN:HB3	15:P:90:SER:H	1.70	0.55
17:R:146:LEU:CG	17:R:147:ASN:H	2.20	0.55
17:R:207:PRO:O	17:R:212:TRP:CD1	2.59	0.55
1:A:1012:TRP:CD1	1:A:1013:ILE:N	2.74	0.55
1:A:1755:LYS:O	1:A:1759:TYR:HD2	1.89	0.55
2:B:1595:ALA:HB1	2:B:1637:VAL:HG11	1.89	0.55
2:B:1905:LEU:HD12	2:B:1908:ARG:HD3	1.87	0.55
2:B:739:GLN:HE22	2:B:823:GLY:HA2	1.71	0.55
3:C:803:VAL:HG22	3:C:813:ILE:HD12	1.88	0.55
9:J:101:PHE:CE2	28:G:219:HIS:CD2	2.95	0.55
6:F:180:THR:O	9:J:83:LYS:HB3	2.07	0.55
1:A:1588:LYS:HE3	11:L:31:A:OP1	2.06	0.55
14:O:115:TYR:HD1	14:O:118:LEU:HD12	1.72	0.55
22:W:188:LEU:CD2	24:Z:415:GLN:CG	2.85	0.55
24:Z:192:GLU:HB3	24:Z:195:GLU:OE2	2.05	0.55
3:C:601:ALA:HB1	3:C:645:LEU:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:778:THR:OG1	3:C:780:PRO:HD2	2.07	0.55
16:Q:257:GLU:HG3	16:Q:258:LEU:N	2.21	0.55
17:R:146:LEU:HG	17:R:147:ASN:H	1.72	0.55
17:R:63:ARG:HH21	19:T:143:HIS:CD2	2.24	0.55
1:A:1270:LEU:HD13	1:A:1275:MET:HG2	1.89	0.55
1:A:2259:ILE:HD11	1:A:2293:ILE:HD11	1.88	0.55
2:B:2098:SER:H	2:B:2147:ASP:CG	2.09	0.55
2:B:739:GLN:NE2	2:B:823:GLY:HA2	2.21	0.55
3:C:309:ASN:HD22	3:C:441:ARG:HH11	1.55	0.55
6:F:496:SER:HB3	6:F:497:PRO:HD3	1.89	0.55
6:F:716:ILE:HG21	6:F:759:ASP:O	2.06	0.55
24:Z:178:ARG:HA	24:Z:198:PHE:CE1	2.42	0.55
1:A:1335:TRP:HB2	1:A:1367:ILE:HD13	1.89	0.55
1:A:2287:ASP:O	1:A:2288:CYS:C	2.46	0.55
2:B:1608:ASP:O	2:B:1609:MET:HG2	2.06	0.55
2:B:1944:GLN:O	2:B:1948:LYS:N	2.29	0.55
2:B:773:ASN:HD22	6:F:754:HIS:CE1	2.22	0.55
6:F:66:LYS:HB3	6:F:1225:VAL:HG22	1.89	0.55
16:Q:208:TYR:O	16:Q:209:ASN:HB3	2.07	0.55
17:R:109:LEU:HD13	17:R:113:GLY:HA2	1.88	0.55
17:R:31:ASN:HB3	17:R:34:TYR:O	2.07	0.55
5:E:28:U:H5”	19:T:118:SER:O	2.07	0.55
19:T:156:THR:HG23	19:T:157:ASP:H	1.72	0.55
24:Z:168:LYS:HZ2	24:Z:171:ASP:HB2	1.71	0.55
1:A:1951:PHE:HB3	1:A:1954:ILE:HD12	1.88	0.55
28:G:277:THR:O	28:G:280:THR:OG1	2.24	0.55
28:G:337:VAL:HG11	28:G:359:ILE:HD11	1.87	0.55
8:I:63:SER:HB3	28:G:810:THR:CG2	2.37	0.55
14:O:197:LEU:HB3	14:O:209:TRP:HB2	1.88	0.55
1:A:2199:VAL:HG13	1:A:2200:LYS:HG3	1.89	0.54
2:B:1362:SER:O	2:B:1386:ASN:ND2	2.40	0.54
2:B:1548:ILE:HG12	2:B:1722:ILE:HD12	1.89	0.54
6:F:547:ASN:ND2	6:F:564:ASP:HB2	2.22	0.54
28:G:442:ILE:HD11	28:G:460:VAL:HB	1.89	0.54
28:G:542:THR:HG22	28:G:582:GLY:HA2	1.89	0.54
28:G:606:LEU:HD22	28:G:646:ILE:HD13	1.89	0.54
8:I:57:TYR:CZ	8:I:70:LEU:HD11	2.42	0.54
13:M:506:U:OP2	28:G:698:ARG:CZ	2.55	0.54
15:P:301:LEU:H	15:P:301:LEU:HD23	1.72	0.54
1:A:2402:GLU:N	1:A:2402:GLU:OE1	2.40	0.54
1:A:354:PRO:O	1:A:355:LEU:HB3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:CG	1:A:396:ARG:HH11	2.19	0.54
28:G:919:ILE:HD11	28:G:937:VAL:HG11	1.89	0.54
7:H:155:ARG:HH21	7:H:155:ARG:HG3	1.72	0.54
16:Q:101:THR:HG22	16:Q:120:LEU:CD2	2.35	0.54
1:A:1424:HIS:CD2	30:X:6:ILE:CD1	2.91	0.54
2:B:1200:PRO:HG2	2:B:1297:TRP:CD1	2.42	0.54
2:B:567:VAL:HG13	2:B:606:VAL:HG12	1.88	0.54
6:F:594:MET:HB3	6:F:656:ILE:HG21	1.88	0.54
6:F:640:THR:OG1	6:F:686:GLN:O	2.21	0.54
28:G:590:LEU:HD11	28:G:594:MET:HE1	1.88	0.54
14:O:206:VAL:HB	14:O:220:TYR:HB2	1.90	0.54
16:Q:217:TRP:CZ3	17:R:187:LYS:CD	2.86	0.54
21:V:35:ILE:HD13	21:V:51:PHE:CE2	2.42	0.54
1:A:2314:TRP:CE2	1:A:2329:PHE:HB2	2.43	0.54
3:C:802:ALA:HB2	3:C:843:LYS:HA	1.89	0.54
28:G:927:ALA:C	28:G:929:ASN:H	2.10	0.54
11:L:25:A:H3'	11:L:26:G:H5"	1.89	0.54
22:W:214:LEU:N	22:W:230:SER:OG	2.41	0.54
1:A:1267:VAL:HG22	1:A:1302:LEU:HD23	1.90	0.54
2:B:1620:TYR:CD1	2:B:1651:ILE:HG23	2.41	0.54
2:B:1929:LEU:HB3	2:B:1947:LEU:HD13	1.90	0.54
6:F:369:ILE:HD13	6:F:421:ILE:HD13	1.89	0.54
6:F:629:GLY:O	6:F:630:ILE:HG13	2.07	0.54
1:A:614:ARG:CZ	12:N:98:A:H5"	2.37	0.54
24:Z:168:LYS:O	24:Z:168:LYS:NZ	2.37	0.54
2:B:1987:VAL:HG22	2:B:1988:TRP:O	2.08	0.54
3:C:772:ASN:HD21	3:C:815:GLY:N	2.06	0.54
6:F:390:LYS:HD2	6:F:410:PHE:HE1	1.73	0.54
28:G:881:MET:O	28:G:885:ILE:HD12	2.07	0.54
8:I:57:TYR:CZ	8:I:70:LEU:CD1	2.89	0.54
11:L:19:U:O2	15:P:175:PRO:CD	2.55	0.54
16:Q:215:PRO:CG	16:Q:217:TRP:CE3	2.91	0.54
1:A:1447:TRP:HB3	1:A:1451:PHE:CE2	2.43	0.54
1:A:2408:GLN:NE2	1:A:2408:GLN:HA	2.21	0.54
2:B:1610:LEU:HD23	2:B:1636:GLY:HA3	1.89	0.54
6:F:368:GLY:HA2	6:F:380:LEU:O	2.08	0.54
6:F:673:ASP:OD1	6:F:674:THR:N	2.41	0.54
28:G:18:GLN:HG3	28:G:19:LEU:N	2.23	0.54
15:P:301:LEU:HG	15:P:302:GLN:O	2.07	0.54
1:A:2262:GLN:HE22	1:A:2266:LEU:HD12	1.73	0.54
2:B:1549:GLN:NE2	2:B:1566:MET:SD	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:492:LEU:HD22	3:C:557:HIS:ND1	2.22	0.54
6:F:192:TYR:HB2	6:F:205:SER:OG	2.08	0.54
9:J:95:ASN:HD21	13:M:503:A:H1'	1.73	0.54
21:V:64:ARG:NH2	21:V:69:GLY:O	2.41	0.54
2:B:1815:VAL:HG23	2:B:1821:GLU:HA	1.90	0.54
2:B:1956:PRO:HA	2:B:1959:ASN:HD22	1.73	0.54
2:B:2049:PRO:HG3	2:B:2097:GLU:OE2	2.08	0.54
3:C:769:TYR:HA	3:C:800:TYR:HE1	1.72	0.54
3:C:697:ARG:CZ	3:C:849:GLY:HA2	2.38	0.54
6:F:324:ASN:ND2	6:F:339:ASP:OD2	2.41	0.54
6:F:780:LEU:HD21	6:F:862:VAL:HG21	1.90	0.54
14:O:332:ARG:HD3	14:O:341:LEU:HD11	1.88	0.54
20:U:40:LEU:O	20:U:44:ASN:ND2	2.40	0.54
15:P:319:HIS:CE1	22:W:264:GLU:CD	2.77	0.54
23:Y:713:GLN:O	23:Y:716:ASN:CG	2.46	0.54
24:Z:177:LEU:CD2	24:Z:194:LEU:CD2	2.73	0.54
1:A:1145:MET:HE3	1:A:1160:LEU:HD13	1.90	0.54
1:A:1308:GLU:HG2	1:A:1311:LYS:HD2	1.90	0.54
1:A:1999:ILE:HD11	1:A:2007:ARG:NH2	2.23	0.54
2:B:2017:TYR:OH	2:B:2049:PRO:O	2.24	0.54
13:M:509:A:N1	28:G:499:ASN:HB3	2.23	0.54
28:G:695:ASN:HD22	28:G:700:VAL:HG21	1.73	0.54
12:N:93:U:O2	12:N:93:U:H2'	2.08	0.54
14:O:152:ASN:HD21	14:O:409:LYS:HB3	1.72	0.54
20:U:145:PHE:HB3	20:U:152:LEU:HD11	1.90	0.54
22:W:224:PHE:O	22:W:225:ALA:HB3	2.07	0.54
24:Z:192:GLU:O	24:Z:195:GLU:HG2	2.08	0.54
2:B:2140:LEU:HD13	2:B:2160:ILE:HG12	1.89	0.53
6:F:653:TYR:HE2	6:F:655:LYS:HZ2	1.54	0.53
28:G:618:GLN:HE21	28:G:657:GLU:HB2	1.73	0.53
10:K:44:GLN:O	10:K:50:LEU:HD12	2.08	0.53
16:Q:226:LEU:CD2	16:Q:262:PHE:HE1	2.20	0.53
21:V:90:ASP:OD2	22:W:241:PHE:CD1	2.62	0.53
1:A:2041:PRO:HG2	1:A:2043:PHE:CE2	2.43	0.53
1:A:2149:LYS:HE3	1:A:2151:GLU:HB3	1.91	0.53
2:B:1933:TYR:HB2	2:B:1947:LEU:HD21	1.89	0.53
2:B:1889:PHE:HE1	2:B:1950:ILE:HG23	1.73	0.53
2:B:1987:VAL:HG13	2:B:2150:LEU:HD22	1.89	0.53
6:F:994:LEU:HB2	6:F:1008:ILE:HD11	1.91	0.53
6:F:1173:LEU:HD21	7:H:268:ASP:OD1	2.08	0.53
8:I:80:SER:O	8:I:83:ARG:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:214:ILE:HD11	16:Q:218:LYS:HG3	1.89	0.53
17:R:13:VAL:HG13	17:R:17:GLU:HB3	1.90	0.53
22:W:213:LYS:HB3	22:W:230:SER:CB	2.38	0.53
1:A:1881:THR:OG1	1:A:1890:PHE:HB2	2.08	0.53
1:A:2359:TYR:HA	1:A:2362:MET:HB2	1.90	0.53
1:A:2409:ILE:HG22	1:A:2411:VAL:CG2	2.39	0.53
6:F:337:VAL:HG22	6:F:346:LEU:HB2	1.90	0.53
6:F:930:LEU:HD13	6:F:984:ILE:HG23	1.89	0.53
28:G:386:TYR:CB	28:G:387:PRO:CD	2.86	0.53
22:W:190:ILE:C	22:W:192:ASP:N	2.57	0.53
1:A:1561:LEU:HD12	1:A:1608:LEU:HD22	1.89	0.53
1:A:2189:LEU:HD13	1:A:2224:VAL:HG23	1.89	0.53
2:B:1214:SER:HB3	2:B:1281:GLN:HE21	1.72	0.53
2:B:1486:ALA:HB2	2:B:1745:TYR:HB3	1.89	0.53
2:B:1524:TRP:HB2	2:B:1780:ARG:HG3	1.90	0.53
2:B:770:LEU:HD22	2:B:799:SER:O	2.08	0.53
24:Z:191:ARG:HE	24:Z:192:GLU:CD	2.12	0.53
3:C:395:LYS:HB2	3:C:395:LYS:HZ3	1.71	0.53
5:E:39:G:N1	17:R:120:TYR:O	2.42	0.53
6:F:1233:SER:O	6:F:1234:LYS:HG2	2.08	0.53
28:G:372:ILE:HD13	28:G:410:LYS:HE3	1.91	0.53
6:F:1091:HIS:CE1	28:G:963:TYR:OH	2.61	0.53
16:Q:207:LEU:HB3	16:Q:210:ILE:HD11	1.90	0.53
22:W:207:THR:C	22:W:214:LEU:CD1	2.66	0.53
1:A:1851:PHE:O	1:A:1881:THR:HA	2.09	0.53
2:B:1091:GLY:O	2:B:1095:ASN:ND2	2.37	0.53
2:B:1372:LYS:HD3	2:B:1708:GLY:HA3	1.89	0.53
2:B:162:ILE:HG22	2:B:165:ARG:HH21	1.72	0.53
2:B:1457:ARG:NH1	2:B:1854:SER:O	2.39	0.53
13:M:515:U:O2	13:M:515:U:H2'	2.08	0.53
15:P:314:ALA:O	22:W:258:GLN:NE2	2.42	0.53
23:Y:704:HIS:CD2	23:Y:847:LEU:CG	2.91	0.53
1:A:1372:LYS:HG2	1:A:1383:PHE:CD2	2.44	0.53
1:A:2184:VAL:HB	1:A:2220:GLU:HG2	1.91	0.53
1:A:681:LYS:O	1:A:684:LYS:HB3	2.08	0.53
1:A:731:THR:HG21	15:P:86:ASN:HD21	1.74	0.53
2:B:1992:ASN:HD21	2:B:2005:LEU:HD13	1.73	0.53
3:C:132:ARG:HG3	3:C:132:ARG:NH1	2.20	0.53
1:A:428:LEU:HD22	3:C:896:GLY:O	2.09	0.53
6:F:1018:ASP:OD1	6:F:1019:ILE:N	2.41	0.53
28:G:945:TYR:HB3	28:G:948:ALA:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:GLU:HG2	1:A:1446:THR:HB	1.91	0.53
2:B:1547:ASN:O	2:B:1722:ILE:N	2.39	0.53
6:F:1163:ALA:HB1	6:F:1165:LYS:NZ	2.23	0.53
6:F:641:GLN:HE22	6:F:705:LEU:HD23	1.73	0.53
6:F:642:LEU:HB3	6:F:654:PHE:HB2	1.90	0.53
28:G:885:ILE:HG23	28:G:888:ILE:HD12	1.91	0.53
9:J:51:PHE:CE2	9:J:54:GLN:HG2	2.44	0.53
10:K:54:SER:HA	10:K:65:THR:HG21	1.89	0.53
15:P:305:SER:HA	22:W:221:GLU:OE1	2.09	0.53
24:Z:203:LYS:O	24:Z:204:ASP:CB	2.57	0.53
1:A:1461:TYR:HD1	1:A:1480:LEU:HD11	1.73	0.53
1:A:401:PRO:O	1:A:402:TRP:HB3	2.09	0.53
2:B:483:LEU:HB2	2:B:488:GLN:HG2	1.90	0.53
3:C:183:GLN:HE22	3:C:654:CYS:HA	1.74	0.53
3:C:200:CYS:SG	3:C:210:ILE:HD12	2.49	0.53
6:F:1117:HIS:O	6:F:1133:ASP:HA	2.08	0.53
28:G:489:VAL:HG12	28:G:491:ARG:H	1.74	0.53
28:G:696:LYS:HG2	28:G:697:HIS:H	1.73	0.53
17:R:117:PHE:O	17:R:129:SER:HA	2.08	0.53
21:V:82:GLN:HB3	22:W:168:GLN:NE2	2.24	0.53
23:Y:258:GLN:NE2	23:Y:290:VAL:HG13	2.22	0.53
1:A:1156:HIS:HD2	1:A:1158:ILE:HB	1.74	0.53
1:A:2409:ILE:CG2	1:A:2411:VAL:HG23	2.38	0.53
2:B:2006:GLU:HA	2:B:2009:LYS:HB3	1.90	0.53
2:B:618:ASN:HB3	2:B:621:ASN:HD22	1.74	0.53
28:G:894:HIS:O	28:G:898:ARG:HG2	2.09	0.53
13:M:516:U:H5'	28:G:291:GLU:OE2	2.09	0.53
16:Q:291:ILE:HG23	16:Q:292:PRO:HA	1.91	0.53
1:A:323:THR:O	1:A:323:THR:HG22	2.08	0.52
2:B:1334:LEU:HD22	2:B:1340:SER:HA	1.91	0.52
6:F:1031:ILE:HD11	6:F:1045:MET:SD	2.49	0.52
6:F:75:CYS:SG	6:F:94:CYS:HB3	2.48	0.52
14:O:115:TYR:HA	14:O:118:LEU:HG	1.91	0.52
14:O:132:SER:HB3	14:O:427:LYS:HB2	1.89	0.52
16:Q:209:ASN:HB3	16:Q:288:ILE:O	2.10	0.52
23:Y:361:LEU:HD21	23:Y:597:LEU:HD13	1.91	0.52
1:A:946:ASN:HB3	1:A:949:ASP:HB3	1.91	0.52
3:C:234:LEU:HD21	3:C:439:ILE:HG23	1.91	0.52
3:C:271:ASP:HB2	3:C:275:LEU:HD23	1.91	0.52
3:C:758:ASP:HB3	3:C:761:ALA:HB3	1.90	0.52
6:F:641:GLN:NE2	6:F:705:LEU:HD23	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ILE:N	18:S:173:HIS:O	2.42	0.52
19:T:104:CYS:N	19:T:153:CYS:SG	2.70	0.52
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.74	0.52
2:B:2103:LEU:HD11	2:B:2140:LEU:HD23	1.91	0.52
2:B:596:ARG:HD2	2:B:599:ILE:HD12	1.92	0.52
6:F:987:PHE:CD2	6:F:1054:LEU:HB2	2.44	0.52
6:F:299:PRO:HD2	6:F:377:PHE:CZ	2.44	0.52
13:M:506:U:H3'	13:M:506:U:O2	2.10	0.52
14:O:224:LEU:HD11	18:S:10:GLU:HA	1.92	0.52
14:O:229:THR:HG21	14:O:272:VAL:N	2.24	0.52
16:Q:253:PHE:HB3	16:Q:258:LEU:HD12	1.90	0.52
1:A:1771:THR:HA	1:A:1789:ASN:HD22	1.74	0.52
2:B:1431:ASP:OD2	2:B:2096:LEU:HG	2.10	0.52
2:B:805:HIS:O	2:B:813:ARG:HD3	2.10	0.52
9:J:101:PHE:CD2	28:G:219:HIS:CG	2.97	0.52
15:P:319:HIS:CD2	15:P:320:GLU:N	2.78	0.52
21:V:17:LEU:HD23	22:W:249:GLN:OE1	2.09	0.52
23:Y:467:LYS:CB	23:Y:494:CYS:CA	2.88	0.52
24:Z:118:LEU:HB3	24:Z:154:VAL:HG22	1.90	0.52
1:A:1069:LEU:HD23	1:A:1120:VAL:HG21	1.90	0.52
1:A:2198:ASP:OD1	1:A:2199:VAL:N	2.42	0.52
1:A:749:ARG:HG3	1:A:753:TYR:CE2	2.45	0.52
2:B:1335:GLY:N	2:B:1360:TYR:OH	2.43	0.52
3:C:251:GLN:NE2	3:C:255:GLN:HE21	2.05	0.52
3:C:486:VAL:HG11	3:C:564:ILE:HD11	1.91	0.52
6:F:332:GLU:HG2	6:F:333:ASN:N	2.25	0.52
6:F:504:HIS:CD2	6:F:511:ILE:HD11	2.45	0.52
28:G:904:GLU:OE2	28:G:940:ASN:HB2	2.10	0.52
11:L:6:U:H2'	11:L:7:C:C6	2.44	0.52
12:N:106:A:H2'	12:N:107:U:O4'	2.08	0.52
1:A:1465:ARG:HG3	15:P:301:LEU:HD13	1.91	0.52
15:P:301:LEU:O	15:P:302:GLN:HG2	2.10	0.52
15:P:318:ARG:HG2	15:P:319:HIS:O	2.09	0.52
21:V:50:VAL:HG12	22:W:237:ARG:CD	2.40	0.52
1:A:1679:GLU:OE2	1:A:1706:VAL:HA	2.10	0.52
1:A:1790:TRP:HZ3	1:A:1798:ILE:HD12	1.75	0.52
1:A:180:PRO:O	1:A:181:HIS:HB2	2.08	0.52
1:A:653:ILE:HD11	1:A:704:TRP:CE2	2.45	0.52
2:B:1343:PHE:HE2	2:B:1385:LEU:HD11	1.75	0.52
2:B:778:LYS:HG2	2:B:782:LYS:HE3	1.90	0.52
2:B:947:ARG:HB3	2:B:955:TYR:CE2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:786:GLY:HA2	28:G:823:MET:HB3	1.91	0.52
16:Q:208:TYR:HB2	16:Q:290:ILE:HD12	1.92	0.52
16:Q:43:LEU:HD11	16:Q:57:LYS:HG3	1.91	0.52
23:Y:240:GLN:HG3	23:Y:373:LYS:HG2	1.92	0.52
23:Y:271:LEU:CG	23:Y:341:SER:OG	2.57	0.52
1:A:1017:ASP:O	1:A:1509:ARG:NH2	2.43	0.52
1:A:1211:SER:OG	1:A:1268:ARG:NH1	2.43	0.52
2:B:828:LEU:HG	2:B:830:CYS:SG	2.50	0.52
3:C:178:LEU:CD1	3:C:214:ASP:HB2	2.40	0.52
3:C:629:TYR:OH	3:C:658:ASP:OD2	2.25	0.52
3:C:681:CYS:HB3	3:C:850:LEU:HD12	1.92	0.52
3:C:869:HIS:HD2	3:C:925:LEU:HB3	1.75	0.52
1:A:947:PRO:HB3	28:G:48:LEU:HD13	1.92	0.52
28:G:801:ILE:HG22	28:G:816:VAL:HG13	1.92	0.52
28:G:794:PRO:HG2	28:G:827:ILE:HD13	1.90	0.52
16:Q:217:TRP:CD2	17:R:187:LYS:HD3	2.44	0.52
24:Z:197:LEU:HD12	24:Z:197:LEU:C	2.29	0.52
2:B:1260:THR:OG1	2:B:1262:ASP:OD1	2.25	0.52
2:B:1400:PRO:HG3	2:B:1478:GLU:HG3	1.91	0.52
2:B:457:LYS:HB3	2:B:458:PRO:HD2	1.92	0.52
7:H:172:VAL:HG23	28:G:934:PHE:CE2	2.45	0.52
8:I:55:ASN:HB2	8:I:56:PRO:CD	2.40	0.52
16:Q:256:SER:O	16:Q:259:GLY:CA	2.58	0.52
18:S:9:LEU:CD2	18:S:11:ALA:N	2.72	0.52
24:Z:181:LEU:CD2	24:Z:191:ARG:HG3	2.39	0.52
1:A:1285:VAL:HG22	1:A:1301:TYR:HD1	1.75	0.52
1:A:1304:VAL:H	1:A:1353:THR:HG21	1.74	0.52
1:A:1372:LYS:HB3	1:A:1377:SER:O	2.10	0.52
1:A:1751:TYR:O	1:A:1755:LYS:HG2	2.10	0.52
1:A:2071:ILE:HG13	1:A:2074:LEU:HD12	1.92	0.52
1:A:701:CYS:SG	1:A:702:GLY:N	2.81	0.52
2:B:1331:THR:HA	2:B:1334:LEU:HD13	1.91	0.52
2:B:2099:TRP:HB2	2:B:2117:VAL:HG23	1.91	0.52
3:C:395:LYS:HZ2	3:C:395:LYS:HB2	1.73	0.52
1:A:389:HIS:HB2	3:C:653:ASP:OD1	2.10	0.52
6:F:71:PHE:O	6:F:430:LEU:HD21	2.10	0.52
6:F:678:LYS:HD2	6:F:727:ASP:HA	1.90	0.52
16:Q:219:ILE:O	16:Q:222:THR:OG1	2.16	0.52
1:A:2309:ASP:HA	1:A:2312:TYR:HD2	1.74	0.52
2:B:1256:VAL:O	2:B:1556:HIS:NE2	2.43	0.52
2:B:1820:ILE:HA	2:B:1846:THR:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ALA:HB2	2:B:704:SER:HB3	1.90	0.52
6:F:180:THR:HG21	6:F:188:SER:CB	2.40	0.52
28:G:894:HIS:O	28:G:898:ARG:CG	2.58	0.52
17:R:143:ASP:O	17:R:146:LEU:N	2.42	0.52
21:V:49:THR:CG2	22:W:233:ASP:HB2	2.40	0.52
1:A:1755:LYS:HE3	1:A:1759:TYR:CE2	2.45	0.51
1:A:1828:SER:HB3	28:G:612:LYS:HD3	1.92	0.51
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.23	0.51
1:A:614:ARG:HG2	1:A:614:ARG:NH1	2.12	0.51
2:B:134:ASP:OD2	2:B:748:LYS:HB2	2.11	0.51
2:B:1554:VAL:HG23	2:B:1557:ILE:HD11	1.92	0.51
3:C:253:ILE:O	3:C:257:ILE:HG13	2.09	0.51
3:C:794:GLN:HE21	3:C:835:LYS:HE3	1.75	0.51
28:G:539:HIS:O	28:G:543:ARG:CG	2.58	0.51
7:H:153:ASP:OD2	11:L:58:A:OP1	2.28	0.51
21:V:105:ASP:OD1	21:V:106:HIS:N	2.43	0.51
24:Z:150:LEU:O	24:Z:154:VAL:HG23	2.10	0.51
24:Z:416:GLY:O	24:Z:420:ILE:HD12	2.10	0.51
1:A:218:SER:HB2	1:A:317:PRO:HG2	1.93	0.51
2:B:569:GLU:OE1	2:B:572:ARG:NH2	2.40	0.51
4:D:81:A:H4'	4:D:82:A:OP2	2.10	0.51
6:F:59:TYR:CD2	6:F:1237:VAL:HG21	2.45	0.51
6:F:333:ASN:O	6:F:350:ILE:HG22	2.10	0.51
15:P:85:SER:O	15:P:87:ASN:N	2.43	0.51
17:R:14:LYS:CE	17:R:14:LYS:CA	2.87	0.51
17:R:161:ARG:O	17:R:165:SER:HB3	2.09	0.51
1:A:1180:GLU:HA	1:A:1183:THR:HG22	1.93	0.51
1:A:1281:ASN:ND2	1:A:1285:VAL:HB	2.25	0.51
1:A:1496:GLN:NE2	1:A:1531:HIS:O	2.42	0.51
1:A:258:ILE:HG22	1:A:259:GLU:O	2.10	0.51
1:A:285:PRO:HD2	1:A:298:TYR:OH	2.10	0.51
2:B:708:CYS:SG	2:B:729:LYS:HE2	2.51	0.51
3:C:277:LEU:HB3	3:C:279:LEU:HD13	1.91	0.51
6:F:929:ILE:HG12	6:F:941:PHE:HD1	1.75	0.51
9:J:51:PHE:CZ	9:J:54:GLN:CB	2.93	0.51
9:J:51:PHE:CZ	9:J:54:GLN:CG	2.93	0.51
15:P:40:LEU:HG	15:P:41:ASP:N	2.23	0.51
23:Y:308:PHE:HA	23:Y:743:GLN:HG3	1.91	0.51
1:A:1038:ILE:HG13	1:A:1039:TRP:N	2.25	0.51
1:A:140:ARG:HH21	1:A:252:GLU:CB	2.24	0.51
1:A:212:VAL:O	1:A:216:GLN:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:TRP:CH2	2:B:177:ILE:HD11	2.46	0.51
2:B:1398:ILE:HB	2:B:1473:TYR:HD1	1.74	0.51
2:B:1342:VAL:HB	2:B:1415:ARG:HH11	1.75	0.51
3:C:145:GLY:O	3:C:149:LEU:N	2.43	0.51
28:G:476:ARG:HG2	28:G:513:LEU:HD22	1.93	0.51
28:G:542:THR:HG22	28:G:582:GLY:CA	2.39	0.51
14:O:156:ILE:HD13	14:O:197:LEU:HD22	1.91	0.51
17:R:212:TRP:O	17:R:215:ARG:HD3	2.10	0.51
24:Z:177:LEU:HD21	24:Z:194:LEU:CD2	2.37	0.51
1:A:1739:ARG:HG2	1:A:1740:TYR:N	2.26	0.51
1:A:922:VAL:HG22	1:A:1519:LEU:HD21	1.93	0.51
2:B:1580:SER:O	2:B:1677:THR:OG1	2.29	0.51
2:B:158:GLU:OE2	2:B:165:ARG:NH2	2.43	0.51
6:F:328:VAL:HG22	6:F:337:VAL:HG12	1.91	0.51
6:F:936:PRO:C	6:F:937:LYS:HD2	2.30	0.51
16:Q:209:ASN:HD21	16:Q:288:ILE:CG2	2.23	0.51
24:Z:179:TYR:CD1	24:Z:179:TYR:C	2.84	0.51
1:A:640:ARG:CG	1:A:640:ARG:HH11	2.23	0.51
3:C:318:LEU:HB3	3:C:425:LEU:HD12	1.93	0.51
3:C:391:MET:HE3	3:C:395:LYS:HE2	1.81	0.51
28:G:408:ARG:HA	28:G:412:LEU:HB2	1.92	0.51
7:H:234:GLN:HB3	7:H:235:PRO:HA	1.93	0.51
13:M:491:C:H2'	13:M:492:U:O4'	2.10	0.51
1:A:161:PHE:CE2	12:N:101:U:C4	37.05	0.51
16:Q:69:ASN:HD22	16:Q:126:THR:HB	1.73	0.51
20:U:40:LEU:CG	20:U:49:ALA:HB2	2.37	0.51
21:V:81:ASP:HB2	22:W:167:VAL:HG21	1.92	0.51
23:Y:651:PHE:HB2	23:Y:783:PHE:HE1	1.76	0.51
1:A:1082:ILE:HG23	1:A:1113:ILE:HD11	1.92	0.51
1:A:1268:ARG:HE	1:A:1301:TYR:HD2	1.57	0.51
1:A:1466:GLN:O	1:A:1470:GLN:HB2	2.11	0.51
1:A:1843:LEU:H	1:A:1843:LEU:HD23	1.74	0.51
3:C:109:LEU:HD21	4:D:43:G:C6	2.45	0.51
6:F:1169:ASP:O	6:F:1172:THR:OG1	2.16	0.51
6:F:666:LEU:HA	6:F:667:THR:OG1	2.10	0.51
28:G:925:HIS:CG	28:G:926:PRO:HD2	2.46	0.51
9:J:95:ASN:HD21	13:M:503:A:C1'	2.24	0.51
12:N:110:U:H2'	12:N:110:U:O2	2.11	0.51
22:W:167:VAL:HG13	22:W:209:LEU:CD2	2.41	0.51
22:W:223:ARG:HG3	22:W:242:GLU:OE2	2.11	0.51
24:Z:368:ASN:HA	24:Z:372:ASP:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1543:ARG:HD3	15:P:328:LEU:HD13	1.93	0.51
1:A:1711:VAL:HG11	1:A:1789:ASN:HB3	1.93	0.51
2:B:1398:ILE:O	2:B:1474:ASP:N	2.36	0.51
2:B:1958:ILE:HD13	2:B:1979:LEU:HD23	1.92	0.51
3:C:141:PRO:O	3:C:146:LYS:NZ	2.44	0.51
3:C:801:TRP:CD1	3:C:843:LYS:HD2	2.46	0.51
3:C:715:MET:HG2	3:C:817:GLN:HB2	1.92	0.51
6:F:67:LYS:NZ	6:F:119:ASN:HD21	2.09	0.51
6:F:704:SER:O	6:F:705:LEU:HD12	2.11	0.51
15:P:301:LEU:HD11	15:P:303:TYR:CZ	2.45	0.51
16:Q:205:PHE:CD2	16:Q:291:ILE:HD11	2.46	0.51
22:W:208:SER:CB	22:W:214:LEU:HD12	2.41	0.51
1:A:1008:LEU:CD2	1:A:1073:ILE:HD11	2.41	0.51
1:A:1211:SER:O	1:A:1257:ASN:ND2	2.44	0.51
1:A:2194:ILE:HD11	1:A:2293:ILE:HG21	1.92	0.51
1:A:329:TYR:CD2	1:A:330:LEU:HG	2.45	0.51
1:A:380:ARG:CZ	1:A:380:ARG:CB	2.89	0.51
1:A:484:PHE:CD1	4:D:81:A:C6	2.99	0.51
1:A:839:HIS:ND1	4:D:95:C:O2	2.43	0.51
28:G:338:GLN:O	28:G:341:GLY:N	2.44	0.51
28:G:591:ASP:OD1	28:G:592:ILE:HD12	2.09	0.51
28:G:823:MET:O	28:G:827:ILE:HG12	2.10	0.51
22:W:217:LYS:HB3	22:W:218:PRO:HD2	1.93	0.51
1:A:1253:LYS:O	1:A:1274:ARG:NH2	2.44	0.51
1:A:1386:ALA:O	1:A:1390:THR:HG23	2.11	0.51
2:B:1476:ALA:HB3	2:B:1512:SER:HB2	1.92	0.51
3:C:104:THR:HG22	3:C:181:LEU:HA	1.93	0.51
6:F:856:ASP:OD1	6:F:857:VAL:N	2.43	0.51
10:K:39:THR:HG22	28:G:950:VAL:HG13	1.92	0.51
20:U:76:THR:OG1	20:U:205:HIS:NE2	2.34	0.51
23:Y:699:GLU:C	23:Y:702:SER:CB	2.79	0.51
1:A:1057:MET:CE	1:A:1114:PHE:CE1	2.92	0.50
1:A:1057:MET:HG3	1:A:1239:THR:CG2	2.41	0.50
1:A:1389:TYR:CE1	1:A:1401:SER:HB3	2.46	0.50
1:A:261:LEU:HD22	1:A:642:GLY:HA2	1.94	0.50
1:A:333:LYS:O	1:A:336:PHE:N	2.44	0.50
2:B:1351:ILE:HD12	2:B:1374:THR:HG21	1.92	0.50
2:B:1686:ASN:HB3	2:B:1695:TYR:HB3	1.93	0.50
2:B:563:LEU:O	2:B:567:VAL:HG23	2.11	0.50
2:B:675:PRO:HD2	2:B:906:LEU:O	2.11	0.50
1:A:461:LEU:HD11	3:C:380:PRO:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:TYR:CD1	3:C:548:ARG:CD	2.94	0.50
6:F:493:VAL:HG13	6:F:499:SER:OG	2.10	0.50
14:O:221:TYR:O	14:O:251:TRP:HH2	1.93	0.50
17:R:22:ILE:CG2	17:R:30:PHE:CE2	2.93	0.50
17:R:72:PHE:HD1	17:R:90:LEU:HB2	1.76	0.50
21:V:19:PRO:HA	21:V:22:SER:OG	2.11	0.50
21:V:33:ILE:HG22	21:V:85:THR:HG23	1.94	0.50
23:Y:353:LEU:HD21	23:Y:582:ILE:HA	1.93	0.50
1:A:928:ARG:CD	1:A:1582:GLU:OE2	2.51	0.50
1:A:228:LYS:HG2	1:A:695:LEU:CD1	2.40	0.50
2:B:1877:LYS:HE3	2:B:1912:ARG:O	2.10	0.50
3:C:711:ALA:HB2	3:C:821:LEU:HD11	1.93	0.50
6:F:1323:CYS:HB3	6:F:1353:ILE:HD12	1.93	0.50
28:G:624:CYS:O	28:G:628:ILE:HG12	2.11	0.50
28:G:763:LEU:O	28:G:766:LEU:N	2.44	0.50
8:I:42:TYR:HB2	8:I:45:GLN:HG3	1.93	0.50
1:A:879:ALA:HB1	15:P:208:LEU:HD21	1.94	0.50
16:Q:222:THR:HA	16:Q:225:GLN:HE21	1.76	0.50
30:X:9:LYS:O	30:X:10:SER:OG	2.26	0.50
1:A:1458:TRP:CD1	28:G:24:SER:O	2.64	0.50
1:A:1889:LEU:HG	1:A:1991:ILE:HG13	1.94	0.50
3:C:667:GLU:OE1	3:C:667:GLU:N	2.44	0.50
3:C:715:MET:HB2	3:C:720:ILE:HD11	1.93	0.50
7:H:192:ARG:CB	7:H:192:ARG:CZ	2.89	0.50
23:Y:699:GLU:H	23:Y:706:LEU:CG	2.24	0.50
2:B:1486:ALA:HB1	2:B:1746:LEU:HA	1.92	0.50
3:C:778:THR:HG23	3:C:781:ASP:H	1.77	0.50
6:F:1295:GLY:O	6:F:1299:ILE:N	2.43	0.50
6:F:820:VAL:HA	6:F:828:VAL:HA	1.93	0.50
10:K:22:GLY:CA	28:G:935:TRP:CZ3	2.92	0.50
7:H:155:ARG:NH2	7:H:156:TYR:HE1	2.08	0.50
7:H:262:HIS:CG	7:H:283:LYS:HZ2	2.28	0.50
8:I:18:SER:O	8:I:21:GLN:N	2.37	0.50
20:U:45:LYS:HD3	20:U:126:VAL:HA	1.92	0.50
24:Z:368:ASN:O	24:Z:373:ILE:HG12	2.11	0.50
1:A:1690:LYS:HE2	1:A:1700:ASP:OD1	2.11	0.50
1:A:1997:ASP:HB2	1:A:1998:ARG:HD2	1.93	0.50
1:A:470:LEU:HD13	3:C:391:MET:SD	2.51	0.50
2:B:1063:ILE:HB	2:B:1081:GLN:NE2	2.26	0.50
2:B:1397:TYR:HD2	2:B:1446:LEU:HG	1.76	0.50
2:B:761:PHE:HD2	2:B:770:LEU:HD12	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1136:GLY:HA2	6:F:1197:ASP:O	2.11	0.50
6:F:610:ILE:CG2	6:F:618:TYR:HB3	2.42	0.50
9:J:100:HIS:O	9:J:103:LYS:HG2	2.12	0.50
13:M:508:U:H3'	13:M:508:U:OP2	2.11	0.50
14:O:391:GLU:HG3	14:O:392:MET:H	1.76	0.50
17:R:142:ILE:CG2	17:R:180:ASN:HD22	2.25	0.50
17:R:63:ARG:HD3	17:R:86:LYS:HA	1.94	0.50
23:Y:223:LEU:HD13	23:Y:251:GLY:HA3	1.94	0.50
23:Y:475:TYR:HE2	23:Y:477:ASN:CG	2.15	0.50
23:Y:699:GLU:O	23:Y:702:SER:CB	2.59	0.50
1:A:487:ASN:OD1	1:A:488:ARG:HG3	2.11	0.50
2:B:1057:LEU:HD21	2:B:1089:PHE:CE1	2.44	0.50
6:F:194:GLU:HG2	6:F:242:VAL:HB	1.93	0.50
6:F:477:ILE:O	6:F:479:SER:N	2.40	0.50
6:F:493:VAL:O	6:F:499:SER:OG	2.18	0.50
8:I:63:SER:HB3	28:G:810:THR:HG22	1.93	0.50
23:Y:429:HIS:O	23:Y:495:ARG:NH1	2.45	0.50
1:A:2208:TYR:HB2	1:A:2223:THR:HB	1.94	0.50
2:B:1429:GLY:HA3	2:B:1451:GLN:NE2	2.26	0.50
2:B:846:ILE:HG12	2:B:887:ILE:HB	1.93	0.50
3:C:660:ARG:HH22	3:C:670:ILE:HD12	1.75	0.50
3:C:287:LYS:NZ	3:C:895:ALA:O	2.26	0.50
6:F:1042:LEU:HD21	6:F:1085:LEU:HD11	1.94	0.50
28:G:177:ASN:OD1	28:G:178:THR:N	2.44	0.50
28:G:855:GLN:HG3	28:G:895:ALA:HA	1.92	0.50
16:Q:205:PHE:O	16:Q:250:GLY:HA2	2.11	0.50
20:U:45:LYS:O	20:U:46:GLU:C	2.51	0.50
22:W:167:VAL:CG1	22:W:209:LEU:HD23	2.42	0.50
1:A:1156:HIS:CD2	1:A:1158:ILE:HB	2.47	0.50
1:A:1368:GLN:NE2	1:A:1389:TYR:OH	2.45	0.50
1:A:2409:ILE:CG2	1:A:2411:VAL:CG2	2.90	0.50
1:A:665:GLY:HA2	1:A:667:TYR:CE2	2.47	0.50
1:A:653:ILE:HD11	1:A:704:TRP:NE1	2.27	0.50
2:B:1994:LEU:HA	2:B:1997:ILE:HD12	1.94	0.50
2:B:772:LYS:NZ	6:F:758:VAL:HG23	2.27	0.50
28:G:232:LEU:HD12	28:G:233:GLY:N	2.27	0.50
28:G:922:GLY:HA3	28:G:934:PHE:CE2	2.47	0.50
28:G:958:ASP:OD1	28:G:959:ASN:N	2.45	0.50
7:H:155:ARG:HH22	7:H:156:TYR:HE1	1.58	0.50
7:H:166:THR:CG2	7:H:167:LYS:N	2.73	0.50
14:O:304:LEU:HD13	14:O:334:TRP:CD2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:105:LEU:O	15:P:108:ASN:N	2.38	0.50
14:O:342:LEU:O	15:P:45:PRO:HB2	2.12	0.50
17:R:164:PHE:HE1	17:R:199:MET:HG3	1.77	0.50
17:R:210:LYS:CG	17:R:211:GLU:N	2.75	0.50
17:R:72:PHE:CE2	17:R:94:PRO:HG3	2.46	0.50
23:Y:277:GLN:O	23:Y:324:ASP:N	2.44	0.50
1:A:1490:ARG:HE	1:A:1536:LEU:HD23	1.76	0.50
2:B:1241:LEU:HD11	2:B:1290:LEU:HD11	1.92	0.50
2:B:1262:ASP:OD1	2:B:1263:ILE:N	2.44	0.50
2:B:479:GLU:O	2:B:482:SER:OG	2.22	0.50
6:F:1065:THR:HG21	6:F:1106:PHE:H	1.77	0.50
28:G:887:ASN:HB3	28:G:899:ILE:HD13	1.93	0.50
7:H:268:ASP:O	28:G:882:ASN:HB3	2.12	0.50
14:O:319:LYS:O	15:P:57:LEU:HG	2.12	0.50
16:Q:215:PRO:CG	16:Q:217:TRP:CZ3	2.91	0.50
20:U:45:LYS:HE3	20:U:46:GLU:N	2.27	0.50
20:U:38:LEU:HD22	21:V:49:THR:HB	1.94	0.50
23:Y:437:ASP:HB2	23:Y:513:ILE:HD13	1.94	0.50
1:A:1458:TRP:NE1	1:A:1489:PRO:HD2	2.27	0.49
1:A:1831:GLN:O	1:A:1833:PRO:N	2.45	0.49
2:B:477:LEU:HD12	6:F:660:SER:HB2	1.94	0.49
3:C:218:HIS:HB3	3:C:221:PHE:CD2	2.46	0.49
3:C:864:VAL:HG12	3:C:866:ILE:HG13	1.94	0.49
6:F:68:GLN:HA	6:F:1223:GLY:O	2.11	0.49
6:F:1224:THR:HG22	6:F:1225:VAL:N	2.27	0.49
6:F:929:ILE:HG12	6:F:941:PHE:CD1	2.47	0.49
28:G:166:LEU:HD21	28:G:195:PHE:CD2	2.47	0.49
14:O:188:VAL:HG13	14:O:197:LEU:HD11	1.93	0.49
17:R:206:LEU:HB3	17:R:209:ASP:CG	2.33	0.49
24:Z:179:TYR:O	24:Z:179:TYR:HD1	1.95	0.49
24:Z:184:GLN:HE21	24:Z:185:GLU:N	2.09	0.49
1:A:1589:LYS:O	8:I:16:ILE:CG1	2.45	0.49
1:A:2412:PHE:HD1	1:A:2413:SER:H	1.58	0.49
1:A:284:ARG:NH1	4:D:33:U:O4	2.46	0.49
1:A:319:ARG:HD3	1:A:486:PHE:CE2	2.46	0.49
1:A:849:LEU:CD1	1:A:973:GLU:HB3	2.42	0.49
2:B:1331:THR:OG1	2:B:1345:PHE:O	2.19	0.49
2:B:517:MET:SD	2:B:666:ARG:NH2	2.85	0.49
6:F:1097:PHE:CE1	6:F:1108:PRO:HB3	2.46	0.49
6:F:157:LEU:O	6:F:176:ASN:HA	2.11	0.49
6:F:369:ILE:HG23	6:F:419:LEU:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:25:A:H3'	11:L:26:G:C5'	2.41	0.49
4:D:96:U:H3	12:N:99:G:H1	1.58	0.49
16:Q:209:ASN:HD21	16:Q:288:ILE:HG23	1.78	0.49
17:R:46:ARG:HH12	17:R:222:LEU:HG	1.77	0.49
24:Z:299:LEU:HD21	24:Z:343:TYR:HE1	1.77	0.49
1:A:1632:ILE:HD11	1:A:1649:PHE:CE2	2.48	0.49
1:A:1711:VAL:CG1	1:A:1789:ASN:HB3	2.43	0.49
1:A:1816:ARG:NH1	1:A:1816:ARG:HG2	2.15	0.49
1:A:2412:PHE:CD1	1:A:2413:SER:N	2.78	0.49
1:A:147:SER:HG	1:A:573:ARG:HH22	1.59	0.49
2:B:1936:ARG:NH2	2:B:1985:GLN:O	2.40	0.49
3:C:292:ILE:O	3:C:296:ASN:ND2	2.45	0.49
6:F:217:ASP:OD1	6:F:218:TYR:N	2.45	0.49
6:F:391:LEU:HA	6:F:406:GLN:O	2.12	0.49
7:H:153:ASP:OD2	11:L:57:A:O3'	2.29	0.49
14:O:197:LEU:O	14:O:209:TRP:N	2.44	0.49
17:R:15:GLU:HA	17:R:18:LEU:HD11	1.92	0.49
20:U:101:ARG:N	20:U:104:TYR:OH	2.38	0.49
23:Y:441:PHE:HE2	23:Y:516:VAL:HG13	1.76	0.49
2:B:1580:SER:N	2:B:1678:ASP:OD2	2.44	0.49
2:B:177:ILE:HD13	2:B:182:PHE:HD1	1.76	0.49
3:C:727:THR:H	3:C:736:ASP:HB2	1.78	0.49
3:C:79:GLU:OE1	15:P:205:SER:OG	49.52	0.49
3:C:918:LEU:HD23	3:C:928:CYS:HB2	1.93	0.49
6:F:1042:LEU:HD13	6:F:1051:LEU:HD13	1.93	0.49
6:F:1305:GLN:O	6:F:1309:SER:HB3	2.12	0.49
6:F:238:LEU:O	6:F:255:LEU:HB2	2.12	0.49
28:G:334:ILE:HG22	28:G:377:THR:HG21	1.94	0.49
28:G:386:TYR:HB3	28:G:387:PRO:HD2	1.95	0.49
17:R:210:LYS:CE	17:R:210:LYS:CA	2.90	0.49
23:Y:224:PRO:HG3	23:Y:401:ARG:HD2	1.95	0.49
23:Y:346:ASP:OD1	23:Y:347:GLU:N	2.45	0.49
1:A:1475:LEU:HD13	15:P:301:LEU:HD12	1.93	0.49
1:A:1511:ARG:O	1:A:1515:LYS:HG2	2.12	0.49
1:A:1664:ASP:OD2	1:A:1809:ASN:ND2	2.45	0.49
1:A:854:ARG:HG2	1:A:854:ARG:NH2	2.20	0.49
2:B:1750:ILE:HD11	2:B:1773:PHE:HE1	1.76	0.49
2:B:714:ASN:HD22	2:B:717:LYS:HE2	1.78	0.49
3:C:736:ASP:OD1	3:C:737:ILE:N	2.45	0.49
6:F:59:TYR:CE2	6:F:1316:LYS:HD2	2.48	0.49
6:F:71:PHE:CD2	6:F:95:VAL:HG11	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:166:LEU:HD11	28:G:195:PHE:HB3	1.94	0.49
1:A:777:LYS:HB3	11:L:18:U:C4	2.48	0.49
16:Q:227:LEU:HD21	16:Q:262:PHE:HD1	1.78	0.49
20:U:176:ARG:HH21	20:U:178:ILE:HD13	1.76	0.49
20:U:38:LEU:HD23	21:V:49:THR:CG2	2.41	0.49
22:W:167:VAL:HG11	22:W:209:LEU:HD23	1.94	0.49
21:V:91:ASN:O	22:W:239:ASN:CB	2.60	0.49
1:A:1932:GLN:HG2	1:A:1955:ALA:HB3	1.95	0.49
1:A:589:THR:HG21	17:R:31:ASN:ND2	2.27	0.49
2:B:493:SER:O	2:B:497:THR:N	2.45	0.49
2:B:618:ASN:OD1	2:B:619:SER:N	2.46	0.49
3:C:706:LEU:HD23	3:C:826:PRO:HD3	1.94	0.49
9:J:8:LEU:HD13	9:J:89:ILE:HG21	1.95	0.49
16:Q:220:THR:HG23	16:Q:240:LEU:HD23	1.94	0.49
17:R:152:LYS:CG	17:R:153:PRO:HD2	2.43	0.49
22:W:167:VAL:CG1	22:W:209:LEU:CD2	2.91	0.49
1:A:763:MET:HE1	1:A:779:ALA:CB	2.43	0.49
3:C:968:MET:O	3:C:972:ARG:NH1	2.46	0.49
19:T:114:THR:OG1	19:T:118:SER:HA	2.13	0.49
1:A:2410:ASP:OD1	1:A:2412:PHE:HE1	1.94	0.49
1:A:394:ARG:CG	1:A:394:ARG:NH1	2.73	0.49
2:B:159:ASP:HB3	2:B:165:ARG:NH1	2.28	0.49
3:C:618:LEU:HD13	3:C:666:ILE:HD11	1.94	0.49
1:A:839:HIS:CE1	4:D:95:C:O2	2.65	0.49
28:G:361:ASP:OD1	28:G:362:CYS:N	2.46	0.49
28:G:368:VAL:N	28:G:369:PRO:HD2	2.28	0.49
7:H:155:ARG:HH21	7:H:155:ARG:CG	2.26	0.49
13:M:506:U:OP2	28:G:698:ARG:CD	2.61	0.49
16:Q:69:ASN:ND2	16:Q:126:THR:CB	2.73	0.49
17:R:206:LEU:HD12	17:R:207:PRO:HD3	1.94	0.49
21:V:91:ASN:O	22:W:239:ASN:HB3	2.12	0.49
1:A:2204:ALA:HA	1:A:2260:HIS:HA	1.95	0.49
2:B:1916:HIS:O	2:B:1917:THR:OG1	2.19	0.49
2:B:727:TYR:HE1	2:B:761:PHE:CE1	2.31	0.49
3:C:539:VAL:HG13	3:C:564:ILE:HG23	1.94	0.49
6:F:977:ILE:HG12	6:F:1004:LEU:HD22	1.94	0.49
28:G:790:LYS:HD2	28:G:826:TYR:HB3	1.94	0.49
9:J:7:ASP:OD1	9:J:8:LEU:N	2.46	0.49
13:M:484:A:H3'	13:M:484:A:H8	1.78	0.49
16:Q:84:ILE:HA	16:Q:87:ARG:HG2	1.94	0.49
17:R:22:ILE:O	17:R:22:ILE:HG13	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:232:PRO:HA	17:R:235:GLN:HB3	1.94	0.49
20:U:50:LEU:CB	20:U:139:GLN:HE22	2.26	0.49
23:Y:277:GLN:N	23:Y:322:MET:O	2.45	0.49
1:A:831:ARG:HH11	1:A:848:ASN:ND2	2.11	0.49
3:C:272:ARG:HG3	3:C:276:ASP:OD2	2.13	0.49
6:F:759:ASP:OD1	6:F:760:GLY:N	2.44	0.49
6:F:831:THR:OG1	6:F:835:VAL:O	2.14	0.49
28:G:674:ASP:OD1	28:G:675:LEU:N	2.46	0.49
7:H:192:ARG:NH1	7:H:192:ARG:CB	2.76	0.49
9:J:8:LEU:CD2	9:J:93:GLY:HA3	2.43	0.49
14:O:229:THR:HG21	14:O:272:VAL:H	1.78	0.49
16:Q:217:TRP:CE3	17:R:187:LYS:HD3	2.47	0.49
22:W:167:VAL:O	22:W:171:GLY:N	2.45	0.49
1:A:1747:ASP:OD1	1:A:1747:ASP:N	2.29	0.48
3:C:567:ILE:HG22	3:C:571:TYR:HE1	1.78	0.48
3:C:772:ASN:HD21	3:C:815:GLY:H	1.61	0.48
6:F:1227:CYS:SG	6:F:1229:ILE:HD11	2.53	0.48
6:F:1233:SER:CB	6:F:1236:ASN:H	2.26	0.48
6:F:819:VAL:O	6:F:819:VAL:HG23	2.13	0.48
5:E:41:A:C8	17:R:34:TYR:CD2	3.01	0.48
1:A:1755:LYS:HE3	1:A:1759:TYR:HE2	1.79	0.48
1:A:194:HIS:CD2	15:P:122:LEU:CD2	2.93	0.48
1:A:2390:VAL:O	1:A:2394:GLN:HG2	2.13	0.48
1:A:309:SER:OG	1:A:475:ASP:CB	2.56	0.48
2:B:1405:ILE:O	2:B:1409:LEU:N	2.45	0.48
2:B:1875:THR:O	2:B:1879:MET:N	2.38	0.48
5:E:66:C:H2'	5:E:66:C:O2	2.10	0.48
5:E:92:C:H4'	5:E:92:C:OP1	2.13	0.48
6:F:1051:LEU:HB3	6:F:1063:SER:HB3	1.95	0.48
8:I:55:ASN:O	8:I:56:PRO:CB	2.61	0.48
19:T:143:HIS:O	19:T:151:ARG:HG2	2.13	0.48
24:Z:148:LEU:HD12	24:Z:190:LEU:HD21	1.95	0.48
1:A:1846:ASN:C	1:A:1847:ASP:O	2.51	0.48
1:A:1999:ILE:CD1	1:A:2007:ARG:NH2	2.76	0.48
1:A:909:THR:OG1	28:G:48:LEU:HB2	2.13	0.48
2:B:1239:PHE:CE1	2:B:1294:SER:HB2	2.48	0.48
2:B:1337:ASP:O	2:B:1341:GLU:N	2.40	0.48
3:C:488:ILE:HD11	3:C:493:LEU:HD12	1.95	0.48
28:G:327:TRP:C	28:G:327:TRP:CD1	2.86	0.48
9:J:67:VAL:HG23	9:J:68:ASN:H	1.78	0.48
14:O:389:THR:HG22	14:O:426:TRP:HZ2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:91:ILE:HB	16:Q:99:VAL:HG21	1.95	0.48
17:R:255:ASN:O	17:R:259:ASN:N	2.40	0.48
1:A:997:GLN:HE21	1:A:1511:ARG:HH22	1.54	0.48
1:A:1839:ASN:HA	1:A:1842:GLU:HG2	1.96	0.48
1:A:1889:LEU:HD21	1:A:1991:ILE:HD11	1.95	0.48
1:A:388:PRO:O	1:A:392:ASN:HB2	2.12	0.48
2:B:1641:TYR:HE1	2:B:1941:VAL:HG11	1.79	0.48
6:F:965:GLY:N	6:F:1016:SER:OG	2.46	0.48
24:Z:179:TYR:C	24:Z:179:TYR:HD1	2.16	0.48
1:A:1070:LEU:HA	1:A:1073:ILE:HG22	1.94	0.48
1:A:1222:LEU:O	1:A:1225:ALA:N	2.47	0.48
1:A:1440:ILE:O	1:A:1442:ARG:N	2.46	0.48
1:A:1911:TRP:NE1	1:A:2324:VAL:HG21	2.29	0.48
1:A:563:ASP:OD1	1:A:564:TRP:N	2.47	0.48
1:A:732:ARG:NH1	5:E:73:A:OP2	2.45	0.48
3:C:328:VAL:HG13	3:C:332:TYR:HB2	1.95	0.48
3:C:635:LYS:HB2	3:C:643:VAL:HB	1.95	0.48
5:E:41:A:C8	17:R:34:TYR:CE2	3.01	0.48
6:F:693:ILE:CG2	6:F:701:LYS:HB2	2.43	0.48
28:G:389:GLY:O	28:G:391:GLU:N	2.46	0.48
7:H:180:LYS:O	7:H:181:GLU:HB2	2.12	0.48
7:H:203:THR:HG22	7:H:250:VAL:HG21	1.95	0.48
16:Q:220:THR:HG23	16:Q:240:LEU:CD2	2.43	0.48
17:R:12:GLN:HG2	17:R:79:GLY:O	2.13	0.48
13:M:520:G:N2	21:V:107:THR:OG1	2.45	0.48
23:Y:550:ALA:HB2	23:Y:563:ARG:HH21	1.78	0.48
1:A:1458:TRP:CE3	28:G:25:ILE:HG22	2.46	0.48
1:A:1697:SER:OG	1:A:1767:TYR:OH	2.26	0.48
2:B:574:PHE:HB3	2:B:585:VAL:HG11	1.96	0.48
2:B:674:LEU:HD22	2:B:906:LEU:HB3	1.96	0.48
3:C:679:GLU:OE1	3:C:807:PRO:HD2	2.14	0.48
6:F:1048:THR:OG1	6:F:1065:THR:O	2.22	0.48
6:F:471:LYS:HE3	6:F:473:GLN:HB3	1.94	0.48
7:H:154:ALA:O	7:H:157:PRO:HD3	2.13	0.48
14:O:392:MET:HG3	14:O:393:VAL:H	1.77	0.48
14:O:389:THR:O	14:O:400:ARG:HD2	2.14	0.48
16:Q:291:ILE:HG23	16:Q:292:PRO:N	2.29	0.48
17:R:145:ALA:O	17:R:146:LEU:HB3	2.14	0.48
20:U:50:LEU:HA	20:U:139:GLN:NE2	2.14	0.48
21:V:124:GLU:O	21:V:128:ARG:HG2	2.14	0.48
21:V:83:ARG:HH12	22:W:224:PHE:HB3	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:209:LEU:HD12	22:W:209:LEU:C	2.34	0.48
1:A:1212:ARG:HG2	1:A:1213:MET:H	1.78	0.48
1:A:1714:PRO:HA	1:A:1788:GLY:O	2.13	0.48
2:B:1039:GLU:OE2	2:B:1042:LYS:HD2	2.13	0.48
2:B:1208:ALA:HB3	2:B:1311:PHE:CE2	2.49	0.48
2:B:677:TYR:HD2	2:B:691:LEU:HD11	1.79	0.48
3:C:362:LYS:CG	3:C:363:PRO:HD2	2.43	0.48
6:F:130:LEU:HB3	6:F:195:ILE:HD13	1.96	0.48
6:F:175:VAL:HG11	6:F:224:ILE:HD12	1.95	0.48
6:F:240:MET:HA	6:F:254:THR:HG22	1.94	0.48
6:F:719:GLN:CG	6:F:762:PHE:HD2	2.23	0.48
28:G:45:LYS:NZ	28:G:53:GLU:OE2	2.47	0.48
9:J:20:GLY:H	9:J:43:VAL:HG23	1.79	0.48
10:K:23:ASP:O	28:G:935:TRP:CB	2.61	0.48
12:N:112:U:H3	17:R:226:ALA:HA	1.79	0.48
15:P:142:GLU:OE1	15:P:142:GLU:N	2.46	0.48
22:W:185:ALA:O	22:W:189:THR:OG1	2.29	0.48
24:Z:459:ARG:HH21	24:Z:485:GLN:HG2	1.77	0.48
1:A:1656:LYS:O	1:A:1660:SER:OG	2.11	0.48
1:A:2238:ILE:HG22	1:A:2239:SER:O	2.14	0.48
1:A:834:ILE:HG12	1:A:840:VAL:HG11	1.95	0.48
2:B:1999:HIS:H	2:B:2089:GLU:CD	2.17	0.48
2:B:767:THR:HA	2:B:771:THR:HG22	1.94	0.48
6:F:197:PRO:HG2	6:F:244:ASP:HA	1.95	0.48
28:G:565:LEU:O	28:G:569:PHE:N	2.46	0.48
8:I:57:TYR:O	8:I:59:TYR:HD1	1.97	0.48
20:U:78:TYR:H	20:U:99:ASN:ND2	2.12	0.48
23:Y:702:SER:CB	23:Y:705:ILE:HB	2.43	0.48
1:A:377:VAL:CG1	1:A:378:PRO:HD2	2.43	0.48
1:A:402:TRP:CG	1:A:402:TRP:O	2.66	0.48
1:A:757:GLU:HG3	1:A:758:LEU:N	2.29	0.48
1:A:770:MET:CE	15:P:165:ILE:HD11	2.43	0.48
1:A:909:THR:HG21	28:G:49:GLN:HG3	1.95	0.48
28:G:191:LYS:HE3	28:G:194:THR:HG21	1.96	0.48
28:G:851:LEU:HD21	28:G:895:ALA:CB	2.44	0.48
7:H:182:TYR:O	7:H:272:GLU:OE1	2.31	0.48
11:L:16:U:C5	11:L:18:U:OP1	2.67	0.48
16:Q:215:PRO:HG3	16:Q:217:TRP:CE3	2.47	0.48
16:Q:3:ASP:N	18:S:20:TYR:HH	2.11	0.48
16:Q:88:ASP:OD1	16:Q:89:HIS:N	2.46	0.48
23:Y:369:ARG:NE	23:Y:372:LEU:HB2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1212:THR:HG22	2:B:1213:ARG:N	2.28	0.48
6:F:339:ASP:OD1	6:F:340:MET:N	2.47	0.48
6:F:839:ARG:HG3	6:F:880:PRO:HG2	1.96	0.48
6:F:97:THR:O	6:F:98:GLU:C	2.51	0.48
9:J:101:PHE:HE2	28:G:219:HIS:CD2	2.31	0.48
1:A:742:VAL:HG11	14:O:224:LEU:HD23	1.94	0.48
16:Q:256:SER:O	16:Q:260:GLU:OE1	2.32	0.48
17:R:206:LEU:CG	17:R:207:PRO:CD	2.90	0.48
23:Y:220:ARG:HD2	23:Y:255:GLN:HE22	1.78	0.48
23:Y:737:VAL:HA	23:Y:740:ILE:HB	1.96	0.48
1:A:1456:ARG:HH22	1:A:1486:ARG:NH1	2.12	0.47
1:A:1831:GLN:O	1:A:1832:GLU:C	2.52	0.47
2:B:1903:VAL:O	2:B:1906:SER:OG	2.25	0.47
5:E:37:U:C4	17:R:47:PHE:CZ	3.02	0.47
6:F:829:SER:HB2	6:F:838:ILE:HG22	1.95	0.47
28:G:686:LEU:HD12	28:G:711:ILE:HG21	1.96	0.47
28:G:805:TYR:HB2	28:G:816:VAL:HG11	1.95	0.47
8:I:55:ASN:ND2	8:I:56:PRO:N	2.56	0.47
15:P:58:PRO:C	15:P:59:THR:HG23	2.34	0.47
16:Q:36:ILE:O	16:Q:110:LYS:HD3	2.14	0.47
17:R:146:LEU:HD23	17:R:147:ASN:H	1.78	0.47
17:R:164:PHE:CE2	17:R:184:VAL:HG21	2.48	0.47
17:R:65:ASP:OD1	17:R:90:LEU:HD22	2.14	0.47
1:A:266:LEU:HD23	1:A:268:LEU:HA	1.96	0.47
1:A:640:ARG:CG	1:A:640:ARG:NH1	2.77	0.47
2:B:2134:THR:O	2:B:2138:HIS:NE2	2.46	0.47
3:C:787:LEU:HD12	3:C:790:LYS:HD2	1.96	0.47
3:C:90:LEU:HD11	14:O:166:VAL:HG21	1.95	0.47
6:F:1090:ILE:O	6:F:1117:HIS:HA	2.13	0.47
6:F:1213:ARG:HD2	6:F:1360:TYR:CD1	2.48	0.47
2:B:160:GLY:HA3	28:G:511:LYS:O	2.15	0.47
7:H:141:VAL:HG12	7:H:143:TYR:N	2.29	0.47
8:I:16:ILE:O	8:I:17:ALA:CB	2.62	0.47
9:J:54:GLN:HA	9:J:54:GLN:OE1	2.14	0.47
20:U:48:ILE:CG2	20:U:49:ALA:N	2.77	0.47
23:Y:298:LEU:HD21	23:Y:304:TYR:HE1	1.79	0.47
1:A:1208:PRO:HB2	1:A:1417:GLN:O	2.14	0.47
1:A:2007:ARG:HG3	1:A:2008:LEU:N	2.28	0.47
1:A:936:GLU:O	1:A:940:ILE:HD12	2.13	0.47
3:C:106:PHE:O	4:D:44:A:H3'	2.13	0.47
6:F:1298:SER:C	6:F:1300:LEU:H	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:406:GLN:HA	6:F:455:LEU:O	2.14	0.47
10:K:32:GLN:HE22	28:G:960:ASN:HB3	1.79	0.47
1:A:872:PRO:HD3	15:P:201:PHE:CE1	2.48	0.47
20:U:76:THR:HG1	20:U:205:HIS:CE1	2.28	0.47
1:A:1041:VAL:O	1:A:1041:VAL:HG12	2.14	0.47
1:A:1233:ARG:HD3	18:S:131:THR:HG21	1.95	0.47
1:A:162:LEU:HD22	1:A:1646:ILE:HG22	38.96	0.47
1:A:1899:TRP:O	1:A:1901:GLY:N	2.47	0.47
1:A:209:ILE:HG13	1:A:493:MET:HE1	1.96	0.47
1:A:244:ASP:OD1	1:A:596:ASN:ND2	2.45	0.47
2:B:114:PRO:O	2:B:118:GLU:N	2.34	0.47
28:G:493:ALA:HA	28:G:499:ASN:OD1	2.15	0.47
28:G:924:PHE:O	28:G:931:ARG:HD3	2.13	0.47
7:H:134:LEU:HD13	7:H:138:LYS:HE2	1.96	0.47
9:J:51:PHE:HE2	9:J:54:GLN:HG2	1.78	0.47
1:A:1475:LEU:O	15:P:304:ASP:HB2	2.14	0.47
16:Q:118:VAL:O	16:Q:119:LYS:CB	2.63	0.47
16:Q:214:ILE:HD11	16:Q:218:LYS:CB	2.44	0.47
17:R:146:LEU:CD1	17:R:211:GLU:OE1	2.62	0.47
20:U:146:ARG:HD3	20:U:155:TYR:CE2	2.49	0.47
20:U:45:LYS:HE3	20:U:45:LYS:HA	1.96	0.47
1:A:1268:ARG:NE	1:A:1301:TYR:HD2	2.12	0.47
1:A:291:LYS:HE2	1:A:292:LYS:HD3	1.96	0.47
1:A:893:ARG:NH1	1:A:893:ARG:CG	2.74	0.47
2:B:1555:GLU:OE2	2:B:1726:HIS:N	2.47	0.47
2:B:1642:LYS:HB2	2:B:1669:ASP:HB3	1.95	0.47
2:B:1685:THR:HG21	2:B:1732:TYR:HE2	1.79	0.47
3:C:347:ARG:O	3:C:352:VAL:HG11	2.15	0.47
3:C:81:LYS:O	3:C:82:ASN:ND2	2.48	0.47
6:F:153:ASP:O	6:F:154:SER:CB	2.62	0.47
28:G:579:ILE:N	28:G:579:ILE:CD1	2.77	0.47
13:M:505:A:O3'	13:M:506:U:O4'	2.32	0.47
5:E:28:U:H1'	16:Q:51:ARG:HH22	1.79	0.47
17:R:146:LEU:CD2	17:R:147:ASN:H	2.27	0.47
17:R:207:PRO:O	17:R:212:TRP:NE1	2.47	0.47
20:U:186:LEU:HB2	20:U:199:LEU:HB2	1.96	0.47
15:P:242:LYS:NZ	20:U:83:TYR:OH	2.37	0.47
23:Y:699:GLU:CA	23:Y:702:SER:CB	2.92	0.47
24:Z:184:GLN:CA	24:Z:184:GLN:NE2	2.77	0.47
1:A:2247:LEU:HB2	1:A:2250:THR:HG21	1.96	0.47
3:C:697:ARG:HH11	3:C:848:VAL:HG12	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:LEU:HD12	6:F:102:GLU:H	1.80	0.47
6:F:205:SER:HB2	6:F:211:LYS:HG2	1.97	0.47
6:F:836:TRP:HZ3	6:F:838:ILE:HG23	1.79	0.47
28:G:550:THR:CG2	28:G:553:LEU:HD22	2.45	0.47
7:H:271:TYR:CZ	7:H:274:ARG:HB2	2.49	0.47
14:O:133:ARG:HH11	14:O:425:ILE:HD12	1.78	0.47
14:O:125:TRP:HE1	14:O:437:GLU:HB3	1.80	0.47
1:A:377:VAL:HG12	1:A:378:PRO:CD	2.44	0.47
1:A:716:ARG:HD3	4:D:111:C:O2	2.15	0.47
1:A:878:GLU:HG2	18:S:133:PHE:HE1	1.80	0.47
2:B:1061:ALA:HB1	2:B:1081:GLN:OE1	2.15	0.47
2:B:1536:SER:HB3	2:B:1539:GLU:HG2	1.95	0.47
2:B:1876:LEU:HA	2:B:1879:MET:HB2	1.96	0.47
3:C:273:LEU:HD21	3:C:284:ALA:HB1	1.95	0.47
1:A:672:LYS:N	4:D:101:C:OP1	2.43	0.47
6:F:1096:LEU:HD13	6:F:1187:PHE:CZ	2.44	0.47
28:G:472:PRO:O	28:G:476:ARG:HG3	2.14	0.47
28:G:458:LEU:HD13	28:G:501:VAL:HG12	1.96	0.47
28:G:637:PHE:O	28:G:641:ASN:ND2	2.48	0.47
7:H:192:ARG:CG	7:H:192:ARG:NH1	2.77	0.47
14:O:191:SER:O	18:S:40:ARG:NH2	2.43	0.47
15:P:301:LEU:CD1	15:P:303:TYR:CE1	2.96	0.47
16:Q:37:CYS:SG	16:Q:39:LEU:HB2	2.55	0.47
17:R:12:GLN:HB3	17:R:79:GLY:O	2.14	0.47
19:T:128:GLN:O	19:T:131:GLU:N	2.41	0.47
22:W:213:LYS:C	22:W:230:SER:OG	2.53	0.47
1:A:1424:HIS:NE2	30:X:6:ILE:HD13	2.29	0.47
1:A:1797:LEU:O	1:A:1800:ASN:N	2.48	0.47
1:A:421:ALA:HB3	1:A:469:ILE:HD12	1.97	0.47
2:B:1123:HIS:HB3	2:B:1124:PRO:HD3	1.96	0.47
3:C:104:THR:CG2	3:C:181:LEU:HD12	2.44	0.47
6:F:1302:ARG:HG2	6:F:1307:TYR:HB2	1.97	0.47
6:F:78:HIS:O	6:F:146:THR:HG22	2.14	0.47
11:L:4:A:H2'	11:L:5:A:C8	2.50	0.47
14:O:437:GLU:N	14:O:438:PRO:HD3	2.30	0.47
1:A:134:MET:CE	19:T:107:ARG:HD2	2.45	0.47
16:Q:24:ARG:CD	19:T:116:ASN:HD22	2.27	0.47
1:A:263:PRO:HD2	19:T:7:ARG:NH2	2.29	0.47
20:U:51:LYS:HG3	20:U:52:HIS:H	1.78	0.47
20:U:96:TYR:CE2	20:U:129:ILE:HG23	2.50	0.47
21:V:83:ARG:NH1	22:W:224:PHE:HB3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:ASN:HB3	24:Z:338:THR:HG21	1.96	0.47
1:A:1227:PHE:CD2	1:A:1243:TRP:HE3	2.33	0.47
1:A:1999:ILE:HG23	1:A:2003:THR:OG1	2.15	0.47
1:A:264:ILE:O	1:A:265:ASN:O	2.33	0.47
2:B:1009:TYR:O	2:B:1107:ARG:NH1	2.44	0.47
1:A:2395:PHE:HB2	2:B:1087:LEU:HD21	1.97	0.47
2:B:1978:ASP:O	2:B:1982:MET:HG3	2.15	0.47
3:C:233:ASP:HB3	3:C:443:TYR:CE1	2.50	0.47
28:G:962:GLU:HG2	28:G:963:TYR:N	2.29	0.47
9:J:4:HIS:HB3	13:M:500:A:O2'	2.14	0.47
15:P:114:VAL:CG1	16:Q:27:LYS:HB2	2.45	0.47
17:R:13:VAL:HG12	17:R:14:LYS:O	2.14	0.47
20:U:84:ARG:HG2	20:U:197:TYR:CE2	2.50	0.47
1:A:2032:ILE:HD13	1:A:2043:PHE:CD1	2.50	0.47
1:A:745:THR:CG2	14:O:203:ASP:HB2	2.45	0.47
2:B:1237:GLU:HB2	2:B:1259:ILE:HB	1.97	0.47
2:B:1387:HIS:CE1	2:B:1392:LYS:HB2	2.49	0.47
2:B:1641:TYR:CE1	2:B:1941:VAL:HG11	2.50	0.47
2:B:2055:TYR:HB2	2:B:2073:ILE:HG12	1.96	0.47
2:B:899:LEU:HD12	2:B:903:ASN:HD21	1.80	0.47
4:D:124:C:H2'	4:D:125:C:O4'	2.15	0.47
1:A:749:ARG:NH1	5:E:76:A:OP2	2.44	0.47
28:G:496:ARG:N	28:G:497:PRO:HD2	2.29	0.47
20:U:81:VAL:HG22	20:U:95:ARG:HG2	1.96	0.47
1:A:1424:HIS:ND1	30:X:22:ARG:HA	2.29	0.47
2:B:1630:ARG:O	2:B:1634:LYS:N	2.47	0.47
2:B:2063:LEU:HD12	2:B:2162:VAL:HG13	1.97	0.47
3:C:625:ILE:HD12	3:C:659:LEU:HD13	1.96	0.47
6:F:71:PHE:CD1	6:F:97:THR:CG2	2.98	0.47
2:B:180:LEU:CD2	28:G:592:ILE:HD13	2.45	0.47
28:G:583:PHE:HZ	28:G:601:ILE:HD13	1.80	0.47
11:L:18:U:C2'	11:L:19:U:OP1	2.63	0.47
15:P:137:PRO:HG3	16:Q:112:PHE:CE1	2.50	0.47
16:Q:222:THR:CA	16:Q:225:GLN:NE2	2.75	0.47
17:R:27:GLY:CA	17:R:37:TRP:HB3	2.45	0.47
1:A:1468:ALA:HA	1:A:1473:ARG:HG2	1.97	0.46
1:A:1831:GLN:C	1:A:1833:PRO:HD2	2.35	0.46
1:A:1857:VAL:HG13	1:A:1894:ILE:HD12	1.97	0.46
1:A:322:VAL:HG21	1:A:327:TYR:CD2	2.49	0.46
2:B:2011:ILE:HG13	2:B:2013:VAL:HG23	1.97	0.46
6:F:564:ASP:OD1	6:F:565:ASN:N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:975:ASP:O	6:F:977:ILE:HD12	2.15	0.46
6:F:98:GLU:OE1	6:F:1196:ASN:ND2	2.48	0.46
13:M:509:A:C2	28:G:503:THR:HG21	2.50	0.46
20:U:38:LEU:CD2	21:V:49:THR:HB	2.45	0.46
24:Z:168:LYS:HZ3	24:Z:171:ASP:CB	2.28	0.46
1:A:266:LEU:HG	1:A:267:PRO:CD	2.44	0.46
1:A:909:THR:O	1:A:913:VAL:HG23	2.16	0.46
2:B:162:ILE:HG22	2:B:165:ARG:NH2	2.31	0.46
2:B:159:ASP:HB3	2:B:165:ARG:HH12	1.80	0.46
2:B:2070:LYS:HA	2:B:2128:LEU:O	2.15	0.46
2:B:673:THR:HG21	2:B:694:PHE:O	2.15	0.46
2:B:932:ARG:NH1	2:B:991:ALA:O	2.36	0.46
3:C:269:LYS:HG2	44:C:1500:GTP:C5	2.51	0.46
3:C:406:VAL:HG13	3:C:427:LEU:HG	1.97	0.46
4:D:175:G:H4'	4:D:176:A:O4'	2.15	0.46
1:A:737:ARG:NH2	5:E:71:G:N7	2.62	0.46
6:F:1233:SER:OG	6:F:1236:ASN:ND2	2.33	0.46
6:F:379:VAL:O	6:F:390:LYS:HA	2.15	0.46
6:F:60:LEU:HB2	6:F:1317:VAL:HG22	1.95	0.46
28:G:334:ILE:HD13	28:G:374:THR:CG2	2.45	0.46
7:H:196:LEU:HD22	7:H:200:ILE:HG21	1.97	0.46
11:L:18:U:H2'	11:L:19:U:OP1	2.16	0.46
14:O:114:ARG:O	14:O:118:LEU:HG	2.16	0.46
16:Q:86:LEU:O	16:Q:89:HIS:N	2.48	0.46
17:R:196:LYS:HA	17:R:223:VAL:HG11	1.98	0.46
23:Y:220:ARG:HH11	23:Y:255:GLN:HE22	1.62	0.46
24:Z:204:ASP:C	24:Z:205:TYR:CD2	2.88	0.46
1:A:1161:TYR:CD1	1:A:1170:MET:HG2	2.48	0.46
1:A:1748:ILE:HD13	1:A:1783:MET:C	2.36	0.46
1:A:1877:GLY:O	1:A:1894:ILE:N	2.41	0.46
1:A:2408:GLN:CA	1:A:2408:GLN:NE2	2.75	0.46
2:B:1551:PHE:CD2	2:B:1563:MET:HG2	2.51	0.46
2:B:1973:ALA:O	2:B:1977:MET:HG3	2.16	0.46
2:B:593:ARG:HH11	2:B:596:ARG:HD3	1.80	0.46
2:B:897:TYR:O	2:B:901:VAL:HG23	2.16	0.46
6:F:683:GLN:N	6:F:683:GLN:OE1	2.48	0.46
28:G:25:ILE:HD11	28:G:30:ARG:HG3	1.98	0.46
28:G:922:GLY:HA3	28:G:934:PHE:HD2	1.79	0.46
9:J:50:SER:O	9:J:51:PHE:CD1	2.69	0.46
11:L:41:C:C5'	11:L:41:C:C6	2.92	0.46
13:M:472:A:O2'	13:M:473:A:H2'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:151:ASP:HB3	14:O:153:GLU:HG2	1.97	0.46
1:A:134:MET:HE3	19:T:107:ARG:CD	2.45	0.46
3:C:471:HIS:HB2	3:C:592:PHE:CZ	2.50	0.46
6:F:1014:LYS:HB2	6:F:1015:LEU:HA	1.96	0.46
6:F:701:LYS:HG2	6:F:718:LEU:CD2	2.45	0.46
6:F:745:LEU:O	6:F:775:VAL:HG23	2.15	0.46
11:L:37:G:N7	28:G:182:ARG:NH2	2.63	0.46
28:G:686:LEU:HD11	28:G:724:TRP:CH2	2.50	0.46
28:G:919:ILE:HD13	28:G:937:VAL:CG1	2.45	0.46
10:K:42:THR:HG22	28:G:947:ASP:CG	2.36	0.46
11:L:36:A:C2	13:M:500:A:C2	3.03	0.46
17:R:126:GLY:HA2	17:R:196:LYS:NZ	2.31	0.46
18:S:6:ARG:O	18:S:7:PRO:O	2.33	0.46
21:V:90:ASP:OD2	22:W:241:PHE:CE1	2.68	0.46
22:W:220:PRO:HG3	22:W:236:HIS:CE1	2.51	0.46
23:Y:276:THR:O	23:Y:346:ASP:HB3	2.15	0.46
23:Y:357:ILE:HD11	23:Y:590:THR:HG23	1.98	0.46
23:Y:429:HIS:HD2	23:Y:495:ARG:HH11	1.62	0.46
1:A:1364:GLU:OE2	1:A:1401:SER:HA	2.16	0.46
1:A:2015:LEU:O	1:A:2019:GLU:HG2	2.16	0.46
2:B:135:ILE:HD12	2:B:139:LEU:HD22	1.98	0.46
2:B:1597:ALA:O	2:B:1601:PHE:N	2.48	0.46
6:F:779:TYR:O	6:F:780:LEU:HD12	2.16	0.46
1:A:909:THR:HG21	28:G:49:GLN:CG	2.45	0.46
8:I:57:TYR:CD1	8:I:70:LEU:CD1	2.80	0.46
21:V:32:TYR:CE1	21:V:78:LYS:HD3	2.51	0.46
23:Y:307:ARG:NE	23:Y:646:PRO:HB2	2.27	0.46
24:Z:191:ARG:HB3	24:Z:192:GLU:OE1	2.15	0.46
1:A:2412:PHE:C	1:A:2413:SER:HG	2.06	0.46
1:A:725:TYR:CD1	5:E:72:C:C1'	2.98	0.46
2:B:1751:HIS:HB3	2:B:1860:PHE:CD1	2.51	0.46
2:B:531:ALA:HB1	2:B:632:ILE:HD13	1.98	0.46
6:F:93:LEU:O	6:F:103:LEU:HD12	2.16	0.46
6:F:267:HIS:HB3	6:F:287:LEU:HA	1.96	0.46
28:G:919:ILE:HD13	28:G:937:VAL:HG11	1.97	0.46
9:J:51:PHE:CE2	9:J:54:GLN:CG	2.99	0.46
15:P:48:GLN:HG3	15:P:49:SER:N	2.29	0.46
16:Q:105:LYS:O	16:Q:109:MET:HB2	2.15	0.46
23:Y:287:ALA:HB2	23:Y:321:TYR:HB2	1.96	0.46
23:Y:807:VAL:HG12	23:Y:841:GLU:HB3	1.97	0.46
1:A:1057:MET:HE2	1:A:1114:PHE:CZ	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1405:ILE:HG23	2:B:1446:LEU:HB3	1.97	0.46
2:B:618:ASN:HB3	2:B:621:ASN:ND2	2.30	0.46
2:B:733:SER:HB3	2:B:738:ASN:HB2	1.98	0.46
14:O:161:ASP:O	14:O:162:THR:OG1	2.23	0.46
20:U:140:HIS:CE1	20:U:161:SER:HG	2.33	0.46
22:W:170:LEU:CD2	22:W:170:LEU:N	2.78	0.46
2:B:1568:PHE:HB2	2:B:1598:PHE:CE1	2.51	0.46
2:B:1782:ILE:HD11	2:B:1791:VAL:HG21	1.98	0.46
2:B:1981:GLN:HA	2:B:2147:ASP:O	2.16	0.46
2:B:562:PRO:HG3	2:B:635:GLU:OE1	2.16	0.46
2:B:513:GLY:O	2:B:666:ARG:NH1	2.49	0.46
3:C:307:ILE:HA	3:C:324:ILE:HD11	1.98	0.46
3:C:722:ASP:OD2	3:C:755:TYR:OH	2.25	0.46
3:C:869:HIS:CD2	3:C:925:LEU:HD22	2.50	0.46
1:A:899:PRO:HD3	1:A:1006:ARG:HH12	1.81	0.46
1:A:1080:ASP:HB3	3:C:82:ASN:HD22	57.91	0.46
1:A:1354:GLU:N	1:A:1355:PRO:HD2	2.31	0.46
1:A:1703:MET:HB2	1:A:1732:MET:H	1.81	0.46
1:A:2262:GLN:OE1	1:A:2292:SER:OG	2.31	0.46
1:A:404:ASN:OD1	3:C:927:MET:HE1	2.15	0.46
1:A:905:TYR:CE2	1:A:907:ASN:HB2	2.51	0.46
2:B:1120:GLY:HA2	2:B:1251:ILE:HB	1.96	0.46
2:B:1368:VAL:HB	2:B:1511:LEU:HD23	1.98	0.46
2:B:2055:TYR:HA	2:B:2073:ILE:HA	1.98	0.46
2:B:899:LEU:O	2:B:903:ASN:ND2	2.21	0.46
3:C:502:LEU:HB3	3:C:576:THR:OG1	2.15	0.46
3:C:539:VAL:HG13	3:C:564:ILE:CG2	2.46	0.46
28:G:467:VAL:HG12	28:G:469:SER:H	1.81	0.46
28:G:922:GLY:C	28:G:934:PHE:HD2	2.19	0.46
7:H:166:THR:CG2	7:H:167:LYS:H	2.29	0.46
9:J:37:VAL:HG13	9:J:38:ARG:HG2	1.98	0.46
15:P:57:LEU:HD23	15:P:58:PRO:HD3	1.91	0.46
1:A:997:GLN:HE22	1:A:1511:ARG:HH21	1.58	0.46
2:B:1796:PRO:HA	2:B:1799:ILE:HD12	1.96	0.46
3:C:110:LYS:HE3	3:C:110:LYS:HB2	1.66	0.46
6:F:111:LEU:HD12	6:F:111:LEU:O	2.17	0.46
6:F:1180:THR:HG23	7:H:168:ASN:OD1	2.15	0.46
14:O:365:PHE:CZ	14:O:373:LEU:HD22	2.50	0.46
14:O:132:SER:HB3	14:O:427:LYS:CB	2.46	0.46
16:Q:118:VAL:O	16:Q:119:LYS:HB2	2.16	0.46
18:S:174:VAL:O	18:S:174:VAL:HG12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:89:VAL:HG21	21:V:106:HIS:CD2	2.52	0.46
23:Y:327:LEU:HD11	23:Y:343:ILE:HD13	1.98	0.46
24:Z:301:SER:O	24:Z:302:SER:OG	2.30	0.46
1:A:134:MET:HB3	1:A:135:PRO:CD	2.45	0.45
1:A:1710:GLU:HB3	1:A:1724:PHE:O	2.16	0.45
1:A:346:ILE:HD11	1:A:385:VAL:HG11	1.98	0.45
2:B:1476:ALA:H	2:B:1512:SER:HB2	1.81	0.45
2:B:1862:THR:OG1	2:B:1887:VAL:HB	2.17	0.45
3:C:274:ILE:CG1	3:C:382:TYR:HE1	2.21	0.45
3:C:670:ILE:HG22	3:C:671:SER:O	2.15	0.45
5:E:95:A:H2'	5:E:96:G:O4'	2.15	0.45
6:F:1198:ILE:HG13	10:K:48:ALA:HB1	1.98	0.45
6:F:1308:ARG:HA	6:F:1308:ARG:HD3	1.70	0.45
6:F:284:ALA:HB1	6:F:286:TYR:CZ	2.51	0.45
6:F:363:VAL:CG1	6:F:364:THR:H	2.13	0.45
28:G:156:LEU:O	28:G:160:GLU:N	2.43	0.45
9:J:43:VAL:CG2	9:J:70:ALA:HB3	2.47	0.45
13:M:480:A:O2'	13:M:481:A:H2'	2.16	0.45
14:O:327:CYS:SG	14:O:328:THR:N	2.89	0.45
15:P:301:LEU:N	15:P:301:LEU:CD2	2.78	0.45
17:R:187:LYS:HD2	17:R:187:LYS:O	2.16	0.45
17:R:210:LYS:HD3	17:R:210:LYS:C	2.37	0.45
17:R:4:TRP:NE1	17:R:92:HIS:HB3	2.31	0.45
23:Y:467:LYS:CB	23:Y:494:CYS:N	2.78	0.45
23:Y:702:SER:O	23:Y:705:ILE:N	2.49	0.45
1:A:1163:ARG:NH1	1:A:1163:ARG:CG	2.78	0.45
1:A:2060:LEU:HD22	1:A:2071:ILE:HD11	1.98	0.45
2:B:1365:SER:HB3	2:B:1508:PHE:HB2	1.97	0.45
2:B:1663:VAL:HG12	2:B:1664:LEU:H	1.80	0.45
2:B:1803:LEU:O	2:B:1807:VAL:HG23	2.16	0.45
2:B:557:ILE:HG22	2:B:630:LEU:HB3	1.98	0.45
2:B:809:THR:HG23	2:B:811:SER:HB3	1.98	0.45
3:C:468:LEU:O	3:C:578:TYR:HA	2.16	0.45
5:E:39:G:N1	17:R:117:PHE:HB2	2.31	0.45
6:F:118:GLN:HB2	6:F:1325:ASN:OD1	2.16	0.45
2:B:497:THR:HG22	6:F:657:ASP:OD2	2.16	0.45
28:G:698:ARG:HE	28:G:739:ASN:HD22	1.64	0.45
28:G:689:LEU:HD21	28:G:707:PHE:CD1	2.52	0.45
7:H:248:HIS:CE1	7:H:252:PHE:CD2	3.02	0.45
10:K:22:GLY:HA3	28:G:935:TRP:CH2	2.50	0.45
1:A:742:VAL:CG1	14:O:224:LEU:HA	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:91:ILE:HD13	16:Q:125:ILE:HD12	1.98	0.45
17:R:143:ASP:O	17:R:146:LEU:HA	2.16	0.45
23:Y:426:PHE:HB3	23:Y:462:LEU:HD11	1.98	0.45
23:Y:807:VAL:CG2	23:Y:843:ILE:HD11	2.47	0.45
24:Z:319:ASN:HA	24:Z:322:LYS:HD3	1.97	0.45
1:A:2208:TYR:HD1	1:A:2255:LEU:HA	1.81	0.45
1:A:695:LEU:HD12	1:A:695:LEU:O	2.16	0.45
3:C:178:LEU:HD12	3:C:214:ASP:HB2	1.97	0.45
3:C:237:ILE:HD13	3:C:253:ILE:HG22	1.99	0.45
6:F:1191:ASN:ND2	6:F:1316:LYS:HB2	2.31	0.45
6:F:509:LYS:HE3	6:F:890:GLU:OE2	2.16	0.45
6:F:643:ILE:HG21	6:F:691:LEU:HD11	1.99	0.45
6:F:71:PHE:CD1	6:F:97:THR:HG21	2.52	0.45
28:G:334:ILE:HD11	28:G:362:CYS:CB	2.46	0.45
11:L:60:A:H2'	11:L:61:A:O4'	2.17	0.45
12:N:113:U:O4'	17:R:183:PHE:CE2	2.69	0.45
21:V:63:SER:HB2	21:V:74:PHE:CD1	2.39	0.45
22:W:215:TYR:CE2	22:W:232:TRP:CZ3	3.04	0.45
1:A:1561:LEU:HD11	1:A:1608:LEU:CD2	2.44	0.45
1:A:1852:VAL:HG22	1:A:1881:THR:HG22	1.97	0.45
1:A:296:THR:CG2	4:D:33:U:OP2	2.64	0.45
1:A:774:ILE:HD12	1:A:775:ARG:H	1.74	0.45
2:B:162:ILE:O	2:B:166:LYS:N	2.48	0.45
2:B:593:ARG:HD2	2:B:596:ARG:HD3	1.99	0.45
6:F:1122:LYS:O	6:F:1129:VAL:HG13	2.16	0.45
28:G:198:GLU:HG2	28:G:239:TYR:OH	2.16	0.45
28:G:67:ARG:HD2	28:G:292:TYR:HB2	1.98	0.45
14:O:201:SER:OG	14:O:202:GLU:N	2.50	0.45
16:Q:209:ASN:CG	16:Q:288:ILE:O	2.54	0.45
17:R:31:ASN:O	17:R:34:TYR:O	2.33	0.45
22:W:208:SER:CA	22:W:214:LEU:HD12	2.47	0.45
1:A:1889:LEU:O	1:A:1988:LEU:HD23	2.16	0.45
1:A:366:GLU:O	1:A:372:ARG:NH1	2.50	0.45
1:A:379:ILE:HA	1:A:383:TYR:HD2	1.82	0.45
1:A:334:LYS:HD3	1:A:400:ILE:O	2.17	0.45
2:B:1797:HIS:O	2:B:1800:SER:OG	2.24	0.45
2:B:717:LYS:HA	2:B:720:LYS:HB3	1.97	0.45
3:C:861:ILE:HG21	3:C:905:GLN:HB3	1.98	0.45
4:D:79:C:H3'	4:D:79:C:O2	2.16	0.45
6:F:643:ILE:HG13	6:F:691:LEU:HD12	1.98	0.45
6:F:630:ILE:HG21	6:F:646:LEU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:676:PRO:HA	6:F:694:ALA:O	2.17	0.45
28:G:256:PRO:HA	28:G:259:ARG:HB2	1.98	0.45
28:G:835:ILE:C	28:G:837:PHE:H	2.20	0.45
28:G:881:MET:HG2	28:G:885:ILE:CD1	2.41	0.45
9:J:11:CYS:HB3	9:J:86:CYS:HB3	1.98	0.45
17:R:256:ASN:HA	17:R:259:ASN:HD22	1.82	0.45
17:R:76:PHE:HB2	17:R:91:HIS:CD2	2.51	0.45
21:V:11:GLU:HG2	21:V:16:ILE:CG2	2.45	0.45
23:Y:308:PHE:CD2	23:Y:740:ILE:HG12	2.51	0.45
23:Y:556:VAL:HG23	23:Y:557:GLY:N	2.32	0.45
23:Y:543:ARG:N	23:Y:575:GLU:O	2.47	0.45
1:A:1008:LEU:HD21	1:A:1073:ILE:HD11	1.98	0.45
1:A:1998:ARG:HD3	1:A:1998:ARG:H	1.82	0.45
1:A:2015:LEU:HD23	1:A:2022:ALA:HB3	1.99	0.45
1:A:380:ARG:NH1	1:A:380:ARG:CG	2.79	0.45
1:A:978:ILE:CG2	18:S:174:VAL:HG22	2.46	0.45
3:C:109:LEU:HD21	4:D:43:G:N1	2.31	0.45
6:F:1088:GLY:HA3	6:F:1118:VAL:HG21	1.99	0.45
6:F:1122:LYS:NZ	6:F:1202:PHE:O	2.48	0.45
6:F:70:ASN:O	6:F:97:THR:HB	2.17	0.45
6:F:703:MET:SD	6:F:715:VAL:HG22	2.57	0.45
28:G:558:GLU:HG2	28:G:597:PHE:HE2	1.82	0.45
1:A:867:ILE:HG21	1:A:1101:TYR:CD1	2.52	0.45
1:A:763:MET:CE	1:A:779:ALA:CB	2.95	0.45
1:A:854:ARG:NH2	1:A:854:ARG:CG	2.72	0.45
3:C:194:ASN:OD1	3:C:478:TYR:OH	2.33	0.45
6:F:1012:LYS:HA	6:F:1013:ASP:HA	1.62	0.45
6:F:1036:LYS:NZ	6:F:1082:TYR:OH	2.50	0.45
6:F:551:PHE:CD2	6:F:591:THR:HG21	2.49	0.45
13:M:506:U:OP1	13:M:506:U:H4'	2.16	0.45
17:R:143:ASP:C	17:R:146:LEU:H	2.19	0.45
1:A:856:TRP:CG	18:S:174:VAL:HG11	2.50	0.45
1:A:1051:GLU:HA	1:A:1168:ILE:O	2.17	0.45
1:A:1882:LEU:HB3	1:A:1889:LEU:HD23	1.99	0.45
2:B:1754:LEU:HD12	2:B:1810:CYS:SG	2.57	0.45
3:C:501:ILE:O	3:C:535:PRO:HG2	2.16	0.45
6:F:1222:GLN:HE22	10:K:48:ALA:N	2.13	0.45
6:F:258:ASP:OD1	6:F:259:ASN:N	2.50	0.45
6:F:490:SER:OG	6:F:491:GLN:N	2.50	0.45
6:F:779:TYR:C	6:F:780:LEU:HD12	2.37	0.45
6:F:71:PHE:HD1	6:F:97:THR:CG2	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:241:HIS:O	28:G:245:VAL:HG23	2.17	0.45
28:G:286:ILE:HD12	28:G:316:PHE:HZ	1.81	0.45
28:G:927:ALA:HB3	28:G:930:VAL:HB	1.99	0.45
14:O:186:ARG:NH1	14:O:202:GLU:OE2	2.49	0.45
16:Q:205:PHE:CD1	16:Q:205:PHE:N	2.85	0.45
21:V:16:ILE:CG2	21:V:17:LEU:N	2.79	0.45
21:V:19:PRO:O	21:V:25:ASN:HB2	2.17	0.45
21:V:58:VAL:HG12	22:W:212:ARG:NH1	2.31	0.45
23:Y:223:LEU:HB2	23:Y:226:HIS:CD2	2.52	0.45
1:A:645:ASP:OD1	1:A:646:ALA:N	2.48	0.45
3:C:343:ASP:O	3:C:347:ARG:CG	2.63	0.45
3:C:883:ARG:NH2	3:C:910:GLU:O	2.50	0.45
6:F:255:LEU:HG	6:F:295:VAL:CG2	2.47	0.45
6:F:542:THR:HG22	6:F:615:LYS:NZ	2.30	0.45
6:F:638:SER:OG	6:F:639:LYS:N	2.50	0.45
7:H:248:HIS:NE2	7:H:252:PHE:CD2	2.85	0.45
16:Q:120:LEU:HG	16:Q:121:GLY:N	2.32	0.45
17:R:142:ILE:HG22	17:R:180:ASN:HD22	1.82	0.45
20:U:57:ASP:CG	20:U:146:ARG:HE	2.20	0.45
21:V:68:THR:HG23	21:V:70:GLU:HG2	1.99	0.45
1:A:236:ARG:CG	1:A:651:ASP:OD2	2.65	0.45
1:A:296:THR:HB	4:D:33:U:OP2	2.17	0.45
2:B:1330:SER:HA	2:B:1347:THR:HA	1.99	0.45
2:B:1338:ASP:HB3	2:B:1419:LEU:HD11	1.99	0.45
2:B:1502:LEU:HD13	2:B:1504:LYS:HD2	1.98	0.45
3:C:163:ASP:OD2	3:C:548:ARG:NH1	2.46	0.45
3:C:315:SER:HB3	3:C:320:PHE:CE1	2.52	0.45
3:C:652:MET:HE1	3:C:655:LEU:HD12	1.99	0.45
3:C:788:LEU:O	3:C:792:LYS:HG2	2.17	0.45
3:C:867:THR:O	3:C:926:GLY:HA2	2.17	0.45
3:C:932:PHE:O	3:C:933:TRP:HD1	1.96	0.45
6:F:1073:LYS:HB2	6:F:1090:ILE:HG13	1.98	0.45
6:F:1093:SER:HB2	6:F:1112:ASP:HB3	1.98	0.45
6:F:822:HIS:ND1	6:F:846:MET:O	2.50	0.45
6:F:962:LEU:HD23	6:F:1016:SER:C	2.37	0.45
14:O:157:THR:HG21	14:O:423:ILE:HD11	1.99	0.45
1:A:742:VAL:HG11	14:O:224:LEU:HA	1.99	0.45
15:P:47:ARG:O	15:P:50:ASN:O	2.34	0.45
17:R:1:MET:HA	17:R:5:ARG:HB2	1.98	0.45
17:R:62:THR:HG23	17:R:64:GLY:H	1.81	0.45
21:V:48:LEU:O	22:W:231:ARG:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:174:TRP:CZ2	24:Z:201:ARG:HB2	2.51	0.45
1:A:1048:VAL:HG22	1:A:1250:VAL:HG22	1.98	0.44
1:A:840:VAL:HG22	1:A:840:VAL:O	2.17	0.44
1:A:843:THR:O	1:A:847:LYS:HB2	2.17	0.44
1:A:939:LEU:HD12	1:A:986:PRO:HB2	1.99	0.44
2:B:1030:ASP:OD1	2:B:1033:ARG:NH1	2.40	0.44
2:B:1555:GLU:O	2:B:1686:ASN:ND2	2.50	0.44
3:C:746:LYS:O	3:C:750:ILE:HG12	2.17	0.44
6:F:660:SER:OG	6:F:661:ASP:N	2.49	0.44
28:G:221:MET:O	28:G:224:THR:OG1	2.25	0.44
10:K:42:THR:CG2	28:G:950:VAL:HG21	2.41	0.44
9:J:26:CYS:O	9:J:29:LYS:HG3	2.17	0.44
17:R:236:LYS:O	17:R:240:GLU:N	2.47	0.44
21:V:110:ARG:HB3	21:V:110:ARG:HE	1.56	0.44
22:W:167:VAL:O	22:W:171:GLY:HA2	2.17	0.44
23:Y:319:LEU:HD12	23:Y:320:LYS:H	1.82	0.44
1:A:1755:LYS:HB3	1:A:1759:TYR:HE2	1.81	0.44
1:A:2281:PHE:HB3	1:A:2285:LYS:O	2.17	0.44
1:A:195:THR:HG23	1:A:556:TYR:O	2.17	0.44
2:B:1137:THR:HG21	2:B:1148:GLN:HE21	1.83	0.44
2:B:1329:ILE:HG21	2:B:1356:PHE:CE1	2.52	0.44
2:B:1329:ILE:HG13	2:B:1356:PHE:CG	2.52	0.44
2:B:1403:GLU:N	2:B:1403:GLU:OE1	2.50	0.44
2:B:1514:CYS:HB2	2:B:1537:PRO:HG3	1.99	0.44
2:B:511:PHE:O	2:B:537:LYS:HD3	2.17	0.44
2:B:136:PRO:HA	2:B:860:TRP:CE2	2.52	0.44
3:C:103:HIS:CD2	3:C:104:THR:HG23	2.52	0.44
8:I:3:TYR:CE2	12:N:99:G:C5	3.05	0.44
14:O:151:ASP:CB	14:O:153:GLU:HG2	2.47	0.44
17:R:15:GLU:HA	17:R:18:LEU:CD1	2.47	0.44
17:R:176:VAL:O	17:R:179:LYS:O	2.34	0.44
21:V:32:TYR:OH	22:W:162:LEU:HD11	2.18	0.44
22:W:170:LEU:O	22:W:172:ILE:CG1	2.62	0.44
22:W:222:ASN:OD1	22:W:223:ARG:N	2.50	0.44
23:Y:290:VAL:HA	23:Y:293:GLU:HB2	1.99	0.44
1:A:2385:GLU:HB3	1:A:2392:PHE:HE2	1.81	0.44
2:B:1345:PHE:HE1	2:B:1348:PHE:HD1	1.65	0.44
2:B:1564:LEU:HG	2:B:1601:PHE:HE2	1.81	0.44
2:B:830:CYS:SG	2:B:834:LEU:HD22	2.57	0.44
2:B:850:THR:O	2:B:863:LEU:N	2.49	0.44
3:C:799:PHE:CZ	3:C:803:VAL:HG21	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:473:LYS:O	28:G:477:GLU:HG2	2.17	0.44
28:G:569:PHE:HE1	28:G:580:PHE:CE1	2.31	0.44
28:G:583:PHE:HE2	28:G:627:LEU:HD21	1.83	0.44
1:A:1814:VAL:HG21	28:G:645:ILE:HG21	1.99	0.44
14:O:406:THR:O	14:O:414:LEU:HD12	2.17	0.44
15:P:323:VAL:CG2	15:P:324:TYR:CD2	3.00	0.44
16:Q:13:CYS:SG	16:Q:16:CYS:N	2.84	0.44
17:R:146:LEU:CD2	17:R:147:ASN:N	2.80	0.44
19:T:138:THR:O	19:T:138:THR:HG22	2.16	0.44
21:V:33:ILE:CG2	21:V:85:THR:HG23	2.48	0.44
23:Y:438:ILE:HB	23:Y:497:VAL:HG22	1.99	0.44
1:A:1835:LEU:CD1	1:A:1836:ASN:ND2	2.78	0.44
1:A:765:ASP:OD1	14:O:312:ARG:NH2	2.44	0.44
2:B:1397:TYR:CD2	2:B:1446:LEU:HG	2.52	0.44
2:B:1881:TYR:CG	2:B:1914:PRO:HG2	2.52	0.44
2:B:2033:LEU:HD13	2:B:2037:GLN:HB3	1.99	0.44
2:B:648:GLU:OE1	2:B:912:PHE:HB2	2.18	0.44
2:B:932:ARG:HD3	2:B:989:TYR:OH	2.17	0.44
3:C:271:ASP:CG	44:C:1500:GTP:HN1	2.20	0.44
6:F:782:GLU:HB3	6:F:783:ILE:H	1.67	0.44
6:F:71:PHE:HD1	6:F:97:THR:HG21	1.82	0.44
1:A:913:VAL:HG21	28:G:46:ASP:OD2	2.17	0.44
28:G:855:GLN:HG2	28:G:898:ARG:HG3	2.00	0.44
11:L:2:C:H2'	11:L:3:G:C8	2.52	0.44
13:M:484:A:C3'	13:M:484:A:C8	3.00	0.44
13:M:487:A:H4'	13:M:487:A:OP2	2.17	0.44
20:U:101:ARG:HB2	20:U:104:TYR:CZ	2.53	0.44
22:W:229:GLY:C	22:W:231:ARG:H	2.21	0.44
1:A:185:GLN:HE21	1:A:263:PRO:HD3	1.81	0.44
1:A:1860:VAL:HG13	1:A:1872:THR:HB	1.99	0.44
1:A:251:TYR:CE2	1:A:256:GLU:HG2	2.52	0.44
1:A:379:ILE:HA	1:A:383:TYR:CD2	2.52	0.44
2:B:1618:VAL:N	2:B:1619:PRO:HD2	2.32	0.44
2:B:1997:ILE:HG12	2:B:2044:PHE:CE2	2.52	0.44
2:B:714:ASN:HB3	2:B:717:LYS:HB2	2.00	0.44
3:C:320:PHE:HB2	3:C:429:PHE:HD2	1.81	0.44
3:C:633:ILE:HB	3:C:645:LEU:HB2	2.00	0.44
6:F:162:ILE:O	6:F:162:ILE:HG13	2.17	0.44
6:F:250:PRO:HG2	6:F:273:LEU:HB3	2.00	0.44
6:F:521:ASN:OD1	6:F:522:LEU:N	2.50	0.44
28:G:286:ILE:HD12	28:G:316:PHE:CZ	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:212:LEU:HD11	28:G:806:THR:CG2	2.48	0.44
16:Q:69:ASN:HB3	16:Q:123:ALA:CB	2.48	0.44
24:Z:464:PHE:CE2	24:Z:468:ILE:HD11	2.53	0.44
1:A:2182:VAL:HA	1:A:2338:GLN:HB2	2.00	0.44
2:B:517:MET:HE1	2:B:519:ILE:HD11	1.99	0.44
3:C:274:ILE:HG12	3:C:382:TYR:CD1	2.45	0.44
4:D:60:U:O2	4:D:60:U:C3'	2.65	0.44
5:E:5:G:O2'	5:E:6:C:H5'	2.18	0.44
6:F:253:VAL:HG22	6:F:270:PHE:CD2	2.53	0.44
6:F:348:VAL:HG12	6:F:407:LEU:HD12	2.00	0.44
2:B:477:LEU:HD11	6:F:659:SER:O	2.17	0.44
14:O:362:ASP:CG	14:O:379:LYS:HZ3	2.20	0.44
1:A:869:LYS:C	15:P:198:ASN:HD21	2.19	0.44
16:Q:290:ILE:HG22	16:Q:292:PRO:HD2	2.00	0.44
21:V:54:TYR:HB3	21:V:87:LEU:HD23	2.00	0.44
21:V:87:LEU:HD21	22:W:222:ASN:ND2	2.31	0.44
23:Y:580:PRO:HB2	23:Y:582:ILE:HG22	1.99	0.44
24:Z:178:ARG:HG2	24:Z:198:PHE:CZ	2.50	0.44
1:A:1082:ILE:CG2	1:A:1113:ILE:HD11	2.48	0.44
1:A:1681:VAL:HG22	1:A:1703:MET:SD	2.58	0.44
1:A:1565:THR:O	1:A:1816:ARG:HG3	2.17	0.44
1:A:518:VAL:O	1:A:521:SER:N	2.50	0.44
1:A:644:VAL:O	1:A:645:ASP:HB2	2.17	0.44
3:C:807:PRO:HG3	3:C:850:LEU:HD23	1.99	0.44
6:F:1188:GLN:O	6:F:1188:GLN:HG3	2.18	0.44
6:F:924:PHE:HD2	6:F:952:ARG:CD	2.28	0.44
6:F:996:ILE:O	6:F:1003:LEU:HD12	2.18	0.44
7:H:242:LEU:HD12	7:H:242:LEU:HA	1.77	0.44
11:L:7:C:O5'	11:L:7:C:H6	2.01	0.44
12:N:113:U:C6	17:R:183:PHE:CZ	3.05	0.44
14:O:248:ILE:HD11	14:O:283:SER:HB3	2.00	0.44
16:Q:106:ASN:HB2	16:Q:109:MET:HG2	1.99	0.44
20:U:108:ARG:NH2	20:U:138:LYS:HE3	2.33	0.44
20:U:64:TYR:OH	20:U:150:GLY:O	2.27	0.44
20:U:182:SER:HB2	20:U:203:ASN:ND2	2.32	0.44
23:Y:807:VAL:HG23	23:Y:843:ILE:HD11	1.99	0.44
1:A:1400:ILE:HG23	1:A:1542:TYR:CE2	2.52	0.44
1:A:1456:ARG:HG3	1:A:1457:VAL:N	2.32	0.44
2:B:1958:ILE:HG21	2:B:1980:ALA:HA	2.00	0.44
2:B:2054:THR:O	2:B:2074:GLN:N	2.40	0.44
2:B:593:ARG:NH2	2:B:615:THR:HA	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:314:LEU:N	28:G:315:PRO:HD2	2.33	0.44
28:G:378:LEU:HD11	28:G:396:VAL:HG11	2.00	0.44
7:H:175:HIS:CD2	7:H:182:TYR:HB2	2.53	0.44
7:H:265:CYS:SG	7:H:266:PHE:N	2.88	0.44
12:N:93:U:O2	12:N:93:U:C2'	2.64	0.44
16:Q:69:ASN:ND2	16:Q:126:THR:CG2	2.79	0.44
16:Q:205:PHE:HB3	16:Q:291:ILE:O	2.17	0.44
16:Q:88:ASP:O	16:Q:99:VAL:HG11	2.18	0.44
20:U:80:LEU:HD12	20:U:200:ILE:O	2.18	0.44
23:Y:657:THR:O	23:Y:661:HIS:CG	2.71	0.44
24:Z:170:HIS:NE2	24:Z:174:TRP:HZ3	1.99	0.44
2:B:1477:HIS:ND1	2:B:1512:SER:OG	2.35	0.44
2:B:428:ASP:HB3	2:B:431:LYS:HG2	1.99	0.44
2:B:842:ALA:O	2:B:876:GLY:N	2.49	0.44
3:C:100:LEU:CD2	3:C:479:GLY:CA	2.96	0.44
3:C:766:TRP:HB2	3:C:776:ASN:HD22	1.82	0.44
6:F:216:VAL:HG12	6:F:217:ASP:N	2.31	0.44
28:G:517:TYR:OH	28:G:521:LYS:NZ	2.50	0.44
16:Q:206:PHE:HB3	16:Q:208:TYR:OH	2.17	0.44
17:R:187:LYS:HG3	17:R:188:TYR:CD1	2.52	0.44
14:O:263:VAL:CG1	18:S:11:ALA:HB2	2.44	0.44
21:V:82:GLN:H	22:W:168:GLN:NE2	2.12	0.44
22:W:208:SER:CA	22:W:214:LEU:CD1	2.95	0.44
24:Z:300:LYS:HD3	24:Z:300:LYS:HA	1.88	0.44
1:A:168:LEU:N	1:A:169:PRO:HD2	2.32	0.43
1:A:1843:LEU:HD13	1:A:1851:PHE:CZ	2.50	0.43
1:A:2061:THR:O	1:A:2065:ARG:HG2	2.18	0.43
2:B:1308:PHE:HA	2:B:1311:PHE:CE2	2.53	0.43
2:B:714:ASN:OD1	2:B:715:SER:N	2.50	0.43
3:C:799:PHE:O	3:C:802:ALA:N	2.49	0.43
6:F:1305:GLN:O	6:F:1309:SER:CB	2.66	0.43
6:F:224:ILE:HG22	6:F:225:SER:O	2.17	0.43
6:F:493:VAL:HG23	6:F:937:LYS:HG2	1.99	0.43
6:F:746:GLU:O	6:F:747:ASN:CG	2.57	0.43
28:G:963:TYR:CG	28:G:964:ILE:N	2.86	0.43
7:H:180:LYS:CA	7:H:180:LYS:CE	2.90	0.43
13:M:484:A:H3'	13:M:484:A:C8	2.53	0.43
16:Q:242:VAL:O	17:R:161:ARG:NH2	2.50	0.43
17:R:14:LYS:HA	17:R:14:LYS:HE3	1.99	0.43
30:X:12:LYS:C	30:X:14:SER:H	2.22	0.43
23:Y:516:VAL:HB	23:Y:561:CYS:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:569:SER:HA	23:Y:573:GLU:HB2	1.99	0.43
24:Z:203:LYS:O	24:Z:204:ASP:HB2	2.18	0.43
1:A:1214:ARG:HB2	1:A:1255:ASN:OD1	2.19	0.43
1:A:371:ASP:O	3:C:969:LYS:HD3	2.18	0.43
2:B:1352:GLN:HE22	2:B:1378:ALA:HB3	1.83	0.43
2:B:168:LYS:O	2:B:172:GLU:N	2.46	0.43
3:C:242:VAL:HG21	3:C:272:ARG:HG2	1.99	0.43
3:C:743:ASN:O	3:C:746:LYS:HB3	2.18	0.43
5:E:67:C:C6	5:E:67:C:H5"	2.41	0.43
6:F:927:ARG:HG2	6:F:979:CYS:SG	2.58	0.43
8:I:55:ASN:O	8:I:56:PRO:HB3	2.18	0.43
10:K:65:THR:O	10:K:69:LEU:HG	2.18	0.43
3:C:77:LEU:HD21	14:O:133:ARG:HD3	2.00	0.43
16:Q:203:LYS:HG3	16:Q:256:SER:OG	2.18	0.43
17:R:245:GLU:HG3	17:R:249:MET:HE2	2.00	0.43
20:U:80:LEU:HD21	20:U:199:LEU:HD23	1.99	0.43
21:V:27:TYR:O	21:V:29:ASP:N	2.47	0.43
22:W:223:ARG:CG	22:W:242:GLU:OE2	2.65	0.43
24:Z:306:ASP:OD1	30:X:25:ALA:HB3	2.18	0.43
12:N:90:A:C2	30:X:2:SER:O	2.71	0.43
24:Z:181:LEU:HD21	24:Z:191:ARG:CG	2.44	0.43
1:A:1233:ARG:NE	18:S:131:THR:HG21	2.33	0.43
1:A:1419:ASP:OD1	1:A:1419:ASP:O	2.35	0.43
1:A:1488:ILE:HA	1:A:1488:ILE:HD12	1.85	0.43
1:A:928:ARG:NH1	1:A:1582:GLU:OE2	2.51	0.43
1:A:1705:SER:O	2:B:1184:ARG:NH2	2.48	0.43
1:A:2318:ASN:ND2	1:A:2327:GLU:OE2	2.51	0.43
1:A:762:VAL:HG21	1:A:786:LEU:CD1	2.48	0.43
3:C:135:ASN:O	3:C:233:ASP:N	2.39	0.43
3:C:362:LYS:HG3	3:C:363:PRO:HD2	2.00	0.43
3:C:544:LEU:HG	3:C:553:VAL:HG21	1.99	0.43
3:C:705:GLY:C	3:C:826:PRO:HG3	2.38	0.43
6:F:756:GLY:HA3	6:F:759:ASP:OD1	2.17	0.43
6:F:82:LEU:HD22	6:F:114:ILE:HD13	2.01	0.43
7:H:248:HIS:NE2	7:H:252:PHE:HD2	2.16	0.43
8:I:57:TYR:O	8:I:59:TYR:CE1	2.72	0.43
15:P:233:GLU:O	15:P:237:LYS:HB2	2.18	0.43
16:Q:246:ALA:O	16:Q:247:LYS:HB2	2.18	0.43
22:W:193:PRO:HG3	24:Z:464:PHE:CE1	2.53	0.43
23:Y:479:PRO:O	23:Y:483:GLN:HG3	2.19	0.43
24:Z:397:LEU:HA	24:Z:397:LEU:HD12	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:O	1:A:143:ILE:HG22	2.19	0.43
1:A:571:LEU:HD23	1:A:629:MET:SD	2.58	0.43
1:A:173:LEU:HD13	1:A:715:LEU:HB3	2.01	0.43
1:A:978:ILE:HG21	18:S:174:VAL:HG22	2.00	0.43
2:B:1481:GLN:CD	2:B:1701:ASN:HD22	2.21	0.43
2:B:1575:ALA:HA	2:B:1579:ASN:O	2.18	0.43
2:B:1663:VAL:HG12	2:B:1664:LEU:N	2.33	0.43
2:B:1882:VAL:O	2:B:1885:THR:OG1	2.28	0.43
2:B:1932:ALA:HB1	2:B:1937:LEU:HB2	1.99	0.43
2:B:1932:ALA:O	2:B:1937:LEU:N	2.39	0.43
6:F:636:THR:HB	6:F:679:VAL:HG23	2.00	0.43
28:G:25:ILE:HD11	28:G:30:ARG:CG	2.49	0.43
28:G:484:PHE:O	28:G:488:TRP:HB2	2.18	0.43
28:G:927:ALA:O	28:G:929:ASN:N	2.50	0.43
16:Q:203:LYS:O	16:Q:251:LEU:O	2.37	0.43
20:U:50:LEU:CB	20:U:139:GLN:NE2	2.81	0.43
20:U:26:ILE:HG22	20:U:28:ILE:H	1.83	0.43
20:U:45:LYS:HG2	20:U:126:VAL:CB	2.44	0.43
1:A:268:LEU:HD23	1:A:273:ASP:CB	2.48	0.43
1:A:268:LEU:HD23	1:A:273:ASP:OD2	2.18	0.43
1:A:855:LEU:HD23	1:A:855:LEU:HA	1.82	0.43
1:A:931:ALA:CA	1:A:934:ARG:NH1	2.55	0.43
2:B:1436:LEU:HD12	2:B:1439:LEU:HD23	1.99	0.43
2:B:1954:VAL:HG13	2:B:1983:LEU:HD13	1.98	0.43
2:B:2048:TYR:CD1	2:B:2049:PRO:HD2	2.53	0.43
2:B:766:ILE:HG22	2:B:767:THR:N	2.26	0.43
3:C:733:ASN:OD1	3:C:734:CYS:N	2.51	0.43
3:C:945:LEU:O	3:C:945:LEU:HD12	2.19	0.43
6:F:353:ARG:NH1	6:F:468:PRO:HG3	2.33	0.43
6:F:730:MET:SD	6:F:739:LEU:HD21	2.58	0.43
6:F:957:ILE:HG22	6:F:962:LEU:CD1	2.45	0.43
17:R:73:CYS:HB2	17:R:89:TYR:HB2	2.01	0.43
22:W:215:TYR:HE2	22:W:232:TRP:CZ3	2.36	0.43
23:Y:387:SER:O	23:Y:392:ASN:N	2.42	0.43
2:B:1651:ILE:O	2:B:1655:LEU:HG	2.17	0.43
2:B:2023:GLU:HB2	2:B:2026:GLU:OE1	2.18	0.43
2:B:479:GLU:HG3	2:B:481:THR:H	1.83	0.43
3:C:491:GLY:O	3:C:492:LEU:HD23	2.17	0.43
6:F:1037:PHE:HB2	6:F:1042:LEU:HB2	2.00	0.43
6:F:208:GLU:HA	6:F:235:MET:O	2.19	0.43
6:F:449:ASN:OD1	6:F:450:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:418:ALA:O	28:G:422:MET:HG2	2.17	0.43
28:G:922:GLY:CA	28:G:934:PHE:HD2	2.32	0.43
7:H:160:LEU:HD12	28:G:925:HIS:H	1.83	0.43
14:O:115:TYR:HA	14:O:118:LEU:CG	2.48	0.43
14:O:198:PHE:CZ	14:O:239:ILE:HD11	2.54	0.43
14:O:359:ASN:HB3	14:O:363:VAL:HB	1.99	0.43
15:P:323:VAL:HG23	15:P:324:TYR:CD2	2.53	0.43
15:P:38:VAL:HG22	15:P:39:LYS:N	2.33	0.43
16:Q:239:SER:O	16:Q:251:LEU:HD12	2.18	0.43
23:Y:257:PRO:O	23:Y:261:VAL:HG23	2.18	0.43
23:Y:279:ARG:HD2	23:Y:507:SER:OG	2.18	0.43
24:Z:191:ARG:NE	24:Z:192:GLU:OE1	2.49	0.43
1:A:1223:GLY:HA2	1:A:1248:VAL:HG11	2.00	0.43
1:A:1699:ALA:HB1	1:A:1733:TRP:HB2	2.00	0.43
1:A:1781:TYR:N	1:A:1781:TYR:CD1	2.87	0.43
1:A:1910:LYS:HB2	1:A:1940:MET:SD	2.59	0.43
1:A:640:ARG:HH11	1:A:640:ARG:HG2	1.83	0.43
1:A:769:MET:SD	1:A:811:ILE:HD11	2.55	0.43
2:B:1624:LEU:HD21	2:B:1629:LEU:HB2	1.99	0.43
2:B:1932:ALA:HA	2:B:1937:LEU:HD13	2.00	0.43
2:B:767:THR:O	2:B:770:LEU:N	2.51	0.43
6:F:1041:LEU:O	6:F:1051:LEU:HD12	2.19	0.43
6:F:520:SER:O	6:F:874:GLY:CA	2.66	0.43
15:P:319:HIS:CE1	22:W:264:GLU:HB2	2.53	0.43
16:Q:251:LEU:HD12	16:Q:252:ARG:N	2.33	0.43
1:A:589:THR:CG2	17:R:31:ASN:ND2	2.82	0.43
20:U:45:LYS:HE3	20:U:45:LYS:CA	2.48	0.43
30:X:2:SER:OG	30:X:4:ASN:ND2	2.43	0.43
23:Y:586:ASN:OD1	23:Y:587:LEU:N	2.51	0.43
1:A:1350:ILE:HG23	1:A:1356:LEU:HD22	2.00	0.43
1:A:375:PHE:HE2	1:A:1414:TRP:HZ2	1.65	0.43
1:A:460:PRO:HB2	1:A:463:ALA:HB2	2.01	0.43
1:A:950:THR:OG1	1:A:953:ARG:NH2	2.52	0.43
2:B:1997:ILE:HD11	2:B:2016:VAL:HG22	2.00	0.43
2:B:503:GLN:HE22	2:B:529:ASN:HB2	1.82	0.43
2:B:770:LEU:HD23	2:B:770:LEU:O	2.17	0.43
2:B:948:MET:HA	2:B:955:TYR:HD2	1.84	0.43
6:F:1133:ASP:OD2	6:F:1137:ASN:HB2	2.18	0.43
6:F:208:GLU:H	6:F:236:VAL:HA	1.83	0.43
6:F:780:LEU:HD23	6:F:782:GLU:OE2	2.18	0.43
28:G:27:GLN:HE22	28:G:30:ARG:HH21	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:698:ARG:HG3	28:G:699:LYS:N	2.34	0.43
10:K:5:GLN:HB3	28:G:230:TYR:OH	2.19	0.43
14:O:224:LEU:N	14:O:245:ASP:OD2	2.51	0.43
5:E:32:U:H5'	16:Q:45:HIS:NE2	2.34	0.43
17:R:146:LEU:CG	17:R:147:ASN:N	2.80	0.43
17:R:187:LYS:HG3	17:R:188:TYR:CE1	2.54	0.43
24:Z:203:LYS:HA	24:Z:203:LYS:HD3	1.66	0.43
1:A:1057:MET:CE	1:A:1114:PHE:CZ	3.02	0.43
1:A:1322:ALA:O	1:A:1323:SER:HB3	2.16	0.43
1:A:1447:TRP:HB3	1:A:1451:PHE:HE2	1.84	0.43
1:A:1711:VAL:HG12	1:A:1712:SER:N	2.33	0.43
1:A:1895:HIS:CD2	1:A:1896:THR:H	2.37	0.43
1:A:806:ALA:N	1:A:807:PRO:HD2	2.33	0.43
1:A:878:GLU:HG2	18:S:133:PHE:CE1	2.54	0.43
2:B:1359:LEU:HA	2:B:1507:ARG:HH22	1.84	0.43
2:B:1484:TYR:O	2:B:1488:TYR:N	2.49	0.43
2:B:1821:GLU:HG2	2:B:1845:SER:O	2.19	0.43
2:B:471:PRO:HD3	2:B:697:SER:O	2.19	0.43
2:B:648:GLU:HA	2:B:683:PHE:HZ	1.82	0.43
2:B:723:ASN:OD1	2:B:848:LYS:NZ	2.41	0.43
3:C:766:TRP:HZ2	3:C:792:LYS:HB3	1.84	0.43
3:C:99:LYS:NZ	4:D:43:G:OP2	2.41	0.43
4:D:96:U:H6	4:D:96:U:O5'	2.01	0.43
6:F:327:VAL:O	6:F:337:VAL:HA	2.19	0.43
6:F:526:SER:HA	6:F:870:ARG:HG3	2.00	0.43
6:F:561:LEU:HG	6:F:569:GLU:O	2.19	0.43
6:F:277:LEU:HD21	28:G:353:THR:HG23	2.01	0.43
28:G:534:ARG:O	28:G:538:VAL:HG23	2.18	0.43
9:J:50:SER:O	9:J:51:PHE:CG	2.72	0.43
13:M:468:A:H5"	13:M:469:A:P	2.59	0.43
14:O:152:ASN:ND2	14:O:409:LYS:HB3	2.33	0.43
14:O:382:HIS:CE1	14:O:442:TRP:H	2.36	0.43
15:P:50:ASN:ND2	15:P:53:LEU:N	2.67	0.43
16:Q:217:TRP:CE3	17:R:187:LYS:HB2	2.54	0.43
16:Q:26:THR:O	16:Q:44:TYR:HA	2.18	0.43
17:R:15:GLU:HG3	17:R:15:GLU:H	1.57	0.43
22:W:208:SER:HB3	22:W:212:ARG:N	2.34	0.43
23:Y:290:VAL:HG21	23:Y:321:TYR:OH	2.18	0.43
24:Z:205:TYR:O	24:Z:207:SER:N	2.52	0.43
1:A:1043:ARG:HB2	1:A:1044:GLY:H	1.71	0.43
1:A:1032:ILE:HG12	1:A:1171:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:GLU:OE1	1:A:1346:PHE:HZ	2.01	0.43
1:A:1376:ASN:O	1:A:1377:SER:OG	2.31	0.43
1:A:1828:SER:O	1:A:1829:SER:CB	2.66	0.43
1:A:1891:LEU:HD11	1:A:1974:LEU:HD22	2.00	0.43
1:A:264:ILE:O	1:A:265:ASN:C	2.56	0.43
1:A:936:GLU:O	1:A:939:LEU:N	2.52	0.43
2:B:1109:LEU:HD13	2:B:1131:LEU:HB3	2.00	0.43
2:B:1148:GLN:HE22	2:B:1297:TRP:HA	1.83	0.43
3:C:576:THR:HG21	3:C:592:PHE:H	1.83	0.43
3:C:675:THR:OG1	3:C:676:VAL:N	2.51	0.43
3:C:888:ILE:O	3:C:888:ILE:HG13	2.18	0.43
4:D:78:A:O2'	4:D:79:C:P	2.77	0.43
6:F:1085:LEU:HD23	6:F:1085:LEU:HA	1.84	0.43
6:F:257:ILE:HG21	6:F:257:ILE:HD13	1.79	0.43
6:F:361:LYS:C	6:F:363:VAL:H	2.23	0.43
6:F:755:ILE:HD12	6:F:762:PHE:CE1	2.54	0.43
6:F:779:TYR:HD1	6:F:819:VAL:HG12	1.84	0.43
28:G:169:LEU:O	28:G:173:ILE:HD12	2.19	0.43
1:A:135:PRO:HG3	19:T:56:HIS:CD2	2.54	0.43
21:V:35:ILE:O	21:V:74:PHE:HA	2.18	0.43
23:Y:341:SER:O	23:Y:372:LEU:HA	2.19	0.43
23:Y:245:MET:CG	23:Y:381:MET:HA	2.49	0.43
24:Z:168:LYS:NZ	24:Z:171:ASP:CB	2.76	0.43
24:Z:67:LYS:HA	24:Z:67:LYS:HE2	2.00	0.43
1:A:134:MET:HB3	1:A:135:PRO:HD2	2.01	0.42
1:A:1739:ARG:HD3	1:A:1778:ASP:OD1	2.19	0.42
1:A:2208:TYR:CD1	1:A:2255:LEU:HA	2.53	0.42
1:A:499:VAL:HG12	1:A:501:LEU:HD12	2.01	0.42
1:A:874:ILE:O	1:A:875:THR:OG1	2.24	0.42
2:B:1453:GLU:O	2:B:1457:ARG:HG3	2.19	0.42
2:B:1804:SER:O	2:B:1808:GLU:HG2	2.19	0.42
2:B:2033:LEU:HB3	2:B:2037:GLN:HB2	2.01	0.42
6:F:242:VAL:HG22	6:F:252:PHE:CB	2.49	0.42
6:F:426:TYR:HD1	6:F:440:GLN:HB3	1.84	0.42
6:F:827:TRP:N	6:F:827:TRP:CD1	2.87	0.42
28:G:349:LEU:HD23	28:G:349:LEU:HA	1.83	0.42
28:G:386:TYR:CD2	28:G:387:PRO:HD3	2.53	0.42
28:G:390:ILE:CD1	28:G:426:MET:HA	2.49	0.42
28:G:435:THR:O	28:G:439:MET:N	2.33	0.42
28:G:56:THR:O	28:G:57:VAL:HB	2.19	0.42
28:G:789:ALA:HA	28:G:797:VAL:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:862:THR:HG22	28:G:902:GLY:HA2	2.01	0.42
14:O:138:HIS:CD2	14:O:159:SER:HB2	2.53	0.42
14:O:397:GLU:HG3	14:O:400:ARG:HH12	1.83	0.42
15:P:44:ILE:HG12	15:P:45:PRO:HD2	2.00	0.42
15:P:51:PHE:N	15:P:51:PHE:CD1	2.86	0.42
15:P:52:GLU:OE1	15:P:52:GLU:HA	2.19	0.42
17:R:222:LEU:HD13	17:R:224:LYS:HE2	2.00	0.42
1:A:978:ILE:HG23	18:S:174:VAL:HG13	2.01	0.42
20:U:48:ILE:HG22	20:U:49:ALA:O	2.18	0.42
22:W:208:SER:CB	22:W:212:ARG:O	2.51	0.42
24:Z:64:THR:HG23	24:Z:73:ILE:HG12	2.01	0.42
1:A:1050:LEU:CD2	1:A:1248:VAL:HG22	2.47	0.42
1:A:1286:TRP:HB2	1:A:1300:ALA:HB3	2.00	0.42
1:A:744:THR:HG22	5:E:75:A:OP1	2.18	0.42
2:B:559:TYR:HB3	2:B:606:VAL:HG22	2.01	0.42
2:B:759:ASN:O	2:B:762:ALA:N	2.52	0.42
3:C:545:LEU:O	3:C:545:LEU:HD12	2.19	0.42
4:D:103:A:O2'	4:D:104:G:H5"	2.19	0.42
6:F:1299:ILE:C	6:F:1300:LEU:HD12	2.39	0.42
6:F:1336:PHE:O	6:F:1339:LYS:HG2	2.20	0.42
6:F:637:SER:OG	6:F:638:SER:N	2.52	0.42
28:G:319:ALA:O	28:G:323:SER:HB2	2.19	0.42
28:G:581:LYS:O	28:G:585:ALA:N	2.52	0.42
22:W:169:LYS:HE3	22:W:169:LYS:HB2	1.88	0.42
23:Y:277:GLN:HB2	23:Y:283:ALA:HB2	2.01	0.42
23:Y:503:ILE:O	23:Y:507:SER:HB2	2.19	0.42
24:Z:105:GLN:HG3	24:Z:113:SER:HB2	2.01	0.42
1:A:992:ASP:OD1	1:A:1085:LYS:NZ	2.52	0.42
1:A:2402:GLU:N	1:A:2402:GLU:CD	2.73	0.42
1:A:803:GLY:O	15:P:166:PRO:HG3	2.19	0.42
2:B:1214:SER:HB3	2:B:1281:GLN:NE2	2.33	0.42
2:B:1564:LEU:HD21	2:B:1597:ALA:HB1	2.01	0.42
2:B:1779:TYR:O	2:B:1782:ILE:HG22	2.19	0.42
2:B:1883:LEU:HG	2:B:1957:LEU:HD13	2.00	0.42
2:B:904:GLN:O	2:B:905:GLN:HG3	2.19	0.42
3:C:393:LYS:HB3	3:C:413:LEU:HD22	2.01	0.42
6:F:1029:SER:OG	6:F:1045:MET:HA	2.18	0.42
6:F:1299:ILE:HG22	6:F:1300:LEU:HD12	2.01	0.42
6:F:702:ILE:HG22	6:F:717:SER:N	2.34	0.42
6:F:729:ILE:O	6:F:741:LEU:HD12	2.19	0.42
6:F:780:LEU:HB3	6:F:782:GLU:OE2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:G:580:PHE:O	28:G:626:ILE:HD13	2.20	0.42
28:G:873:HIS:O	28:G:875:ASP:N	2.46	0.42
13:M:480:A:HO2'	13:M:481:A:P	2.42	0.42
13:M:514:U:HO2'	13:M:515:U:P	2.30	0.42
14:O:193:ARG:HH22	14:O:237:ASP:H	1.67	0.42
14:O:274:CYS:HA	14:O:280:GLN:O	2.19	0.42
14:O:304:LEU:HD22	14:O:334:TRP:CZ3	2.55	0.42
17:R:255:ASN:O	17:R:259:ASN:ND2	2.53	0.42
1:A:589:THR:HG21	17:R:38:SER:OG	2.19	0.42
17:R:83:LEU:HB2	17:R:87:CYS:HB2	2.01	0.42
24:Z:338:THR:HG22	24:Z:339:PHE:N	2.34	0.42
1:A:1115:GLN:HE22	1:A:1165:LEU:HD23	1.84	0.42
2:B:2043:ALA:HA	2:B:2046:ASN:HD22	1.84	0.42
3:C:317:LYS:HB2	44:C:1500:GTP:C5	2.55	0.42
4:D:80:G:OP1	4:D:114:G:O2'	2.27	0.42
6:F:1080:TRP:NE1	6:F:1126:GLU:HB2	2.34	0.42
6:F:1223:GLY:O	6:F:1224:THR:OG1	2.37	0.42
6:F:332:GLU:CG	6:F:333:ASN:N	2.82	0.42
6:F:741:LEU:HG	6:F:743:VAL:HG23	2.01	0.42
28:G:386:TYR:CD1	28:G:387:PRO:N	2.88	0.42
28:G:667:TYR:HE1	28:G:710:LEU:HB2	1.85	0.42
7:H:213:PRO:HB2	8:I:42:TYR:CE2	2.55	0.42
13:M:514:U:O4'	13:M:515:U:C5	2.73	0.42
16:Q:205:PHE:CE1	16:Q:293:TRP:HD1	2.37	0.42
17:R:4:TRP:NE1	17:R:91:HIS:O	2.51	0.42
19:T:133:ALA:HB1	19:T:140:VAL:H	1.84	0.42
24:Z:174:TRP:HZ2	24:Z:197:LEU:CD1	2.28	0.42
1:A:1158:ILE:HG12	1:A:1172:PHE:CE2	2.55	0.42
1:A:1567:PHE:CZ	1:A:1820:ARG:HD2	2.55	0.42
1:A:869:LYS:O	15:P:198:ASN:ND2	2.40	0.42
2:B:1363:ASN:HD21	2:B:1390:GLN:HE22	1.66	0.42
2:B:1412:TRP:HB3	2:B:1424:ILE:HD13	2.00	0.42
2:B:583:ILE:HG23	2:B:603:GLN:HB2	2.02	0.42
3:C:576:THR:HG22	3:C:592:PHE:HB2	2.01	0.42
3:C:864:VAL:HG22	3:C:930:LEU:CD2	2.49	0.42
3:C:287:LYS:HD2	3:C:896:GLY:HA3	2.01	0.42
6:F:105:ASP:HB2	6:F:114:ILE:CD1	2.47	0.42
6:F:816:MET:HE1	6:F:830:TYR:CD2	2.55	0.42
28:G:494:LEU:HD21	28:G:532:PRO:HG3	2.02	0.42
28:G:835:ILE:C	28:G:837:PHE:N	2.72	0.42
7:H:189:LEU:O	8:I:43:THR:HG21	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CE	19:T:107:ARG:CD	2.97	0.42
20:U:40:LEU:HA	20:U:49:ALA:HB2	2.02	0.42
21:V:24:HIS:HB3	21:V:86:ILE:HG12	2.01	0.42
22:W:188:LEU:C	22:W:190:ILE:N	2.73	0.42
24:Z:174:TRP:CH2	24:Z:205:TYR:OH	2.69	0.42
1:A:900:PHE:N	1:A:1075:ASP:OD2	2.52	0.42
1:A:1011:ASN:HB2	1:A:1144:PHE:HA	2.02	0.42
1:A:1320:LEU:HA	1:A:1320:LEU:HD23	1.81	0.42
1:A:1364:GLU:OE2	1:A:1401:SER:CB	2.67	0.42
1:A:1369:ASN:OD1	1:A:1378:LYS:HE2	2.19	0.42
1:A:1935:VAL:HG11	1:A:1940:MET:CB	2.48	0.42
1:A:1944:LEU:HB3	1:A:1956:ILE:HD13	2.02	0.42
1:A:2352:PRO:HA	1:A:2374:PHE:HD1	1.85	0.42
1:A:557:PHE:HE1	15:P:121:PRO:HG2	1.84	0.42
1:A:712:LEU:HD12	1:A:712:LEU:HA	1.78	0.42
2:B:1211:ILE:HD12	2:B:1215:VAL:HG12	2.02	0.42
2:B:1477:HIS:HB3	2:B:1515:LEU:HD21	2.02	0.42
2:B:1902:LEU:HB3	2:B:1928:LEU:HD12	2.00	0.42
3:C:305:SER:OG	3:C:307:ILE:HG12	2.19	0.42
6:F:636:THR:OG1	6:F:681:ILE:HG22	2.19	0.42
28:G:682:ILE:H	28:G:682:ILE:HD12	1.85	0.42
16:Q:208:TYR:HB2	16:Q:290:ILE:HB	2.02	0.42
17:R:251:VAL:HG12	17:R:255:ASN:ND2	2.34	0.42
17:R:72:PHE:HE1	17:R:90:LEU:HD12	1.84	0.42
1:A:1066:LEU:O	1:A:1067:ASN:C	2.58	0.42
1:A:1477:PHE:O	1:A:1481:GLU:HB2	2.20	0.42
1:A:1461:TYR:CD1	1:A:1480:LEU:HD11	2.53	0.42
1:A:2329:PHE:HA	1:A:2333:PHE:CE2	2.55	0.42
1:A:316:THR:N	1:A:317:PRO:HD2	2.35	0.42
1:A:744:THR:HG23	1:A:746:THR:HG23	2.01	0.42
1:A:835:LYS:HD2	18:S:173:HIS:CE1	2.54	0.42
1:A:932:SER:O	1:A:936:GLU:HG3	2.20	0.42
2:B:850:THR:OG1	2:B:862:GLN:NE2	2.53	0.42
3:C:150:MET:SD	3:C:178:LEU:CD1	2.91	0.42
3:C:100:LEU:CD2	3:C:479:GLY:HA3	2.50	0.42
1:A:367:PHE:CD1	3:C:608:GLN:OE1	2.72	0.42
6:F:1002:ARG:NH2	6:F:1024:GLN:OE1	2.48	0.42
7:H:153:ASP:OD2	11:L:58:A:P	2.77	0.42
7:H:252:PHE:O	7:H:256:ALA:HB2	2.19	0.42
12:N:90:A:N1	30:X:6:ILE:HD11	2.34	0.42
20:U:110:LEU:HA	20:U:132:PRO:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:ASP:H	30:X:6:ILE:HG22	1.84	0.42
24:Z:195:GLU:O	24:Z:198:PHE:HB2	2.19	0.42
1:A:1458:TRP:CH2	1:A:1491:ILE:HD13	2.55	0.42
1:A:1590:LEU:HD13	1:A:1590:LEU:N	2.35	0.42
1:A:378:PRO:HB2	1:A:380:ARG:HG3	2.02	0.42
2:B:2142:ILE:HG13	2:B:2158:PHE:HE1	1.84	0.42
2:B:561:ALA:O	2:B:609:PRO:HD3	2.20	0.42
2:B:767:THR:HG1	2:B:768:HIS:N	2.18	0.42
2:B:707:PHE:HZ	2:B:902:LEU:HD12	1.85	0.42
3:C:106:PHE:CD1	3:C:548:ARG:O	2.73	0.42
3:C:168:VAL:HG12	3:C:173:LYS:HB2	2.02	0.42
3:C:885:GLY:HA2	3:C:907:PRO:HD3	2.01	0.42
6:F:1115:LYS:HD2	28:G:951:PRO:O	2.20	0.42
6:F:666:LEU:HB3	6:F:668:THR:N	2.35	0.42
6:F:116:LYS:HD3	6:F:883:ASP:OD1	2.20	0.42
28:G:213:LEU:O	28:G:213:LEU:HD12	2.19	0.42
28:G:682:ILE:O	28:G:685:ILE:N	2.47	0.42
9:J:3:ARG:HH12	28:G:901:GLU:CD	2.19	0.42
15:P:323:VAL:HG23	15:P:324:TYR:CD1	2.55	0.42
17:R:210:LYS:CG	17:R:211:GLU:H	2.32	0.42
17:R:72:PHE:CD1	17:R:90:LEU:HB2	2.53	0.42
15:P:241:LEU:CD1	20:U:204:VAL:HA	2.49	0.42
1:A:1687:HIS:CG	1:A:1688:PRO:HD2	2.55	0.42
1:A:2228:PRO:HB3	1:A:2359:TYR:CE1	2.54	0.42
1:A:282:ASP:HB2	1:A:285:PRO:HA	2.01	0.42
1:A:388:PRO:HB2	1:A:398:VAL:HG11	2.02	0.42
1:A:1707:HIS:C	2:B:1184:ARG:HH21	2.23	0.42
2:B:1661:VAL:HG12	2:B:1663:VAL:O	2.18	0.42
2:B:2074:GLN:HA	2:B:2125:GLN:HB3	2.02	0.42
3:C:834:MET:HB2	3:C:837:GLN:HG2	2.01	0.42
6:F:1356:VAL:HA	6:F:1360:TYR:CD2	2.55	0.42
6:F:590:HIS:CD2	6:F:591:THR:N	2.88	0.42
28:G:606:LEU:HD21	28:G:643:LEU:HD23	2.01	0.42
8:I:3:TYR:CE2	12:N:99:G:C6	3.07	0.42
14:O:142:VAL:HG13	14:O:157:THR:CG2	2.49	0.42
14:O:118:LEU:CD2	15:P:49:SER:O	2.68	0.42
1:A:1156:HIS:CG	1:A:1157:PRO:HD2	2.55	0.42
2:B:1614:GLU:O	2:B:1618:VAL:HG23	2.20	0.42
3:C:269:LYS:HG2	44:C:1500:GTP:C6	2.55	0.42
6:F:738:GLN:HG3	6:F:754:HIS:CD2	2.55	0.42
6:F:77:GLY:HA3	6:F:146:THR:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:924:PHE:HD1	6:F:945:HIS:HA	1.85	0.42
10:K:23:ASP:O	28:G:935:TRP:HB3	2.20	0.42
11:L:41:C:C6	11:L:41:C:H5"	2.32	0.42
14:O:270:ASN:HD21	14:O:286:THR:HG22	1.85	0.42
22:W:232:TRP:CZ3	22:W:234:GLY:HA2	2.54	0.42
1:A:1835:LEU:HD11	1:A:2006:SER:OG	2.20	0.41
1:A:639:PHE:CB	1:A:649:LEU:HD22	2.50	0.41
2:B:1399:ASN:HB2	2:B:1474:ASP:HB3	2.02	0.41
2:B:1614:GLU:HA	2:B:1617:ILE:HG22	2.02	0.41
2:B:1655:LEU:HB3	2:B:1661:VAL:HG23	2.02	0.41
3:C:325:LYS:HD3	3:C:441:ARG:HH12	1.85	0.41
6:F:1096:LEU:HB3	6:F:1109:TYR:CE1	2.55	0.41
6:F:239:ASP:OD2	6:F:295:VAL:N	2.26	0.41
6:F:441:PHE:HB3	6:F:475:LEU:CD2	2.42	0.41
6:F:507:ASN:ND2	6:F:509:LYS:HE2	2.34	0.41
6:F:517:VAL:HG21	6:F:828:VAL:HG21	2.01	0.41
28:G:772:VAL:HG11	28:G:777:LEU:HD12	2.02	0.41
8:I:20:SER:HB2	28:G:772:VAL:HG13	2.01	0.41
6:F:1178:PRO:HB3	7:H:145:GLN:NE2	2.34	0.41
7:H:193:PRO:O	7:H:194:PHE:HB2	2.20	0.41
7:H:203:THR:CG2	7:H:250:VAL:HG21	2.50	0.41
17:R:164:PHE:HD2	17:R:184:VAL:HG21	1.83	0.41
17:R:251:VAL:HA	17:R:254:ILE:HG12	2.02	0.41
17:R:54:GLN:H	17:R:58:HIS:CD2	2.29	0.41
20:U:105:LEU:HD23	20:U:127:ALA:HA	2.02	0.41
21:V:43:THR:OG1	21:V:44:GLU:OE1	2.37	0.41
23:Y:780:ILE:O	23:Y:784:PRO:HB3	2.18	0.41
24:Z:179:TYR:CD1	24:Z:179:TYR:O	2.72	0.41
1:A:1591:THR:O	1:A:1594:GLN:HB3	2.20	0.41
1:A:1969:MET:HE1	1:A:1978:VAL:HB	2.02	0.41
1:A:304:ASP:OD1	1:A:305:LEU:N	2.48	0.41
1:A:614:ARG:HA	1:A:614:ARG:HD3	1.69	0.41
1:A:995:LEU:HD11	1:A:1078:ILE:HG23	2.02	0.41
2:B:1252:LEU:HD22	2:B:1274:TYR:CZ	2.54	0.41
2:B:126:TRP:NE1	2:B:181:LYS:O	2.52	0.41
2:B:1897:GLY:O	2:B:1901:LEU:HD13	2.20	0.41
2:B:1946:ASP:O	2:B:1950:ILE:N	2.50	0.41
2:B:707:PHE:CZ	2:B:902:LEU:HD12	2.54	0.41
3:C:369:LYS:O	3:C:369:LYS:HG3	2.19	0.41
6:F:94:CYS:SG	6:F:101:LEU:HD11	2.59	0.41
6:F:126:SER:HB2	6:F:151:THR:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:268:LEU:HD13	6:F:329:ILE:CD1	2.50	0.41
6:F:950:GLN:HE21	6:F:973:ILE:HG21	1.85	0.41
28:G:252:ILE:HD13	28:G:296:VAL:HG22	2.01	0.41
28:G:580:PHE:HB3	28:G:626:ILE:HD11	2.02	0.41
11:L:64:G:H2'	11:L:65:A:C8	2.55	0.41
16:Q:3:ASP:HB3	16:Q:7:GLU:OE2	2.20	0.41
17:R:147:ASN:O	17:R:148:SER:C	2.59	0.41
1:A:861:GLN:HE21	1:A:1097:HIS:HB3	1.85	0.41
1:A:520:VAL:O	1:A:524:LYS:HG2	2.20	0.41
2:B:1376:LYS:NZ	2:B:1512:SER:O	2.54	0.41
2:B:1889:PHE:HA	2:B:1892:VAL:HG23	2.02	0.41
2:B:451:GLY:HA3	2:B:466:PRO:HG3	2.01	0.41
1:A:1034:ASN:ND2	28:G:20:GLY:CA	2.66	0.41
28:G:685:ILE:O	28:G:688:THR:OG1	2.29	0.41
28:G:740:LYS:O	28:G:741:GLU:C	2.59	0.41
16:Q:13:CYS:SG	16:Q:16:CYS:HB3	2.60	0.41
16:Q:261:ARG:O	16:Q:264:SER:HB2	2.19	0.41
20:U:61:PRO:O	20:U:65:MET:HG2	2.20	0.41
21:V:48:LEU:C	22:W:231:ARG:CZ	2.88	0.41
23:Y:713:GLN:HA	23:Y:716:ASN:HB3	2.01	0.41
24:Z:152:ILE:HD13	24:Z:194:LEU:CA	2.42	0.41
1:A:1051:GLU:HB3	1:A:1167:ARG:NH2	2.34	0.41
1:A:1145:MET:SD	1:A:1160:LEU:HD22	2.61	0.41
1:A:1348:GLU:CG	1:A:1446:THR:HB	2.49	0.41
1:A:1611:SER:OG	1:A:1612:PRO:HD3	2.21	0.41
1:A:1738:LEU:HD22	1:A:1779:LEU:HD21	2.02	0.41
1:A:2411:VAL:HG11	2:B:564:LYS:NZ	2.35	0.41
2:B:503:GLN:HG2	2:B:530:ILE:HG13	2.02	0.41
3:C:323:THR:O	3:C:326:GLU:N	2.53	0.41
6:F:1096:LEU:HD23	6:F:1109:TYR:OH	2.20	0.41
6:F:118:GLN:HE21	6:F:1299:ILE:CD1	2.34	0.41
6:F:539:ASP:OD2	6:F:541:ALA:HB3	2.21	0.41
6:F:864:SER:OG	6:F:865:ILE:N	2.54	0.41
6:F:889:HIS:CG	6:F:890:GLU:N	2.88	0.41
28:G:900:LEU:O	28:G:904:GLU:HG2	2.20	0.41
7:H:185:GLY:N	8:I:72:ASN:HD21	2.19	0.41
9:J:39:PRO:HB2	9:J:71:PHE:HD2	1.85	0.41
14:O:433:THR:O	14:O:437:GLU:HB2	2.20	0.41
15:P:141:ASP:OD1	15:P:142:GLU:N	2.51	0.41
15:P:50:ASN:HD21	15:P:53:LEU:N	2.17	0.41
17:R:152:LYS:HG2	17:R:153:PRO:CD	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:HG2	19:T:49:LEU:HD23	2.02	0.41
21:V:25:ASN:HD22	28:G:490:ARG:HH22	1.68	0.41
21:V:50:VAL:HG12	22:W:237:ARG:HD2	2.01	0.41
23:Y:650:GLU:CG	23:Y:651:PHE:N	2.83	0.41
23:Y:705:ILE:O	23:Y:708:LEU:HB3	2.20	0.41
23:Y:807:VAL:HA	23:Y:841:GLU:HB2	2.03	0.41
1:A:1999:ILE:HD13	1:A:1999:ILE:HG21	1.89	0.41
1:A:934:ARG:NH2	1:A:1587:PHE:CE1	2.88	0.41
2:B:704:SER:N	2:B:884:GLY:O	2.52	0.41
3:C:237:ILE:HD12	3:C:265:PHE:HE1	1.84	0.41
3:C:460:GLY:HA3	3:C:461:LYS:HA	1.80	0.41
3:C:477:ASP:HB2	3:C:628:TYR:CE1	2.55	0.41
3:C:951:ILE:HB	3:C:952:PRO:HD3	2.03	0.41
6:F:242:VAL:HG22	6:F:252:PHE:HB3	2.01	0.41
6:F:70:ASN:OD1	6:F:70:ASN:O	2.39	0.41
6:F:826:THR:HG23	6:F:845:ASN:HA	2.03	0.41
28:G:801:ILE:CG2	28:G:816:VAL:HG13	2.49	0.41
14:O:402:VAL:HG22	14:O:418:GLU:HG2	2.01	0.41
1:A:426:PRO:HB3	24:Z:201:ARG:HG3	2.02	0.41
1:A:1440:ILE:HD13	1:A:1440:ILE:HG21	1.80	0.41
1:A:1693:LYS:HE3	1:A:1693:LYS:HB2	1.89	0.41
1:A:1783:MET:HE2	1:A:1783:MET:HB3	1.98	0.41
1:A:1861:THR:HG1	1:A:1863:HIS:CE1	2.34	0.41
1:A:1865:THR:HG21	1:A:1869:ASN:HD22	1.86	0.41
1:A:1948:MET:HG3	1:A:1956:ILE:HD11	2.01	0.41
1:A:1991:ILE:HG21	1:A:1991:ILE:HD13	1.88	0.41
1:A:561:THR:O	1:A:562:ILE:HB	2.19	0.41
3:C:758:ASP:OD1	3:C:759:SER:N	2.54	0.41
3:C:89:PRO:HA	14:O:212:GLU:O	2.20	0.41
6:F:1315:ARG:HG2	6:F:1316:LYS:HG2	2.03	0.41
6:F:160:VAL:HG11	6:F:171:LEU:HG	2.03	0.41
6:F:765:ILE:HD12	6:F:765:ILE:H	1.85	0.41
28:G:525:PRO:HB3	28:G:533:PHE:CZ	2.56	0.41
7:H:180:LYS:O	7:H:181:GLU:CB	2.67	0.41
9:J:6:PHE:HZ	28:G:897:MET:HE1	1.85	0.41
13:M:468:A:C8	13:M:469:A:N7	2.89	0.41
16:Q:263:VAL:O	16:Q:263:VAL:HG12	2.20	0.41
16:Q:69:ASN:CB	16:Q:123:ALA:CB	2.96	0.41
19:T:156:THR:HG23	19:T:157:ASP:N	2.36	0.41
1:A:1196:GLU:HB3	1:A:1199:ILE:HD12	2.03	0.41
1:A:1854:ASP:HA	1:A:1857:VAL:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:O	1:A:288:GLU:HG2	2.21	0.41
2:B:1548:ILE:HA	2:B:1722:ILE:HB	2.03	0.41
2:B:1554:VAL:HG21	2:B:1563:MET:SD	2.61	0.41
2:B:1573:ALA:O	2:B:1577:ASN:N	2.53	0.41
2:B:1654:ARG:HG2	2:B:1658:TYR:CE2	2.56	0.41
1:A:460:PRO:HG3	3:C:375:GLU:HG3	2.03	0.41
6:F:1002:ARG:HH22	6:F:1004:LEU:HD11	1.85	0.41
6:F:104:TYR:HE1	6:F:113:LEU:HD12	1.86	0.41
6:F:561:LEU:HD21	6:F:568:MET:HG3	2.02	0.41
6:F:716:ILE:HG22	6:F:716:ILE:O	2.21	0.41
28:G:840:PRO:O	28:G:843:GLU:HB3	2.21	0.41
21:V:3:LYS:O	21:V:7:ILE:HD12	2.20	0.41
22:W:167:VAL:HG13	22:W:209:LEU:HD21	2.02	0.41
1:A:1080:ASP:HB3	3:C:82:ASN:ND2	57.71	0.41
1:A:1568:ASN:HB2	1:A:1832:GLU:OE2	2.21	0.41
1:A:2060:LEU:HB3	1:A:2071:ILE:CD1	2.50	0.41
2:B:119:THR:HA	2:B:122:GLN:HG2	2.03	0.41
2:B:1777:TYR:OH	2:B:1781:ARG:HD3	2.20	0.41
2:B:1962:VAL:HG13	2:B:1973:ALA:HB1	2.02	0.41
2:B:2033:LEU:HB2	2:B:2038:LEU:HG	2.03	0.41
2:B:767:THR:HG1	2:B:768:HIS:H	1.69	0.41
2:B:834:LEU:HD12	2:B:838:VAL:HB	2.03	0.41
3:C:306:PRO:HG2	3:C:349:TRP:CE3	2.55	0.41
3:C:348:LEU:O	3:C:372:THR:HB	2.20	0.41
6:F:1173:LEU:HA	6:F:1173:LEU:HD23	1.76	0.41
6:F:347:LYS:HB3	6:F:460:PRO:HB3	2.01	0.41
6:F:444:LEU:O	6:F:444:LEU:HD23	2.21	0.41
6:F:679:VAL:HG12	6:F:693:ILE:HD12	2.03	0.41
6:F:766:LYS:HD3	6:F:836:TRP:CE2	2.55	0.41
6:F:995:ILE:HG13	6:F:1041:LEU:HD21	2.03	0.41
28:G:321:CYS:O	28:G:330:ARG:HG2	2.21	0.41
28:G:373:VAL:O	28:G:377:THR:HG23	2.21	0.41
28:G:378:LEU:CD1	28:G:396:VAL:HG11	2.51	0.41
28:G:583:PHE:CE2	28:G:627:LEU:HD21	2.56	0.41
6:F:1315:ARG:NH2	28:G:872:GLY:O	2.54	0.41
28:G:941:MET:HE3	28:G:945:TYR:HD2	1.85	0.41
8:I:18:SER:O	8:I:19:GLU:C	2.58	0.41
16:Q:217:TRP:C	16:Q:217:TRP:CD1	2.93	0.41
17:R:251:VAL:HG12	17:R:255:ASN:HD21	1.85	0.41
1:A:1018:SER:OG	1:A:1019:GLU:HG3	2.21	0.41
1:A:1169:TYR:CE2	1:A:1262:MET:HG2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1890:PHE:CE1	1:A:1988:LEU:HD21	2.56	0.41
1:A:2215:HIS:HB2	1:A:2218:VAL:HG23	2.03	0.41
1:A:2185:LEU:O	1:A:2341:LEU:HD12	2.20	0.41
1:A:775:ARG:O	1:A:778:LYS:HB2	2.21	0.41
1:A:923:TYR:CD1	1:A:926:LYS:HD3	2.56	0.41
1:A:930:ASN:C	1:A:934:ARG:NH1	2.74	0.41
2:B:1481:GLN:OE1	2:B:1701:ASN:ND2	2.54	0.41
6:F:104:TYR:CD1	6:F:113:LEU:HA	2.54	0.41
6:F:122:ALA:HB3	6:F:1300:LEU:HD22	2.03	0.41
6:F:1353:ILE:O	6:F:1356:VAL:HG22	2.21	0.41
6:F:125:THR:HG22	6:F:191:SER:HA	2.03	0.41
6:F:200:ARG:NH2	6:F:247:PHE:HA	2.36	0.41
28:G:25:ILE:HG21	28:G:25:ILE:HD13	1.85	0.41
28:G:503:THR:O	28:G:507:VAL:HG23	2.20	0.41
28:G:839:THR:N	28:G:840:PRO:HD2	2.36	0.41
28:G:850:ASP:OD1	28:G:853:HIS:CD2	2.73	0.41
28:G:908:GLN:HG2	28:G:945:TYR:OH	2.20	0.41
7:H:222:GLU:OE1	7:H:223:LYS:N	2.53	0.41
9:J:67:VAL:HG23	9:J:68:ASN:N	2.36	0.41
9:J:8:LEU:HB3	9:J:89:ILE:HG23	2.03	0.41
14:O:200:VAL:HG21	14:O:227:VAL:HG12	2.03	0.41
14:O:422:SER:OG	14:O:424:LYS:NZ	2.53	0.41
16:Q:69:ASN:HB3	16:Q:123:ALA:HB1	2.01	0.41
23:Y:290:VAL:HG11	23:Y:319:LEU:HD23	2.01	0.41
1:A:1212:ARG:HG2	1:A:1213:MET:N	2.35	0.41
1:A:1585:MET:HG3	1:A:1586:GLN:OE1	2.21	0.41
1:A:2177:VAL:HG12	1:A:2179:GLU:H	1.85	0.41
1:A:2380:LEU:HD22	1:A:2384:ASN:ND2	2.36	0.41
2:B:1345:PHE:CE1	2:B:1348:PHE:HD1	2.39	0.41
2:B:1641:TYR:HD1	2:B:1642:LYS:O	2.04	0.41
2:B:2007:LYS:HB3	2:B:2030:ILE:HG12	2.03	0.41
3:C:314:ALA:CB	3:C:321:THR:HG22	2.51	0.41
5:E:39:G:C6	17:R:117:PHE:CD2	3.09	0.41
6:F:62:HIS:HD2	6:F:1228:PHE:CE1	2.39	0.41
6:F:61:TYR:CE2	6:F:63:LEU:HD11	2.56	0.41
28:G:843:GLU:OE1	28:G:879:HIS:NE2	2.54	0.41
15:P:241:LEU:O	15:P:245:SER:HB3	2.18	0.41
19:T:129:LEU:HA	19:T:129:LEU:HD23	1.93	0.41
1:A:1506:ARG:O	1:A:1511:ARG:NH1	2.53	0.41
1:A:404:ASN:OD1	1:A:405:ASN:N	2.54	0.41
1:A:173:LEU:HD22	1:A:719:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1463:LYS:HG3	2:B:1466:GLN:NE2	2.36	0.41
3:C:596:ASP:OD1	3:C:597:TYR:N	2.54	0.41
4:D:114:G:O2'	4:D:115:G:H5'	2.21	0.41
6:F:215:LEU:HB3	6:F:225:SER:HB3	2.02	0.41
6:F:839:ARG:HG3	6:F:880:PRO:CG	2.50	0.41
28:G:416:LEU:HD11	28:G:441:ILE:HG21	2.02	0.41
28:G:538:VAL:CG1	28:G:578:ILE:HG13	2.51	0.41
13:M:504:C:N4	28:G:776:GLN:NE2	2.69	0.41
14:O:279:PRO:HG3	14:O:301:MET:SD	2.60	0.41
15:P:302:GLN:HG3	15:P:303:TYR:N	2.35	0.41
16:Q:103:GLU:HG2	16:Q:104:ALA:HB3	2.02	0.41
16:Q:291:ILE:HG23	16:Q:292:PRO:CA	2.50	0.41
19:T:13:PRO:HG2	19:T:77:LEU:HA	2.02	0.41
22:W:229:GLY:C	22:W:231:ARG:N	2.73	0.41
1:A:1144:PHE:CD2	1:A:1145:MET:HG2	2.56	0.40
1:A:1774:MET:O	1:A:1786:ALA:HA	2.21	0.40
1:A:2410:ASP:OD1	1:A:2412:PHE:CE1	2.74	0.40
1:A:254:HIS:O	1:A:258:ILE:HD12	2.21	0.40
2:B:1647:ASN:O	2:B:1651:ILE:HG12	2.20	0.40
3:C:501:ILE:HD11	3:C:567:ILE:HD12	2.03	0.40
4:D:43:G:H2'	4:D:45:A:H5'	2.02	0.40
5:E:65:U:OP1	18:S:12:ARG:NH1	2.54	0.40
6:F:838:ILE:H	6:F:838:ILE:HG13	1.58	0.40
28:G:928:LYS:O	28:G:928:LYS:HG3	2.21	0.40
8:I:88:LYS:HE2	8:I:88:LYS:HB3	1.92	0.40
13:M:509:A:H2	28:G:503:THR:CG2	2.34	0.40
14:O:333:SER:HB3	14:O:343:THR:HG22	2.02	0.40
14:O:373:LEU:HD21	14:O:402:VAL:HG21	2.02	0.40
23:Y:384:LYS:O	23:Y:387:SER:N	2.54	0.40
23:Y:308:PHE:CE2	23:Y:740:ILE:HG12	2.56	0.40
24:Z:204:ASP:O	24:Z:205:TYR:CD2	2.73	0.40
24:Z:449:PHE:CE1	24:Z:465:PHE:HE2	2.39	0.40
1:A:1087:ASN:ND2	1:A:1099:ASN:O	2.54	0.40
1:A:1755:LYS:HB3	1:A:1759:TYR:CE2	2.55	0.40
1:A:271:GLN:C	1:A:271:GLN:NE2	2.74	0.40
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.87	0.40
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.84	0.40
2:B:1149:PHE:CD2	2:B:1195:LEU:HB3	2.56	0.40
2:B:1425:ILE:HB	2:B:1442:SER:OG	2.21	0.40
2:B:1872:ASN:OD1	2:B:1873:THR:HG23	2.21	0.40
2:B:557:ILE:HD11	2:B:604:VAL:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:274:ILE:HD13	3:C:385:PHE:CD2	2.55	0.40
3:C:365:GLU:CG	3:C:366:ASN:H	2.32	0.40
3:C:624:LYS:HB3	3:C:628:TYR:HE2	1.86	0.40
3:C:769:TYR:OH	3:C:774:LEU:HD22	2.22	0.40
1:A:503:LYS:HE3	4:D:82:A:OP1	2.21	0.40
5:E:67:C:C6	5:E:67:C:C4'	3.05	0.40
6:F:1120:VAL:HG22	6:F:1121:LEU:N	2.36	0.40
6:F:1221:LEU:C	6:F:1223:GLY:H	2.25	0.40
6:F:161:GLN:HE21	6:F:163:ILE:HG22	1.87	0.40
6:F:831:THR:HG23	6:F:831:THR:O	2.22	0.40
28:G:349:LEU:O	28:G:352:LEU:HB2	2.21	0.40
7:H:196:LEU:HD22	7:H:200:ILE:CG2	2.51	0.40
7:H:288:HIS:ND1	7:H:288:HIS:N	2.69	0.40
6:F:186:ARG:N	10:K:41:ASN:ND2	2.70	0.40
15:P:53:LEU:CD2	15:P:53:LEU:C	2.89	0.40
15:P:58:PRO:O	15:P:59:THR:CB	2.70	0.40
16:Q:80:TRP:HE3	16:Q:82:ILE:HD12	1.85	0.40
16:Q:82:ILE:HG23	16:Q:86:LEU:HD23	2.03	0.40
24:Z:284:THR:HB	24:Z:286:THR:HG23	2.02	0.40
1:A:1790:TRP:HE3	1:A:1794:LEU:HB3	1.85	0.40
1:A:1849:LYS:HG2	1:A:1932:GLN:HB2	2.03	0.40
1:A:505:TRP:CE3	1:A:690:LYS:HD3	2.57	0.40
1:A:782:ILE:HD12	1:A:782:ILE:C	2.36	0.40
2:B:170:GLN:CD	2:B:177:ILE:HG22	2.42	0.40
5:E:9:A:H2'	5:E:10:G:C8	2.56	0.40
6:F:163:ILE:HD13	6:F:172:LYS:CD	2.49	0.40
6:F:373:LEU:O	6:F:376:ASP:HB3	2.21	0.40
6:F:519:TYR:CE1	6:F:874:GLY:HA3	2.56	0.40
6:F:528:PRO:HG2	6:F:554:PHE:CZ	2.56	0.40
28:G:215:ASP:N	28:G:215:ASP:OD1	2.54	0.40
8:I:24:LEU:HA	8:I:24:LEU:HD23	1.94	0.40
13:M:500:A:OP2	28:G:775:ARG:NH2	2.46	0.40
14:O:210:ASP:HB2	14:O:217:ILE:CG1	2.46	0.40
20:U:80:LEU:HD23	20:U:129:ILE:HD13	2.02	0.40
23:Y:810:HIS:CG	23:Y:811:PRO:HD2	2.56	0.40
24:Z:125:PHE:CZ	24:Z:132:GLU:HB2	2.57	0.40
1:A:1375:LEU:O	1:A:1376:ASN:CB	2.69	0.40
1:A:138:HIS:O	1:A:142:ILE:HG12	2.22	0.40
1:A:1689:ARG:HG2	1:A:1692:TYR:OH	2.20	0.40
1:A:1835:LEU:CD1	1:A:1836:ASN:CG	2.90	0.40
1:A:2060:LEU:HB3	1:A:2071:ILE:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1469:GLU:HA	2:B:1506:ILE:HG12	2.02	0.40
3:C:120:ARG:O	3:C:123:MET:HB3	2.21	0.40
3:C:606:VAL:HB	3:C:671:SER:HB2	2.03	0.40
3:C:89:PRO:O	3:C:91:VAL:N	2.52	0.40
1:A:756:LEU:HD11	5:E:63:G:H4'	2.04	0.40
6:F:208:GLU:CG	6:F:209:GLN:H	2.35	0.40
6:F:832:TRP:CG	6:F:833:LYS:N	2.89	0.40
28:G:396:VAL:O	28:G:396:VAL:HG12	2.20	0.40
28:G:740:LYS:O	28:G:743:ARG:N	2.55	0.40
9:J:51:PHE:CD2	9:J:52:GLY:N	2.74	0.40
9:J:22:LEU:HG	9:J:70:ALA:HB2	2.03	0.40
10:K:44:GLN:HB3	10:K:69:LEU:HD12	2.03	0.40
15:P:131:ALA:HA	18:S:18:ALA:HA	2.02	0.40
19:T:31:ARG:O	19:T:35:LYS:HG3	2.22	0.40
23:Y:357:ILE:O	23:Y:361:LEU:HG	2.21	0.40
24:Z:296:TYR:HD1	24:Z:332:SER:HG	1.68	0.40
24:Z:449:PHE:CE1	24:Z:465:PHE:CE2	3.09	0.40
1:A:1288:LEU:HB2	1:A:1298:ALA:HB3	2.04	0.40
1:A:1740:TYR:CE1	1:A:1780:ALA:HB2	2.57	0.40
1:A:375:PHE:O	3:C:956:PRO:HA	2.22	0.40
1:A:470:LEU:O	1:A:473:THR:HG22	2.22	0.40
1:A:609:GLU:OE2	5:E:44:A:H5'	2.22	0.40
2:B:1955:VAL:HG12	2:B:1959:ASN:HD21	1.86	0.40
2:B:2011:ILE:HD11	2:B:2030:ILE:HD11	2.02	0.40
2:B:890:THR:HG1	2:B:894:ASN:HD22	1.59	0.40
3:C:362:LYS:O	3:C:364:PHE:N	2.55	0.40
3:C:368:GLU:OE2	3:C:370:TYR:N	2.54	0.40
3:C:701:GLU:OE1	3:C:706:LEU:N	2.48	0.40
3:C:840:PRO:O	3:C:843:LYS:HB3	2.20	0.40
6:F:670:PRO:HB3	6:F:713:LEU:HD21	2.04	0.40
28:G:894:HIS:O	28:G:898:ARG:HG3	2.22	0.40
15:P:330:VAL:O	15:P:333:ASP:N	2.54	0.40
16:Q:240:LEU:HD12	16:Q:241:ILE:H	1.85	0.40
16:Q:24:ARG:HD2	19:T:116:ASN:HD22	1.87	0.40
17:R:153:PRO:HD3	17:R:177:GLU:OE1	2.22	0.40
21:V:11:GLU:OE2	21:V:22:SER:HA	2.20	0.40
23:Y:458:ILE:HA	23:Y:461:LYS:HB2	2.03	0.40
23:Y:701:GLU:HB3	23:Y:848:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2192/2287 (96%)	2037 (93%)	134 (6%)	21 (1%)	19 66
2	B	1803/2163 (83%)	1687 (94%)	112 (6%)	4 (0%)	52 88
3	C	872/1008 (86%)	800 (92%)	62 (7%)	10 (1%)	17 63
6	F	1164/1361 (86%)	1042 (90%)	110 (10%)	12 (1%)	19 66
7	H	147/436 (34%)	139 (95%)	6 (4%)	2 (1%)	14 58
8	I	98/266 (37%)	87 (89%)	9 (9%)	2 (2%)	9 51
9	J	101/107 (94%)	87 (86%)	14 (14%)	0	100 100
10	K	82/85 (96%)	78 (95%)	3 (4%)	1 (1%)	16 61
14	O	335/451 (74%)	302 (90%)	26 (8%)	7 (2%)	9 50
15	P	236/379 (62%)	209 (89%)	23 (10%)	4 (2%)	11 54
16	Q	177/364 (49%)	157 (89%)	16 (9%)	4 (2%)	8 48
17	R	259/339 (76%)	238 (92%)	18 (7%)	3 (1%)	16 61
18	S	65/175 (37%)	53 (82%)	9 (14%)	3 (5%)	3 29
19	T	155/157 (99%)	139 (90%)	13 (8%)	3 (2%)	10 51
20	U	172/207 (83%)	162 (94%)	9 (5%)	1 (1%)	30 75
21	V	126/148 (85%)	118 (94%)	6 (5%)	2 (2%)	12 55
22	W	98/266 (37%)	89 (91%)	6 (6%)	3 (3%)	5 41
23	Y	570/876 (65%)	548 (96%)	21 (4%)	1 (0%)	52 88
24	Z	443/577 (77%)	399 (90%)	32 (7%)	12 (3%)	6 44
25	a	119/259 (46%)	104 (87%)	13 (11%)	2 (2%)	11 54
26	b	146/301 (48%)	134 (92%)	9 (6%)	3 (2%)	9 50
27	c	291/587 (50%)	276 (95%)	9 (3%)	6 (2%)	9 50
28	G	871/971 (90%)	820 (94%)	41 (5%)	10 (1%)	17 63
29	d	234/687 (34%)	214 (92%)	19 (8%)	1 (0%)	39 81
30	X	25/135 (18%)	20 (80%)	5 (20%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	v	120/859 (14%)	110 (92%)	5 (4%)	5 (4%)	3 32
32	e	141/213 (66%)	114 (81%)	16 (11%)	11 (8%)	1 14
33	f	98/215 (46%)	95 (97%)	3 (3%)	0	100 100
34	o	118/503 (24%)	113 (96%)	4 (3%)	1 (1%)	24 70
34	p	122/503 (24%)	116 (95%)	6 (5%)	0	100 100
34	q	349/503 (69%)	321 (92%)	16 (5%)	12 (3%)	5 39
34	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	7 46
35	t	149/175 (85%)	133 (89%)	13 (9%)	3 (2%)	9 51
36	n	21/455 (5%)	19 (90%)	1 (5%)	1 (5%)	3 28
37	k	76/196 (39%)	69 (91%)	7 (9%)	0	100 100
38	i	71/94 (76%)	65 (92%)	6 (8%)	0	100 100
39	h	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	13 56
40	j	65/77 (84%)	64 (98%)	1 (2%)	0	100 100
41	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	15 60
42	m	78/146 (53%)	74 (95%)	4 (5%)	0	100 100
43	g	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	17 63
All	All	12546/19315 (65%)	11559 (92%)	831 (7%)	156 (1%)	21 61

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	1376	ASN
1	A	1405	ILE
1	A	1829	SER
1	A	1830	VAL
1	A	1847	ASP
1	A	2288	CYS
2	B	696	SER
2	B	697	SER
2	B	905	GLN
3	C	364	PHE
3	C	602	VAL
6	F	363	VAL
6	F	413	ILE
6	F	1299	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	55	ASN
8	I	56	PRO
16	Q	99	VAL
18	S	7	PRO
19	T	140	VAL
21	V	17	LEU
22	W	172	ILE
22	W	191	GLU
25	a	139	PHE
26	b	167	ILE
27	c	204	LYS
28	G	57	VAL
28	G	386	TYR
28	G	681	PRO
28	G	830	MET
28	G	831	SER
28	G	835	ILE
28	G	836	TYR
31	v	616	PRO
32	e	83	VAL
32	e	117	ASP
32	e	144	SER
32	e	148	LEU
32	e	170	ASN
34	q	53	ILE
34	q	77	ILE
34	q	172	PRO
34	q	174	TRP
34	q	239	PRO
34	q	246	PRO
34	q	362	PRO
34	q	442	SER
34	r	64	GLU
35	t	77	PRO
1	A	1323	SER
1	A	1746	HIS
3	C	460	GLY
6	F	961	CYS
16	Q	255	SER
17	R	44	ASN
17	R	146	LEU
17	R	218	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	U	52	HIS
22	W	230	SER
24	Z	69	ASN
24	Z	206	LYS
24	Z	234	GLU
24	Z	235	ALA
24	Z	398	PRO
25	a	168	PHE
27	c	230	THR
31	v	601	VAL
31	v	618	GLU
31	v	634	HIS
32	e	147	LYS
32	e	149	LYS
32	e	171	GLN
34	q	196	PRO
35	t	110	GLU
36	n	61	LYS
1	A	645	ASP
1	A	1585	MET
3	C	952	PRO
6	F	364	THR
10	K	19	ILE
14	O	124	GLU
14	O	391	GLU
14	O	442	TRP
15	P	59	THR
18	S	131	THR
24	Z	67	LYS
24	Z	204	ASP
26	b	68	THR
27	c	82	ASN
32	e	82	LYS
34	o	17	PRO
34	r	20	ARG
35	t	80	ASN
1	A	540	THR
1	A	562	ILE
2	B	1609	MET
3	C	84	GLN
14	O	278	ASP
14	O	279	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	O	435	GLU
15	P	86	ASN
19	T	119	THR
24	Z	304	SER
26	b	8	GLN
27	c	224	MET
27	c	231	SER
32	e	33	ASN
41	l	82	PRO
43	g	82	LYS
1	A	1015	PRO
1	A	1490	ARG
3	C	366	ASN
3	C	854	ILE
6	F	92	GLN
6	F	247	PHE
6	F	248	ASN
6	F	434	ASN
6	F	773	LYS
7	H	194	PHE
7	H	235	PRO
15	P	312	ALA
16	Q	52	SER
16	Q	119	LYS
21	V	18	SER
24	Z	229	VAL
28	G	873	HIS
34	q	60	ALA
3	C	363	PRO
18	S	22	PRO
19	T	104	CYS
23	Y	783	PHE
24	Z	146	ASN
28	G	348	VAL
28	G	892	SER
1	A	1964	PRO
29	d	166	VAL
34	q	36	GLY
39	h	15	PRO
1	A	407	VAL
1	A	741	ILE
1	A	802	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	704	PRO
3	C	829	VAL
24	Z	471	GLY
31	v	617	PRO
34	q	175	PRO
6	F	523	ILE
24	Z	214	ILE
32	e	18	PRO
1	A	644	VAL
1	A	771	PRO
6	F	1031	ILE
14	O	277	VAL
15	P	143	VAL
27	c	218	VAL
34	r	36	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1994/2066 (96%)	1916 (96%)	78 (4%)	39 76
2	B	1632/1955 (84%)	1632 (100%)	0	100 100
3	C	791/910 (87%)	778 (98%)	13 (2%)	70 89
6	F	1088/1244 (88%)	1071 (98%)	17 (2%)	70 89
7	H	139/392 (36%)	129 (93%)	10 (7%)	18 57
8	I	89/236 (38%)	82 (92%)	7 (8%)	15 53
9	J	93/97 (96%)	85 (91%)	8 (9%)	13 49
10	K	76/77 (99%)	67 (88%)	9 (12%)	6 31
14	O	295/397 (74%)	293 (99%)	2 (1%)	88 96
15	P	218/328 (66%)	202 (93%)	16 (7%)	17 57
16	Q	171/332 (52%)	159 (93%)	12 (7%)	19 59
17	R	224/296 (76%)	209 (93%)	15 (7%)	20 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	S	58/151 (38%)	56 (97%)	2 (3%)	44 79
19	T	141/141 (100%)	138 (98%)	3 (2%)	61 86
20	U	157/189 (83%)	150 (96%)	7 (4%)	34 73
21	V	114/132 (86%)	112 (98%)	2 (2%)	66 88
22	W	91/240 (38%)	77 (85%)	14 (15%)	3 20
23	Y	299/789 (38%)	291 (97%)	8 (3%)	52 83
24	Z	417/538 (78%)	383 (92%)	34 (8%)	14 51
25	a	112/237 (47%)	108 (96%)	4 (4%)	42 77
26	b	134/273 (49%)	134 (100%)	0	100 100
27	c	196/316 (62%)	190 (97%)	6 (3%)	47 81
28	G	778/867 (90%)	768 (99%)	10 (1%)	76 91
29	d	215/249 (86%)	213 (99%)	2 (1%)	84 94
30	X	21/121 (17%)	21 (100%)	0	100 100
31	v	59/152 (39%)	49 (83%)	10 (17%)	2 15
32	e	48/189 (25%)	43 (90%)	5 (10%)	9 39
33	f	92/193 (48%)	92 (100%)	0	100 100
34	o	61/451 (14%)	54 (88%)	7 (12%)	7 33
34	p	62/451 (14%)	54 (87%)	8 (13%)	5 27
34	q	121/451 (27%)	105 (87%)	16 (13%)	5 27
34	r	59/451 (13%)	54 (92%)	5 (8%)	13 49
35	t	39/165 (24%)	28 (72%)	11 (28%)	0 3
36	n	20/413 (5%)	12 (60%)	8 (40%)	0 1
37	k	70/176 (40%)	70 (100%)	0	100 100
38	i	65/83 (78%)	60 (92%)	5 (8%)	16 54
39	h	61/77 (79%)	60 (98%)	1 (2%)	70 89
40	j	58/66 (88%)	55 (95%)	3 (5%)	29 68
41	l	69/89 (78%)	67 (97%)	2 (3%)	50 81
42	m	77/129 (60%)	71 (92%)	6 (8%)	16 53
43	g	79/87 (91%)	74 (94%)	5 (6%)	22 63
All	All	10583/16196 (65%)	10212 (96%)	371 (4%)	47 78

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	PRO
1	A	228	LYS
1	A	236	ARG
1	A	238	ARG
1	A	256	GLU
1	A	261	LEU
1	A	263	PRO
1	A	266	LEU
1	A	268	LEU
1	A	270	SER
1	A	271	GLN
1	A	309	SER
1	A	324	ASP
1	A	331	PHE
1	A	377	VAL
1	A	380	ARG
1	A	392	ASN
1	A	394	ARG
1	A	396	ARG
1	A	451	ASP
1	A	452	PHE
1	A	461	LEU
1	A	497	GLN
1	A	570	GLN
1	A	614	ARG
1	A	640	ARG
1	A	715	LEU
1	A	716	ARG
1	A	737	ARG
1	A	750	LEU
1	A	769	MET
1	A	773	SER
1	A	774	ILE
1	A	775	ARG
1	A	777	LYS
1	A	782	ILE
1	A	854	ARG
1	A	893	ARG
1	A	928	ARG
1	A	934	ARG
1	A	1011	ASN
1	A	1043	ARG
1	A	1325	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1370	ARG
1	A	1376	ASN
1	A	1378	LYS
1	A	1379	MET
1	A	1442	ARG
1	A	1456	ARG
1	A	1470	GLN
1	A	1499	ARG
1	A	1509	ARG
1	A	1521	ARG
1	A	1589	LYS
1	A	1590	LEU
1	A	1605	ARG
1	A	1608	LEU
1	A	1629	LEU
1	A	1739	ARG
1	A	1747	ASP
1	A	1748	ILE
1	A	1749	SER
1	A	1783	MET
1	A	1794	LEU
1	A	1809	ASN
1	A	1816	ARG
1	A	1830	VAL
1	A	1831	GLN
1	A	1843	LEU
1	A	1899	TRP
1	A	1998	ARG
1	A	2006	SER
1	A	2255	LEU
1	A	2402	GLU
1	A	2403	GLU
1	A	2408	GLN
1	A	2409	ILE
1	A	2412	PHE
3	C	100	LEU
3	C	108	GLN
3	C	115	LYS
3	C	132	ARG
3	C	150	MET
3	C	160	ARG
3	C	170	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	176	ARG
3	C	177	TYR
3	C	180	ASN
3	C	275	LEU
3	C	395	LYS
3	C	548	ARG
6	F	80	VAL
6	F	97	THR
6	F	147	PHE
6	F	153	ASP
6	F	162	ILE
6	F	203	ILE
6	F	257	ILE
6	F	294	PHE
6	F	410	PHE
6	F	444	LEU
6	F	770	LEU
6	F	885	TRP
6	F	1195	VAL
6	F	1231	LEU
6	F	1239	MET
6	F	1302	ARG
6	F	1318	ILE
7	H	155	ARG
7	H	179	LYS
7	H	180	LYS
7	H	181	GLU
7	H	192	ARG
7	H	195	GLU
7	H	233	VAL
7	H	242	LEU
7	H	246	LYS
7	H	288	HIS
8	I	11	LYS
8	I	18	SER
8	I	51	GLN
8	I	53	ARG
8	I	55	ASN
8	I	77	SER
8	I	83	ARG
9	J	2	SER
9	J	4	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	J	54	GLN
9	J	78	ARG
9	J	97	LEU
9	J	98	ASP
9	J	99	ARG
9	J	102	GLU
10	K	8	LEU
10	K	24	GLU
10	K	27	THR
10	K	28	ARG
10	K	42	THR
10	K	44	GLN
10	K	57	ARG
10	K	60	LEU
10	K	63	ARG
14	O	138	HIS
14	O	228	ARG
15	P	37	ASN
15	P	40	LEU
15	P	44	ILE
15	P	48	GLN
15	P	52	GLU
15	P	55	VAL
15	P	57	LEU
15	P	60	LYS
15	P	111	HIS
15	P	133	LYS
15	P	243	GLU
15	P	244	LEU
15	P	247	ARG
15	P	300	ASP
15	P	302	GLN
15	P	325	ASP
16	Q	119	LYS
16	Q	120	LEU
16	Q	209	ASN
16	Q	213	SER
16	Q	217	TRP
16	Q	220	THR
16	Q	222	THR
16	Q	226	LEU
16	Q	227	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Q	245	LYS
16	Q	248	CYS
16	Q	252	ARG
17	R	7	LYS
17	R	10	LYS
17	R	12	GLN
17	R	14	LYS
17	R	15	GLU
17	R	17	GLU
17	R	18	LEU
17	R	31	ASN
17	R	41	PHE
17	R	66	ASN
17	R	67	ASP
17	R	121	ARG
17	R	181	CYS
17	R	210	LYS
17	R	215	ARG
18	S	10	GLU
18	S	40	ARG
19	T	54	GLN
19	T	122	CYS
19	T	126	ARG
20	U	38	LEU
20	U	40	LEU
20	U	42	SER
20	U	44	ASN
20	U	45	LYS
20	U	46	GLU
20	U	50	LEU
21	V	6	GLN
21	V	110	ARG
22	W	160	LYS
22	W	168	GLN
22	W	174	VAL
22	W	187	SER
22	W	188	LEU
22	W	189	THR
22	W	191	GLU
22	W	196	THR
22	W	207	THR
22	W	208	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	W	209	LEU
22	W	212	ARG
22	W	214	LEU
22	W	262	LEU
23	Y	266	THR
23	Y	367	PRO
23	Y	413	PRO
23	Y	578	PRO
23	Y	606	PRO
23	Y	614	PRO
23	Y	784	PRO
23	Y	826	PRO
24	Z	12	LYS
24	Z	16	GLU
24	Z	34	MET
24	Z	67	LYS
24	Z	94	LEU
24	Z	132	GLU
24	Z	138	ILE
24	Z	145	LYS
24	Z	149	ARG
24	Z	151	VAL
24	Z	162	LEU
24	Z	168	LYS
24	Z	174	TRP
24	Z	177	LEU
24	Z	179	TYR
24	Z	181	LEU
24	Z	184	GLN
24	Z	185	GLU
24	Z	186	LEU
24	Z	190	LEU
24	Z	192	GLU
24	Z	193	SER
24	Z	194	LEU
24	Z	195	GLU
24	Z	197	LEU
24	Z	198	PHE
24	Z	199	GLU
24	Z	201	ARG
24	Z	216	ASP
24	Z	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	Z	243	GLU
24	Z	245	CYS
24	Z	303	LEU
24	Z	398	PRO
25	a	134	THR
25	a	167	ASP
25	a	168	PHE
25	a	178	TRP
27	c	504	PRO
27	c	505	PRO
27	c	517	VAL
27	c	523	LEU
27	c	532	PRO
27	c	550	PRO
28	G	22	GLN
28	G	327	TRP
28	G	386	TYR
28	G	469	SER
28	G	543	ARG
28	G	553	LEU
28	G	681	PRO
28	G	740	LYS
28	G	849	ARG
28	G	936	ARG
29	d	120	ASN
29	d	134	LYS
31	v	616	PRO
31	v	617	PRO
31	v	641	PRO
31	v	706	LEU
31	v	712	CYS
31	v	722	PRO
31	v	723	SER
31	v	725	THR
31	v	726	ARG
31	v	733	ILE
32	e	10	THR
32	e	13	VAL
32	e	87	THR
32	e	153	VAL
32	e	179	THR
34	o	17	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	o	26	SER
34	o	44	PRO
34	o	63	THR
34	o	96	PHE
34	o	109	LEU
34	o	134	SER
34	p	17	PRO
34	p	44	PRO
34	p	63	THR
34	p	80	LEU
34	p	85	GLN
34	p	93	LEU
34	p	99	ARG
34	p	109	LEU
34	q	17	PRO
34	q	44	PRO
34	q	55	PRO
34	q	56	SER
34	q	61	SER
34	q	102	LEU
34	q	126	LEU
34	q	172	PRO
34	q	175	PRO
34	q	196	PRO
34	q	215	CYS
34	q	235	THR
34	q	239	PRO
34	q	262	PRO
34	q	350	PRO
34	q	412	PRO
34	r	17	PRO
34	r	44	PRO
34	r	63	THR
34	r	93	LEU
34	r	99	ARG
35	t	5	SER
35	t	7	VAL
35	t	13	PRO
35	t	77	PRO
35	t	96	PRO
35	t	100	THR
35	t	105	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	t	108	SER
35	t	133	PRO
35	t	136	VAL
35	t	150	THR
36	n	51	PHE
36	n	55	GLU
36	n	57	LYS
36	n	58	ARG
36	n	59	ARG
36	n	61	LYS
36	n	62	THR
36	n	66	ASP
38	i	16	CYS
38	i	18	PHE
38	i	25	THR
38	i	79	LYS
38	i	81	LEU
39	h	79	LEU
40	j	18	ASN
40	j	41	ASP
40	j	71	LEU
41	l	10	LEU
41	l	76	ASP
42	m	20	LYS
42	m	26	TRP
42	m	30	GLN
42	m	77	ASP
42	m	99	ASP
42	m	104	ASP
43	g	24	PHE
43	g	49	ARG
43	g	77	THR
43	g	99	ASP
43	g	100	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (173) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	392	ASN
1	A	429	ASN
1	A	541	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	574	GLN
1	A	785	HIS
1	A	848	ASN
1	A	868	GLN
1	A	997	GLN
1	A	1034	ASN
1	A	1045	GLN
1	A	1115	GLN
1	A	1156	HIS
1	A	1231	GLN
1	A	1295	GLN
1	A	1368	GLN
1	A	1376	ASN
1	A	1789	ASN
1	A	1836	ASN
1	A	1845	ASN
1	A	1895	HIS
1	A	2229	GLN
1	A	2355	ASN
1	A	2394	GLN
1	A	2408	GLN
2	B	116	ASN
2	B	122	GLN
2	B	170	GLN
2	B	191	ASN
2	B	529	ASN
2	B	706	GLN
2	B	739	GLN
2	B	773	ASN
2	B	862	GLN
2	B	904	GLN
2	B	1003	ASN
2	B	1148	GLN
2	B	1219	ASN
2	B	1281	GLN
2	B	1352	GLN
2	B	1386	ASN
2	B	1390	GLN
2	B	1430	ASN
2	B	1435	ASN
2	B	1531	ASN
2	B	1701	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1959	ASN
2	B	2046	ASN
2	B	2050	ASN
2	B	2139	ASN
2	B	2161	ASN
3	C	82	ASN
3	C	112	ASN
3	C	183	GLN
3	C	251	GLN
3	C	289	ASN
3	C	309	ASN
3	C	432	GLN
3	C	772	ASN
3	C	776	ASN
3	C	794	GLN
6	F	62	HIS
6	F	119	ASN
6	F	248	ASN
6	F	382	GLN
6	F	384	ASN
6	F	420	HIS
6	F	481	GLN
6	F	547	ASN
6	F	590	HIS
6	F	609	HIS
6	F	641	GLN
6	F	686	GLN
6	F	687	HIS
6	F	738	GLN
6	F	754	HIS
6	F	944	ASN
6	F	950	GLN
6	F	1011	ASN
6	F	1091	HIS
6	F	1117	HIS
6	F	1192	HIS
6	F	1222	GLN
6	F	1304	HIS
6	F	1359	ASN
7	H	145	GLN
7	H	175	HIS
7	H	262	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	2	ASN
8	I	25	GLN
8	I	55	ASN
8	I	72	ASN
9	J	95	ASN
9	J	100	HIS
10	K	32	GLN
10	K	37	ASN
10	K	41	ASN
10	K	44	GLN
10	K	46	HIS
14	O	138	HIS
14	O	382	HIS
15	P	50	ASN
15	P	86	ASN
15	P	302	GLN
15	P	313	ASN
15	P	319	HIS
15	P	322	GLN
16	Q	67	GLN
16	Q	69	ASN
16	Q	106	ASN
16	Q	209	ASN
16	Q	225	GLN
17	R	31	ASN
17	R	58	HIS
17	R	69	GLN
17	R	91	HIS
17	R	201	ASN
17	R	248	ASN
17	R	259	ASN
18	S	173	HIS
19	T	54	GLN
19	T	57	HIS
19	T	116	ASN
19	T	143	HIS
20	U	44	ASN
20	U	52	HIS
20	U	99	ASN
20	U	139	GLN
21	V	5	GLN
22	W	168	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	W	173	ASN
22	W	236	HIS
22	W	239	ASN
23	Y	272	GLN
23	Y	349	HIS
23	Y	429	HIS
24	Z	170	HIS
24	Z	184	GLN
24	Z	354	HIS
24	Z	362	ASN
24	Z	457	HIS
24	Z	463	ASN
25	a	140	GLN
25	a	175	ASN
25	a	176	GLN
27	c	82	ASN
27	c	214	ASN
28	G	17	HIS
28	G	58	GLN
28	G	59	ASN
28	G	65	HIS
28	G	216	GLN
28	G	219	HIS
28	G	295	ASN
28	G	311	ASN
28	G	407	HIS
28	G	572	GLN
28	G	618	GLN
28	G	695	ASN
28	G	697	HIS
28	G	760	HIS
28	G	853	HIS
29	d	79	HIS
29	d	120	ASN
29	d	147	ASN
29	d	179	GLN
29	d	258	GLN
33	f	200	ASN
38	i	34	GLN
38	i	86	ASN
40	j	66	ASN
41	l	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	m	30	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	L	65/1175 (5%)	12 (18%)	0
12	N	24/25 (96%)	9 (37%)	0
13	M	47/61 (77%)	21 (44%)	5 (10%)
4	D	114/214 (53%)	24 (21%)	2 (1%)
5	E	102/112 (91%)	17 (16%)	0
All	All	352/1587 (22%)	83 (23%)	7 (1%)

All (83) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	29	G
4	D	31	G
4	D	42	A
4	D	43	G
4	D	45	A
4	D	46	C
4	D	74	U
4	D	75	A
4	D	77	A
4	D	79	C
4	D	81	A
4	D	84	A
4	D	92	U
4	D	101	C
4	D	127	U
4	D	164	C
4	D	165	A
4	D	166	U
4	D	170	U
4	D	171	U
4	D	172	U
4	D	173	U
4	D	174	G
4	D	175	G
5	E	14	C
5	E	35	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	36	U
5	E	51	A
5	E	60	G
5	E	66	C
5	E	67	C
5	E	68	C
5	E	80	U
5	E	81	G
5	E	85	C
5	E	86	G
5	E	88	U
5	E	91	A
5	E	92	C
5	E	93	A
5	E	103	A
11	L	15	C
11	L	17	U
11	L	18	U
11	L	19	U
11	L	26	G
11	L	32	G
11	L	38	U
11	L	41	C
11	L	46	C
11	L	48	U
11	L	52	A
11	L	66	A
12	N	96	U
12	N	98	A
12	N	100	G
12	N	102	A
12	N	109	U
12	N	110	U
12	N	111	U
12	N	112	U
12	N	114	U
13	M	471	A
13	M	473	A
13	M	481	A
13	M	484	A
13	M	493	A
13	M	497	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	501	A
13	M	502	C
13	M	505	A
13	M	506	U
13	M	507	U
13	M	508	U
13	M	509	A
13	M	510	A
13	M	512	U
13	M	515	U
13	M	516	U
13	M	518	U
13	M	520	G
13	M	521	U
13	M	522	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	78	A
4	D	172	U
13	M	472	A
13	M	480	A
13	M	500	A
13	M	514	U
13	M	515	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 18 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
44	GTP	C	1500	-	26,34,34	0.84	0	29,54,54	1.65	5 (17%)
47	ADP	Y	902	45	24,29,29	1.06	1 (4%)	23,45,45	1.80	1 (4%)

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
44	GTP	C	1500	-	-	0/18/38/38	0/3/3/3
47	ADP	Y	902	45	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y	902	ADP	C5-C4	3.23	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Y	902	ADP	N3-C2-N1	-7.16	123.24	128.87
44	C	1500	GTP	N3-C2-N1	-4.33	121.67	127.56
44	C	1500	GTP	C6-C5-C4	-3.50	116.86	120.86
44	C	1500	GTP	C5-C6-N1	-2.13	120.74	123.52
44	C	1500	GTP	C1'-N9-C4	-2.01	124.57	126.81
44	C	1500	GTP	C6-N1-C2	4.15	120.75	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	C	1500	GTP	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	Y	902	ADP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.