



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:54 AM UTC

PDB ID : 6CNB / pdb_00006cnb
EMDB ID : EMD-7530
Title : Yeast RNA polymerase III initial transcribing complex
Authors : Han, Y.; He, Y.
Deposited on : 2018-03-08
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

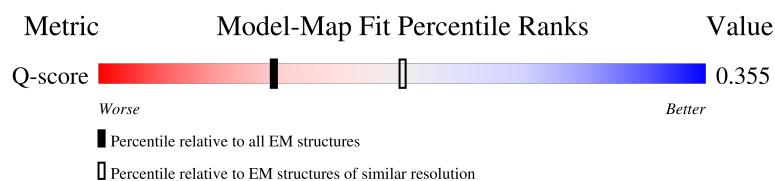
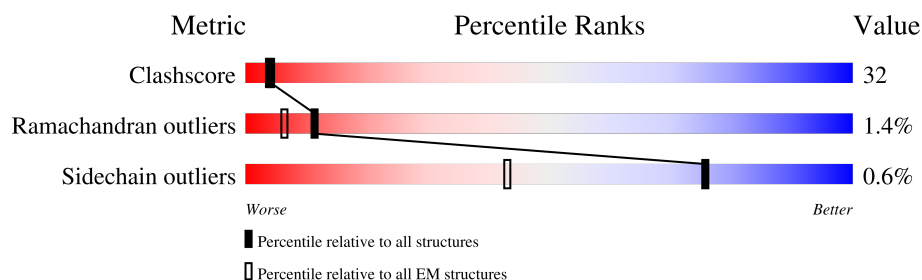
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



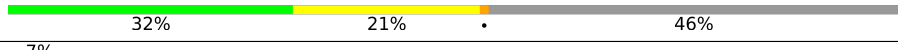
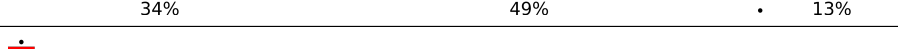
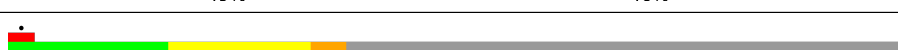
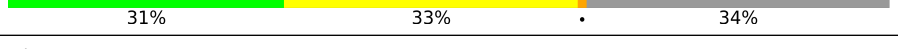
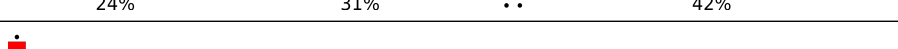
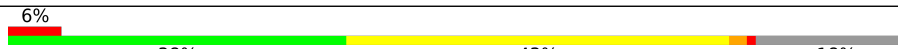
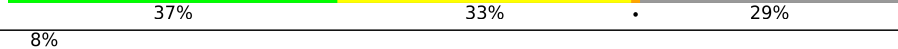
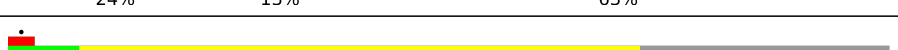
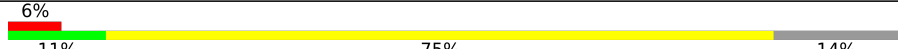
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	1460	
2	B	1149	
3	C	335	
4	D	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	R	736	
19	S	594	
20	X	71	
21	Y	71	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 47837 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 DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11159	7029	1972	2099	59		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	184	Total	C	N	O	S	0	0
			1484	972	239	267	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	277	Total	C	N	O	S	0	0
			2242	1438	368	425	11		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7,DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	54	Total	C	N	O	0	0
			368	238	64	66		

- Molecule 18 is a protein called Transcription factor IIIB 70 kDa subunit,TATA-box-binding protein,Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	522	Total	C	N	O	S	0	0
			4131	2621	733	757	20		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	383	ALA	-	linker	UNP P29056
R	384	MET	-	linker	UNP P29056
R	385	PRO	-	linker	UNP P29056
R	386	TRP	-	linker	UNP P29056
R	567	GLY	-	linker	UNP P13393
R	568	SER	-	linker	UNP P13393
R	569	GLY	-	linker	UNP P13393
R	570	SER	-	linker	UNP P13393
R	571	GLY	-	linker	UNP P13393

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	572	SER	-	linker	UNP P13393
R	573	GLY	-	linker	UNP P13393
R	574	SER	-	linker	UNP P13393
R	575	GLY	-	linker	UNP P13393
R	576	SER	-	linker	UNP P13393
R	577	GLY	-	linker	UNP P13393
R	578	SER	CYS	engineered mutation	UNP P29056

- Molecule 19 is a protein called Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B",Transcription factor TFIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	217	Total	C	N	O	S	0	0
			1649	1035	286	321	7		

- Molecule 20 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	51	Total	C	N	O	P	0	0
			1036	501	177	308	50		

- Molecule 21 is a DNA chain called DNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	61	Total	C	N	O	P	0	0
			1254	603	228	363	60		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	I	1	Total	Zn	0
			1	1	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

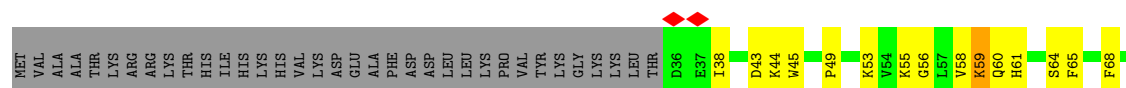
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	R	1	1	1	0

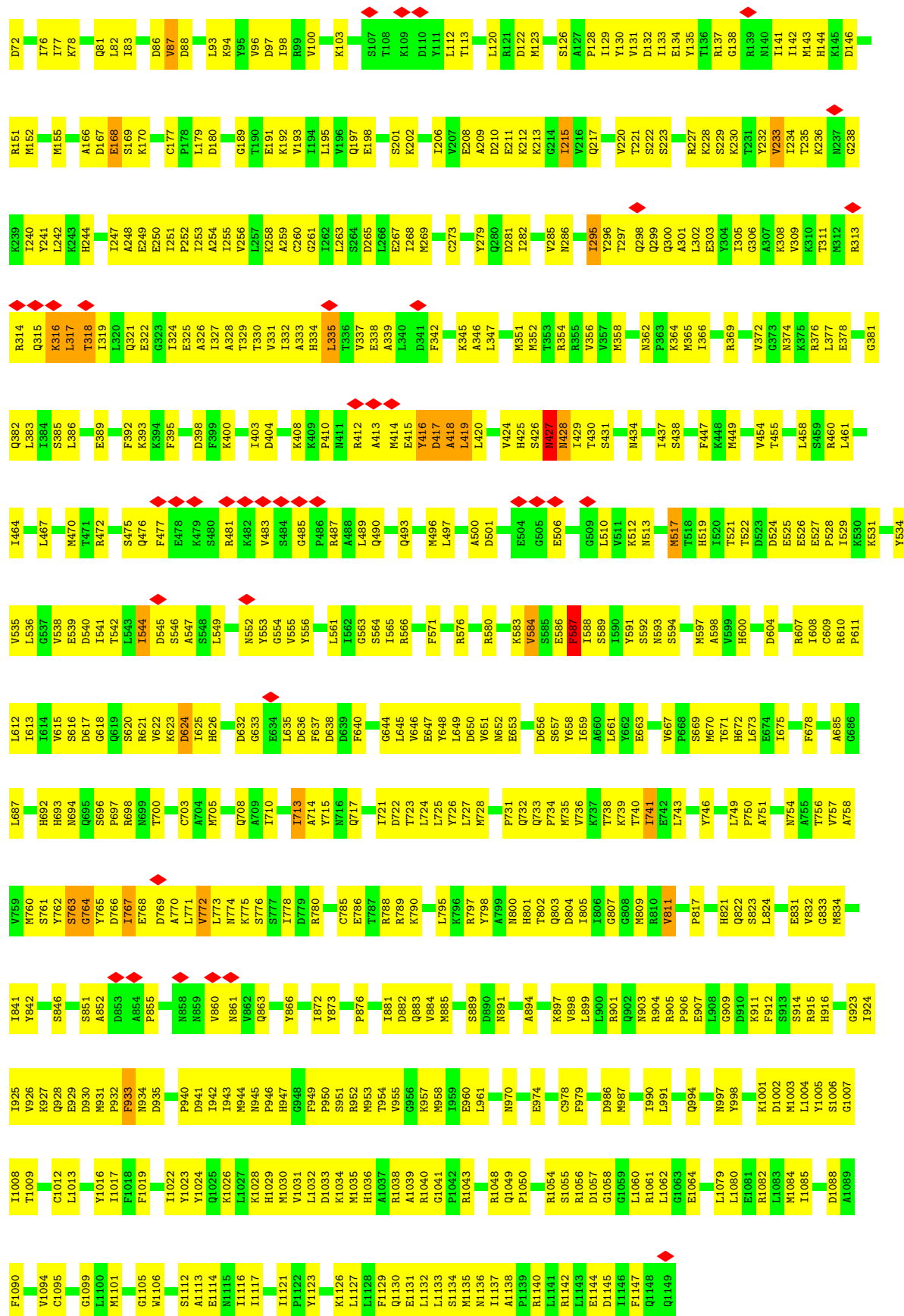
3 Residue-property plots

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

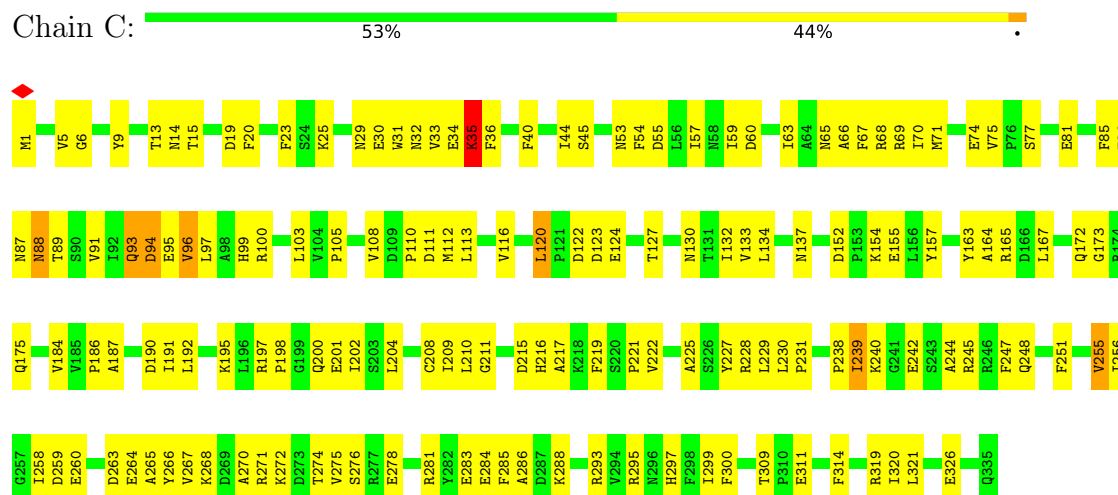
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



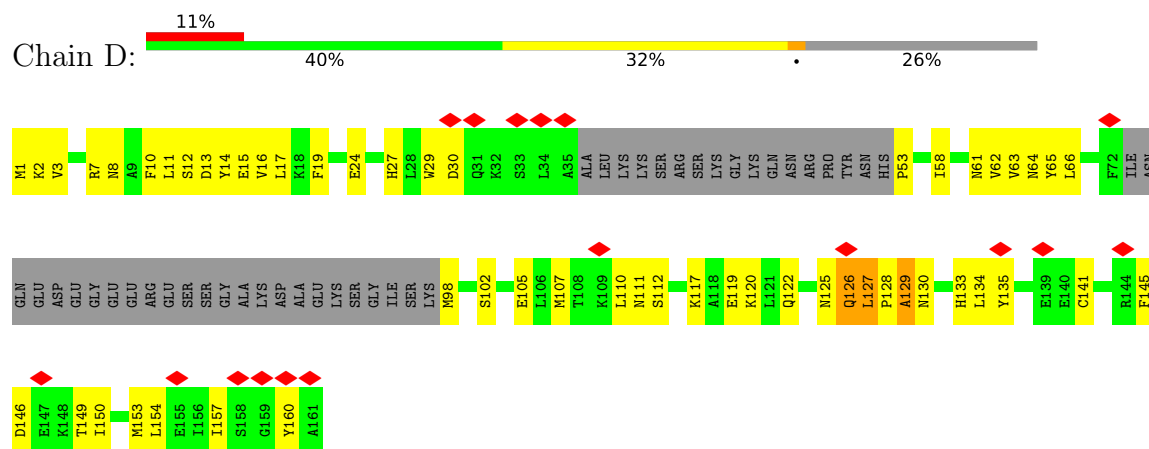




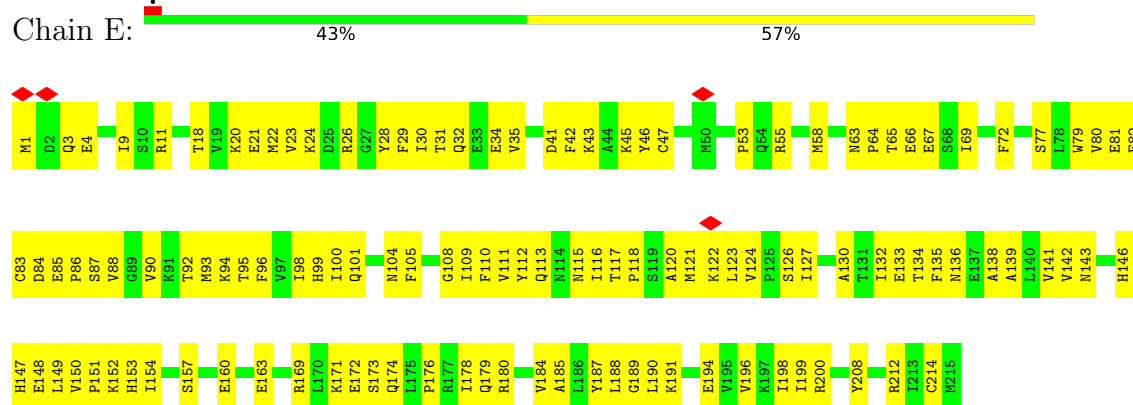
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



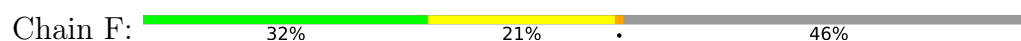
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

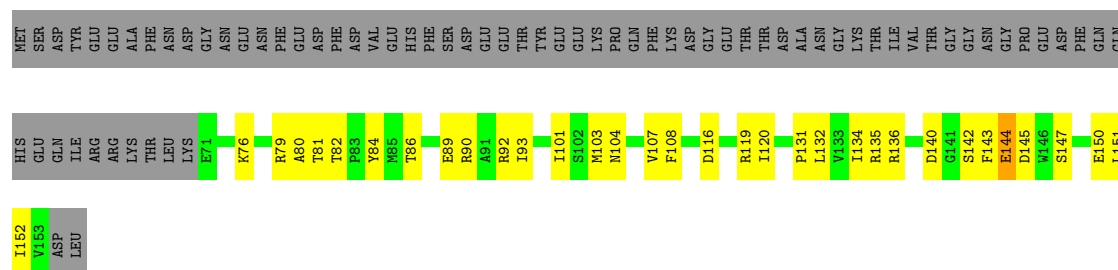


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

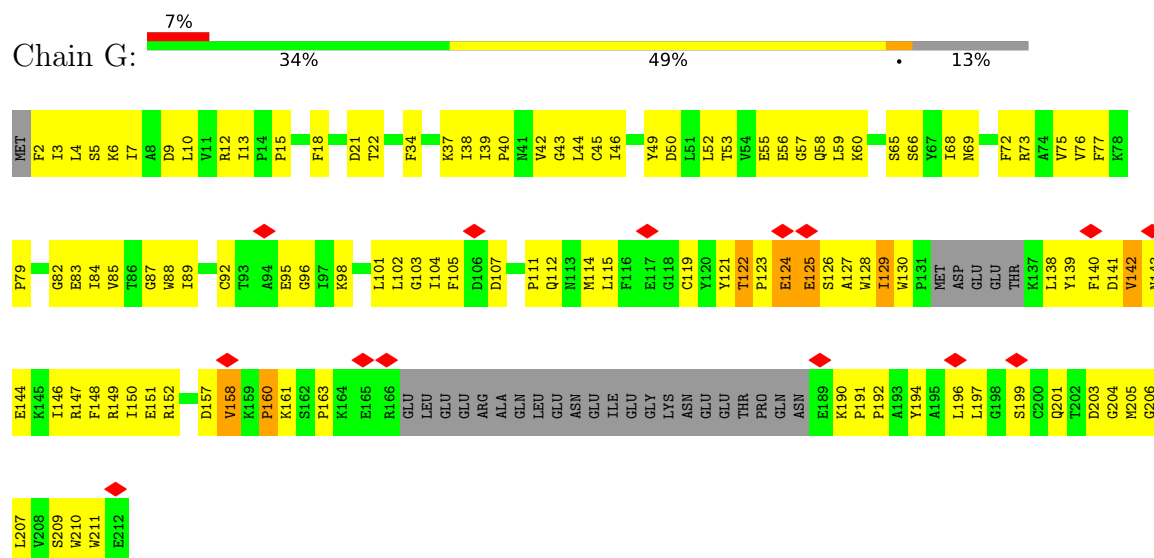


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

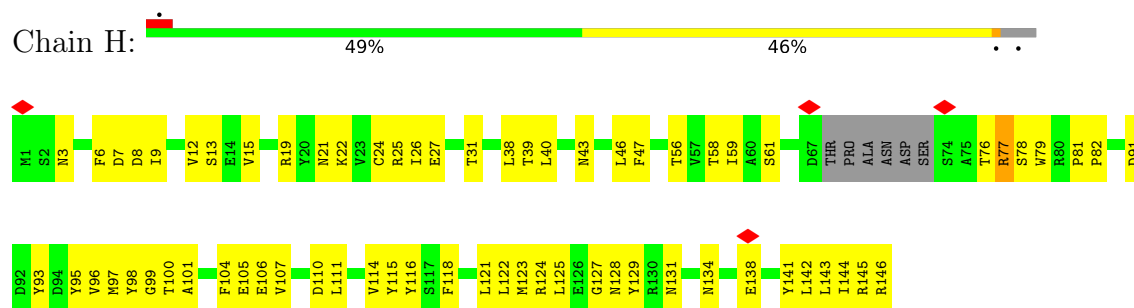




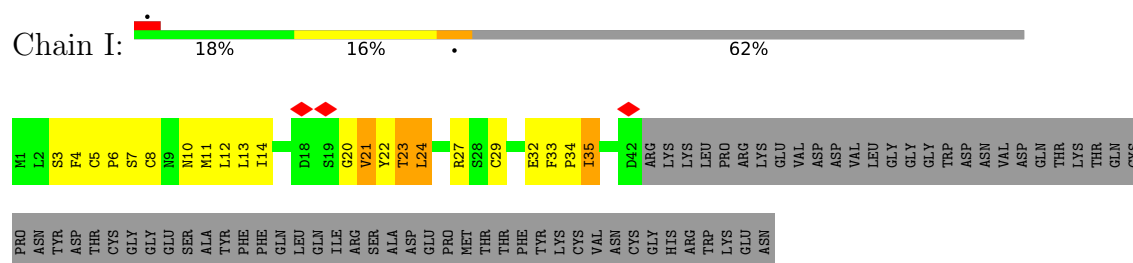
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



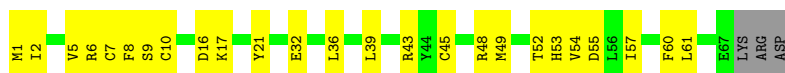
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



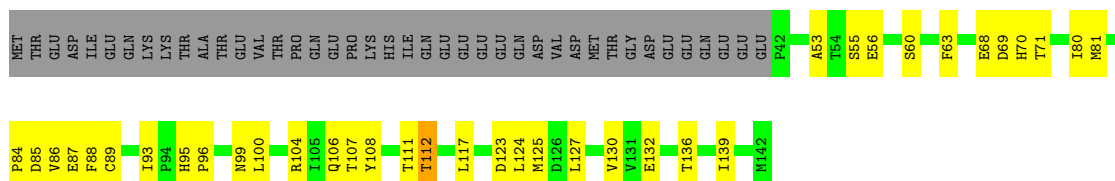
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10

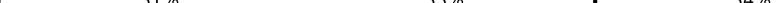


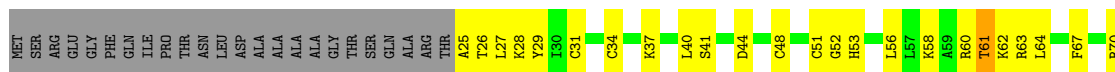
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



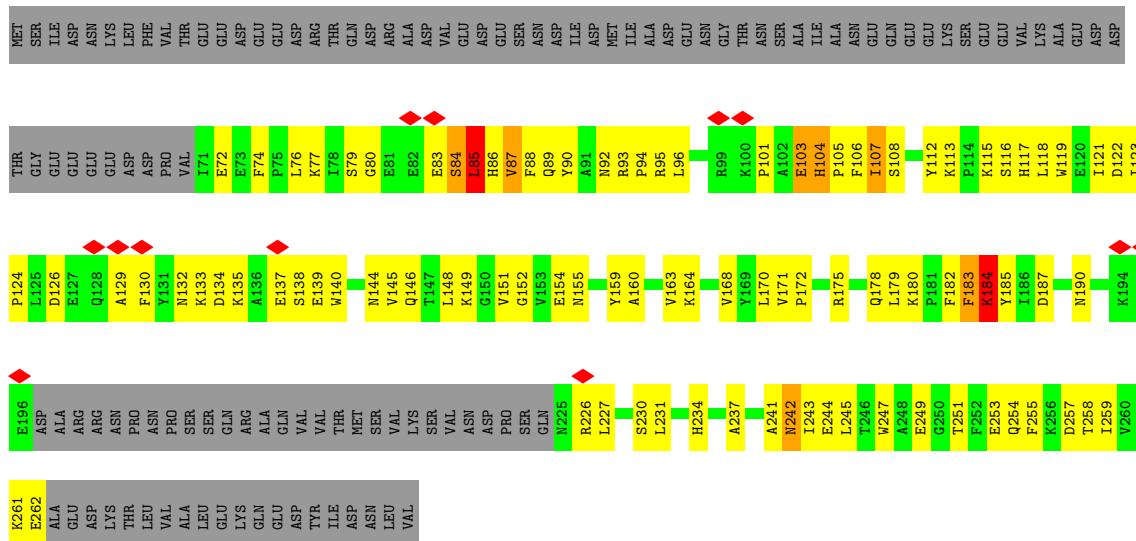
- Chain K: 45% 25% . 29%

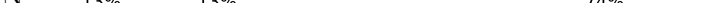


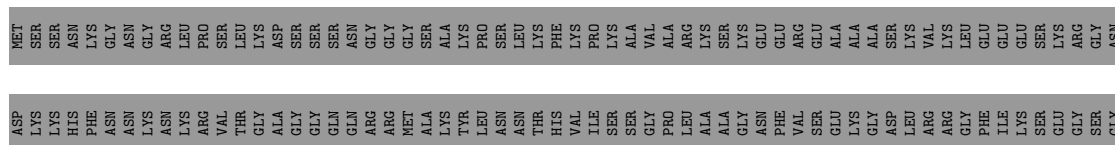
- Chain L:  31% 33% . 34%

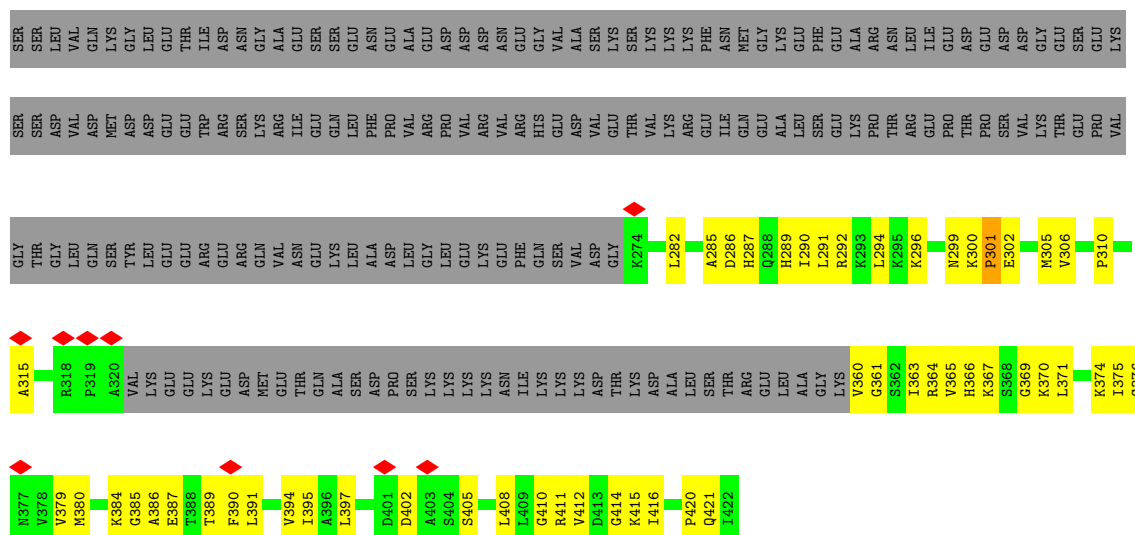


- Chain M:  24% 31% .. 42%

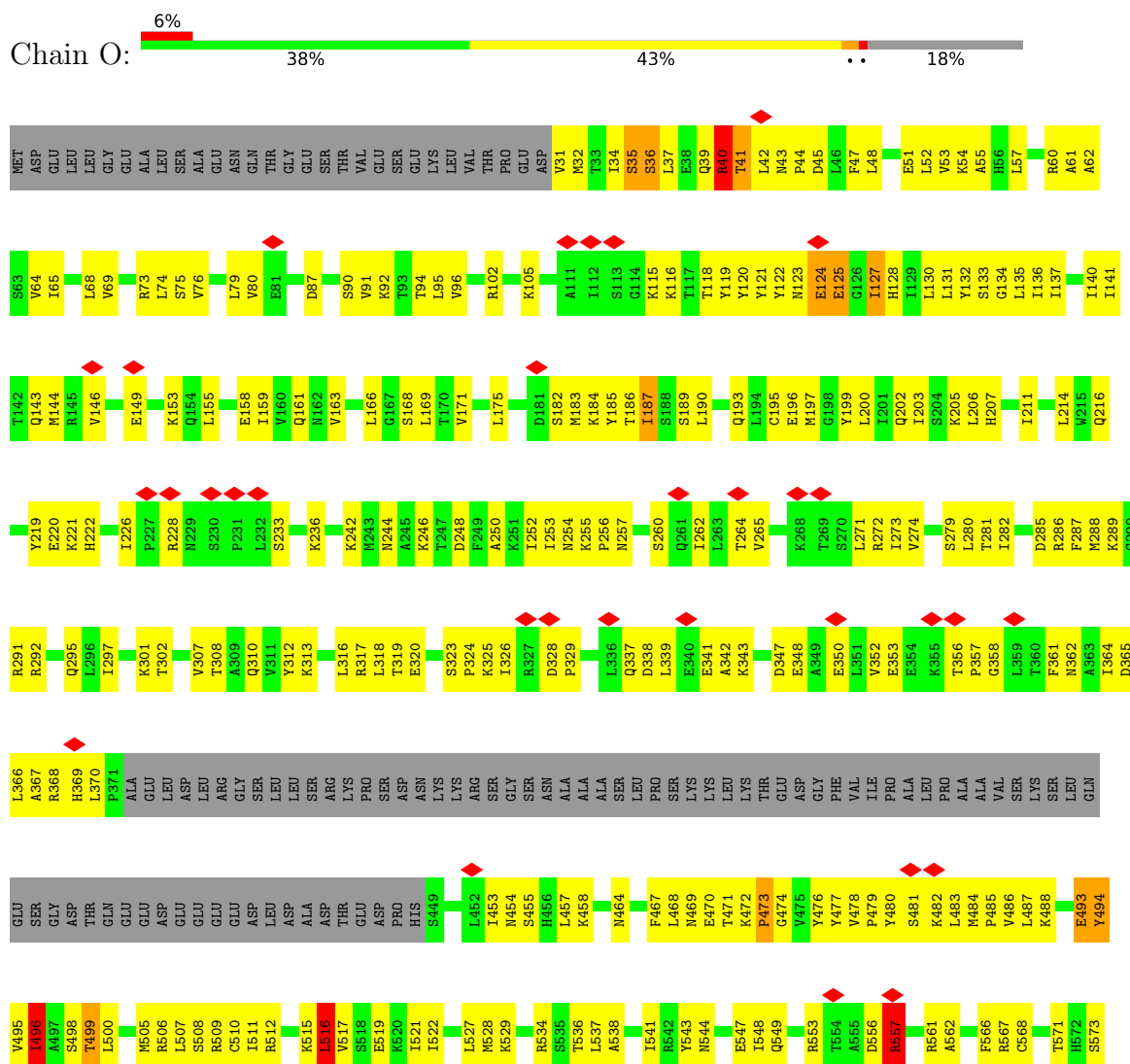


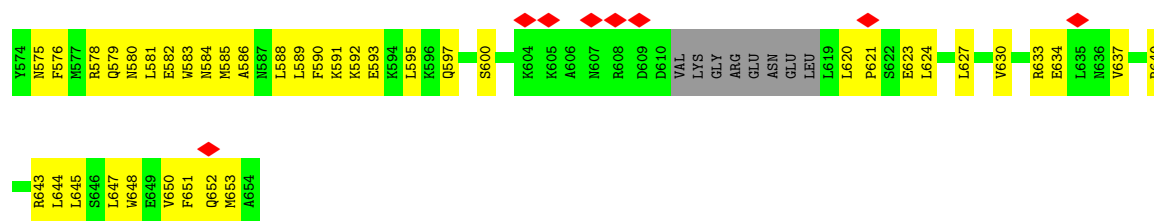
- Chain N:  13% 13% 74%



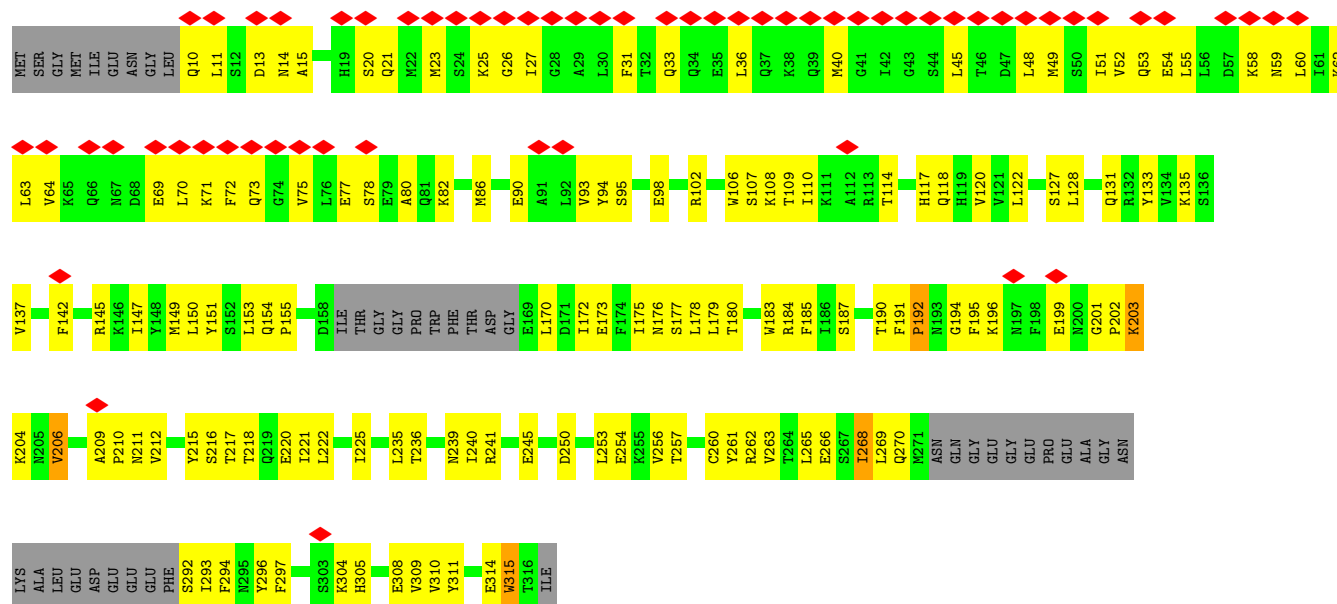


• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

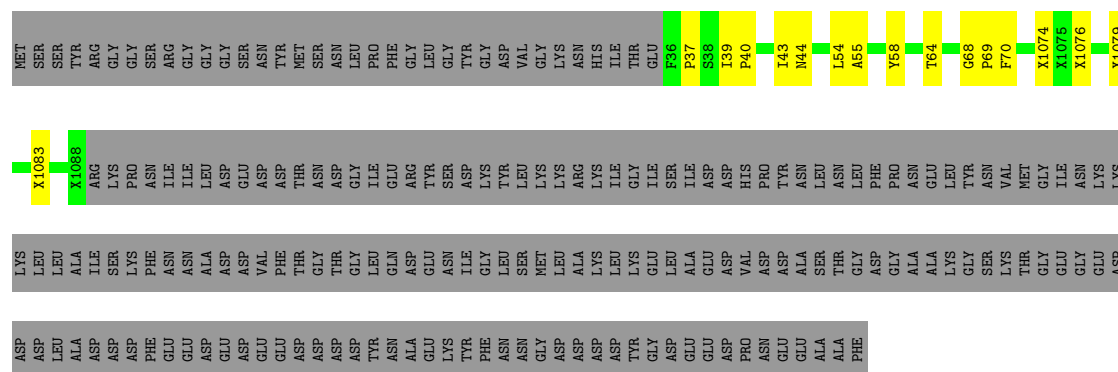




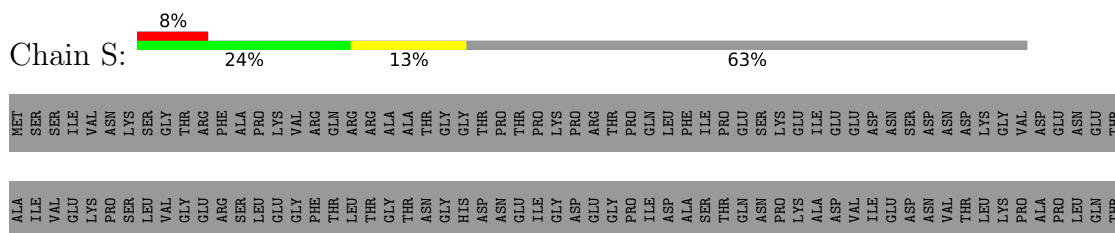
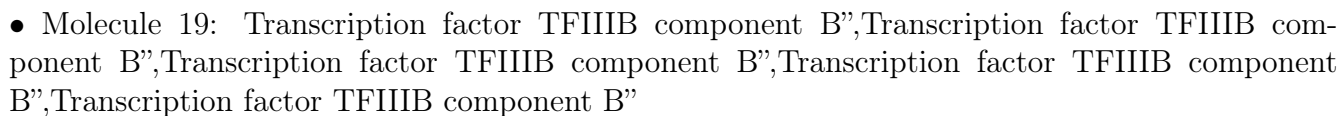
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

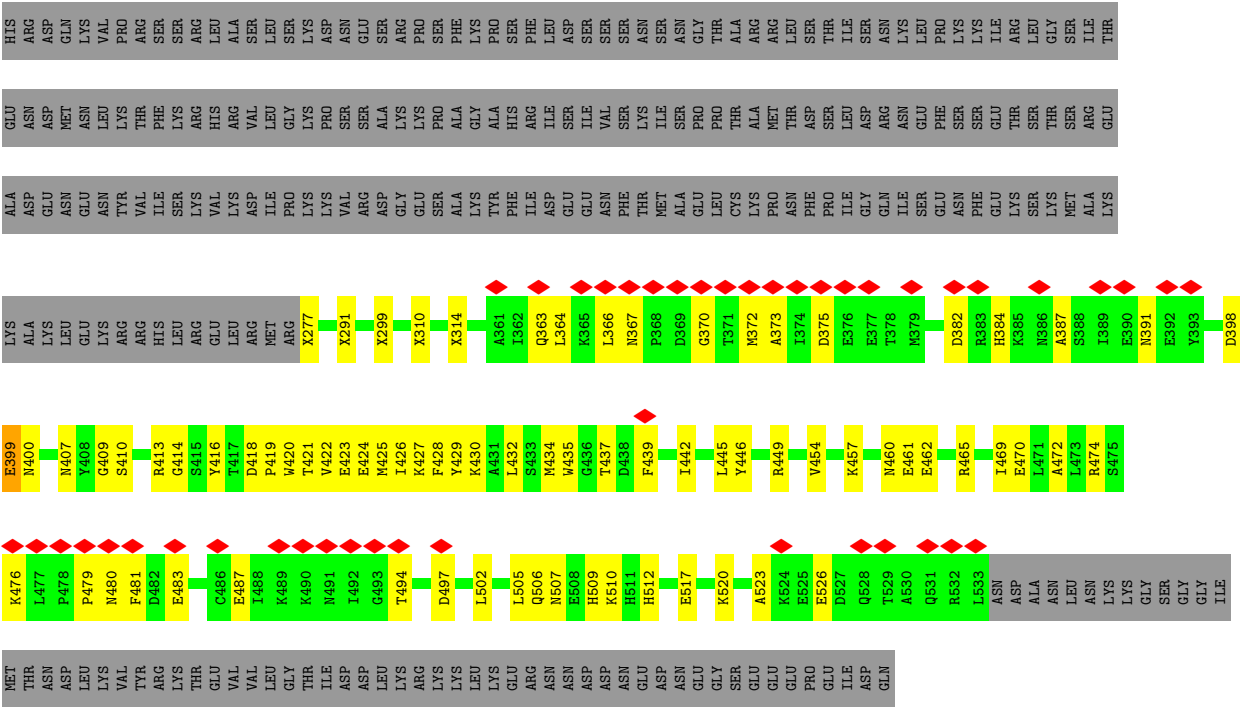


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7, DNA-directed RNA polymerase III subunit RPC7

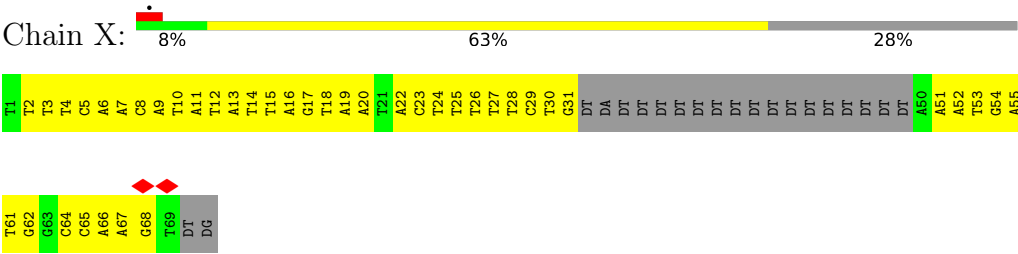


• Molecule 18: Transcription factor IIIB 70 kDa subunit, TATA-box-binding protein, Transcription factor IIIB 70 kDa subunit

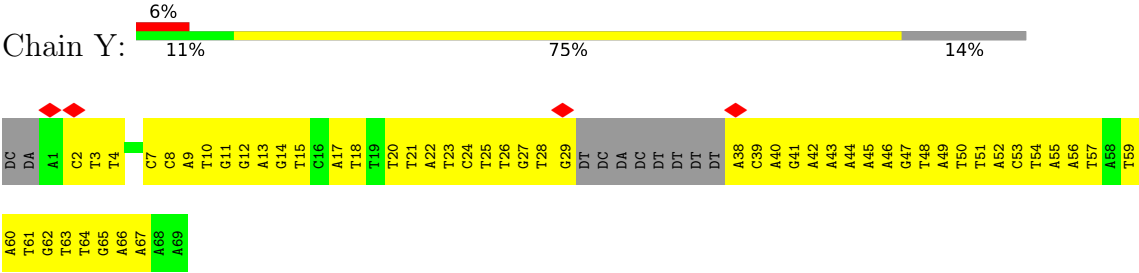




• Molecule 20: DNA (71-MER)



• Molecule 21: DNA (71-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0334	Depositor
Map size ($\text{\AA}$)	339.84, 339.84, 339.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.18, 1.18, 1.18	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/11358	0.79	16/15345 (0.1%)
2	B	0.41	1/8943 (0.0%)	0.79	15/12068 (0.1%)
3	C	0.40	0/2711	0.78	7/3676 (0.2%)
4	D	0.21	0/991	0.66	1/1328 (0.1%)
5	E	0.32	0/1795	0.65	0/2416
6	F	0.40	0/683	0.76	0/923
7	G	0.28	0/1523	0.70	2/2066 (0.1%)
8	H	0.34	0/1138	0.65	0/1540
9	I	0.34	0/328	0.77	0/445
10	J	0.45	0/558	0.75	0/750
11	K	0.42	0/803	0.79	1/1083 (0.1%)
12	L	0.33	0/365	0.81	1/485 (0.2%)
13	M	0.32	1/1369 (0.1%)	0.82	5/1851 (0.3%)
14	N	0.24	0/855	0.73	2/1149 (0.2%)
15	O	0.32	0/4394	0.76	5/5928 (0.1%)
16	P	0.25	0/2282	0.69	6/3075 (0.2%)
17	Q	0.26	0/281	0.55	0/381
18	R	0.27	1/4200 (0.0%)	0.63	3/5659 (0.1%)
19	S	0.18	0/1464	0.60	3/1971 (0.2%)
20	X	0.28	0/1158	0.51	0/1782
21	Y	0.28	0/1407	0.50	0/2169
All	All	0.35	3/48606 (0.0%)	0.73	67/66090 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	151	GLN	CA-C	7.22	1.62	1.52
2	B	517	MET	CA-CB	-5.59	1.45	1.53
13	M	103	GLU	CA-C	5.00	1.59	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	184	LYS	N-CA-C	-10.46	100.52	113.18
3	C	96	VAL	N-CA-C	9.77	120.39	110.23
2	B	335	LEU	N-CA-C	-9.44	100.71	112.88
2	B	428	ASN	N-CA-C	-9.26	101.09	112.38
15	O	556	ASP	N-CA-C	-9.14	100.25	111.40
19	S	399	GLU	N-CA-C	8.81	123.60	107.73
3	C	35	LYS	N-CA-C	-8.79	101.65	112.38
13	M	104	HIS	CA-C-N	8.67	130.68	119.84
13	M	104	HIS	C-N-CA	8.67	130.68	119.84
18	R	151	GLN	CA-C-O	8.61	129.84	120.20
15	O	35	SER	N-CA-C	-8.51	102.92	113.38
18	R	150	LEU	N-CA-C	8.35	121.98	109.95
15	O	493	GLU	CB-CA-C	-8.08	107.25	116.63
1	A	282	GLU	N-CA-C	-8.06	100.20	110.19
1	A	229	ASN	N-CA-C	-7.80	102.77	111.82
3	C	120	LEU	CA-C-N	-7.75	110.16	119.84
3	C	120	LEU	C-N-CA	-7.75	110.16	119.84
1	A	227	THR	N-CA-C	7.73	121.81	112.38
16	P	270	GLN	N-CA-C	-7.67	102.61	110.97
3	C	94	ASP	N-CA-C	-7.61	103.88	113.01
15	O	127	ILE	N-CA-C	-7.45	102.15	112.50
2	B	1135	MET	CA-C-N	-7.21	112.84	122.42
2	B	1135	MET	C-N-CA	-7.21	112.84	122.42
1	A	247	THR	N-CA-C	-6.93	104.40	112.92
16	P	268	ILE	N-CA-C	6.81	117.57	110.62
1	A	190	SER	CA-C-N	-6.65	110.22	122.06
1	A	190	SER	C-N-CA	-6.65	110.22	122.06
18	R	152	VAL	N-CA-C	6.65	123.17	109.34
16	P	315	TRP	N-CA-C	-6.60	103.28	112.12
7	G	129	ILE	CA-C-N	6.56	132.20	121.57
7	G	129	ILE	C-N-CA	6.56	132.20	121.57
1	A	36	THR	CB-CA-C	-6.48	109.09	116.54
2	B	329	THR	N-CA-C	6.36	119.89	111.75
1	A	1445	ARG	N-CA-C	-6.25	99.22	108.79
15	O	498	SER	N-CA-C	-6.23	104.38	112.23
3	C	187	ALA	CB-CA-C	-6.22	109.39	116.54
11	K	112	THR	N-CA-CB	-6.21	101.28	110.85
1	A	1449	GLU	N-CA-C	6.08	123.75	110.80
13	M	183	PHE	N-CA-C	6.06	119.01	108.76
2	B	764	GLY	N-CA-C	-6.06	106.67	114.85
1	A	31	GLU	N-CA-C	5.78	117.66	111.36
2	B	933	PHE	CA-C-N	5.67	132.37	121.54
2	B	933	PHE	C-N-CA	5.67	132.37	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	544	ILE	CA-C-N	5.59	128.55	120.38
2	B	544	ILE	C-N-CA	5.59	128.55	120.38
3	C	93	GLN	N-CA-C	5.59	118.17	110.35
2	B	419	LEU	CA-C-N	-5.53	110.23	121.18
2	B	419	LEU	C-N-CA	-5.53	110.23	121.18
1	A	1448	PHE	N-CA-C	-5.46	99.17	110.80
1	A	79	GLY	N-CA-C	-5.38	106.26	112.29
2	B	418	ALA	N-CA-C	-5.37	104.03	111.28
14	N	301	PRO	CA-C-N	-5.30	115.48	122.85
14	N	301	PRO	C-N-CA	-5.30	115.48	122.85
1	A	168	ALA	CB-CA-C	-5.22	109.58	115.79
2	B	317	LEU	N-CA-C	-5.19	106.05	112.38
19	S	398	ASP	CA-C-N	-5.16	115.27	123.12
19	S	398	ASP	C-N-CA	-5.16	115.27	123.12
12	L	52	GLY	N-CA-C	-5.16	108.56	115.32
13	M	85	LEU	N-CA-C	5.10	121.66	110.80
1	A	31	GLU	N-CA-CB	-5.08	102.64	110.16
16	P	270	GLN	N-CA-CB	5.07	117.31	109.91
4	D	126	GLN	N-CA-C	5.07	117.78	110.28
1	A	538	LYS	N-CA-C	5.06	119.72	111.37
2	B	522	THR	N-CA-CB	-5.04	102.77	110.49
1	A	495	TRP	CB-CA-C	-5.03	109.25	115.89
16	P	199	GLU	CA-C-N	-5.02	115.87	122.85
16	P	199	GLU	C-N-CA	-5.02	115.87	122.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11159	0	11285	815	0
2	B	8788	0	8901	659	0
3	C	2655	0	2628	170	0
4	D	977	0	983	87	0
5	E	1759	0	1788	109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	671	0	692	35	0
7	G	1484	0	1485	130	0
8	H	1120	0	1089	68	0
9	I	321	0	303	43	0
10	J	549	0	559	37	0
11	K	792	0	790	38	0
12	L	363	0	386	35	0
13	M	1338	0	1307	148	0
14	N	845	0	891	68	0
15	O	4329	0	4497	364	0
16	P	2242	0	2265	146	0
17	Q	368	0	307	14	0
18	R	4131	0	4230	261	0
19	S	1649	0	1456	72	0
20	X	1036	0	584	76	0
21	Y	1254	0	695	94	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	R	1	0	0	0	0
All	All	47837	0	47121	3055	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (3055) 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)
20:X:4:DT:H2''	20:X:5:DC:C5'	1.26	1.57
2:B:587:PHE:CZ	2:B:607:ARG:HD3	1.32	1.56
20:X:4:DT:C2'	20:X:5:DC:H5'	1.35	1.54
1:A:200:GLU:HB3	15:O:516:LEU:CD2	1.48	1.43
1:A:235:LYS:HD3	15:O:44:PRO:CG	1.49	1.40
2:B:587:PHE:HZ	2:B:607:ARG:CD	1.35	1.38
1:A:154:CYS:HB3	1:A:157:CYS:SG	1.66	1.36
4:D:127:LEU:HD22	4:D:133:HIS:CD2	1.66	1.29
15:O:495:VAL:O	15:O:496:ILE:HG12	1.36	1.26
12:L:34:CYS:SG	12:L:51:CYS:HB3	1.75	1.25
7:G:82:GLY:HA2	7:G:150:ILE:O	1.32	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:NZ	15:O:44:PRO:CB	2.04	1.21
1:A:200:GLU:CB	15:O:516:LEU:HD21	1.72	1.19
1:A:598:MET:O	1:A:599:LYS:HG2	1.38	1.19
1:A:599:LYS:HB2	1:A:600:PRO:CD	1.73	1.19
1:A:232:LYS:O	1:A:235:LYS:HE3	1.42	1.16
1:A:235:LYS:HA	1:A:252:ARG:HD3	1.22	1.16
1:A:235:LYS:NZ	15:O:44:PRO:HB2	1.61	1.16
1:A:235:LYS:CD	15:O:44:PRO:HG2	1.77	1.15
21:Y:20:DT:C7	21:Y:21:DT:H73	1.75	1.15
1:A:599:LYS:HB2	1:A:600:PRO:HD2	1.15	1.14
1:A:235:LYS:HZ3	15:O:44:PRO:HB3	1.12	1.13
15:O:495:VAL:O	15:O:496:ILE:CG1	1.96	1.12
9:I:8:CYS:HB3	9:I:29:CYS:SG	1.87	1.12
1:A:235:LYS:CD	15:O:44:PRO:CG	2.28	1.11
1:A:102:ILE:HD12	1:A:242:LEU:CD1	1.79	1.10
18:R:219:ARG:HA	18:R:514:GLU:CG	1.81	1.10
8:H:58:THR:O	8:H:143:LEU:HB3	1.50	1.09
7:G:126:SER:CB	7:G:139:TYR:HB2	1.82	1.09
1:A:235:LYS:HD3	15:O:44:PRO:CB	1.83	1.08
20:X:3:DT:H2"	20:X:4:DT:C7	1.82	1.08
1:A:256:TYR:CE2	1:A:1401:PHE:CE1	2.42	1.08
1:A:102:ILE:HD12	1:A:242:LEU:HD13	1.14	1.07
3:C:93:GLN:HB3	3:C:95:GLU:HG2	1.34	1.07
4:D:127:LEU:CD2	4:D:133:HIS:HD2	1.66	1.07
1:A:252:ARG:HB3	1:A:253:PRO:HD2	1.31	1.06
7:G:87:GLY:O	7:G:146:ILE:HB	1.55	1.06
15:O:184:LYS:HA	15:O:187:ILE:HD11	1.35	1.06
15:O:584:ASN:O	15:O:588:LEU:HB3	1.56	1.05
20:X:3:DT:H2"	20:X:4:DT:H71	1.35	1.05
18:R:219:ARG:HA	18:R:514:GLU:HG3	1.36	1.05
1:A:598:MET:O	1:A:599:LYS:CG	2.05	1.05
11:K:111:THR:HG22	11:K:112:THR:H	1.18	1.04
1:A:102:ILE:CD1	1:A:242:LEU:HD13	1.88	1.04
1:A:1174:GLN:HB3	1:A:1185:GLN:O	1.54	1.04
19:S:470:GLU:O	19:S:474:ARG:HB3	1.56	1.04
1:A:235:LYS:CD	15:O:44:PRO:HB2	1.88	1.04
4:D:11:LEU:HD21	4:D:16:VAL:HG21	1.40	1.03
7:G:126:SER:HB3	7:G:139:TYR:CB	1.89	1.02
15:O:73:ARG:HG2	15:O:121:TYR:CE1	1.94	1.01
15:O:36:SER:O	15:O:40:ARG:HB2	1.60	1.01
2:B:521:THR:HG21	2:B:587:PHE:CD1	1.96	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:125:GLU:HB3	15:O:128:HIS:HB2	1.40	0.99
2:B:316:LYS:HZ2	13:M:226:ARG:HH21	0.99	0.99
1:A:235:LYS:CA	1:A:252:ARG:HD3	1.93	0.99
1:A:100:ILE:O	1:A:104:GLN:HB2	1.63	0.98
1:A:235:LYS:HA	1:A:252:ARG:CD	1.94	0.97
7:G:126:SER:HB3	7:G:139:TYR:HB2	1.00	0.97
1:A:102:ILE:CD1	1:A:242:LEU:CD1	2.41	0.97
20:X:4:DT:C2'	20:X:5:DC:C5'	2.12	0.97
18:R:558:PRO:O	18:R:562:GLU:HB2	1.65	0.97
8:H:105:GLU:HG2	8:H:106:GLU:H	1.28	0.97
1:A:599:LYS:CB	1:A:600:PRO:CD	2.41	0.97
2:B:135:TYR:CE1	2:B:419:LEU:HB3	1.99	0.97
4:D:14:TYR:CD1	4:D:15:GLU:N	2.32	0.97
3:C:172:GLN:H	3:C:175:GLN:HB3	1.29	0.96
13:M:85:LEU:O	14:N:397:LEU:O	1.84	0.96
19:S:483:GLU:O	19:S:487:GLU:HB2	1.63	0.95
1:A:235:LYS:CD	15:O:44:PRO:CB	2.43	0.95
2:B:419:LEU:HD12	2:B:420:LEU:N	1.81	0.95
1:A:252:ARG:HB3	1:A:253:PRO:CD	1.96	0.95
18:R:83:ALA:O	18:R:87:LEU:HG	1.67	0.94
19:S:418:ASP:HB3	19:S:449:ARG:HH12	1.32	0.94
2:B:772:VAL:HG13	2:B:943:ILE:HG23	1.47	0.94
18:R:219:ARG:HD3	18:R:514:GLU:HG3	1.50	0.94
9:I:24:LEU:HD23	9:I:33:PHE:CD1	2.04	0.93
2:B:521:THR:CG2	2:B:609:CYS:SG	2.56	0.93
1:A:235:LYS:HZ2	15:O:44:PRO:HB2	1.19	0.93
2:B:417:ASP:HB3	2:B:419:LEU:HG	1.50	0.93
1:A:235:LYS:HD3	15:O:44:PRO:HG2	0.93	0.92
13:M:182:PHE:O	13:M:183:PHE:HD1	1.51	0.92
14:N:371:LEU:HD22	14:N:384:LYS:HD3	1.52	0.92
1:A:228:LEU:HB3	1:A:257:ILE:HD11	1.52	0.92
1:A:256:TYR:CZ	1:A:1401:PHE:CD1	2.59	0.91
1:A:179:ILE:CD1	15:O:557:ARG:HH21	1.82	0.91
2:B:315:GLN:O	2:B:316:LYS:HB2	1.68	0.91
2:B:552:ASN:ND2	2:B:566:ARG:HA	1.86	0.91
12:L:48:CYS:SG	12:L:51:CYS:O	2.29	0.90
15:O:143:GLN:HE21	15:O:196:GLU:HG2	1.34	0.90
15:O:470:GLU:HB2	15:O:479:PRO:HG3	1.52	0.90
11:K:111:THR:CG2	11:K:112:THR:H	1.83	0.90
1:A:228:LEU:HD12	1:A:229:ASN:N	1.87	0.89
3:C:94:ASP:O	12:L:67:PHE:HE2	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HG3	1:A:275:GLN:HG2	1.51	0.89
2:B:143:MET:SD	19:S:399:GLU:HB2	2.12	0.89
2:B:587:PHE:CZ	2:B:607:ARG:CD	2.24	0.89
9:I:29:CYS:HB3	13:M:183:PHE:CE2	2.08	0.89
1:A:235:LYS:NZ	15:O:44:PRO:HB3	1.78	0.88
4:D:14:TYR:CD1	4:D:15:GLU:HG2	2.08	0.88
2:B:55:LYS:NZ	2:B:59:LYS:HE3	1.89	0.88
2:B:55:LYS:HZ3	2:B:59:LYS:HE3	1.37	0.88
15:O:44:PRO:HA	15:O:582:GLU:HG2	1.54	0.88
15:O:184:LYS:HA	15:O:187:ILE:CD1	2.03	0.88
1:A:235:LYS:CE	15:O:44:PRO:CB	2.51	0.88
2:B:552:ASN:HD21	2:B:566:ARG:HA	1.37	0.88
13:M:85:LEU:HD23	13:M:86:HIS:O	1.74	0.88
15:O:105:LYS:HG2	15:O:123:ASN:HA	1.56	0.88
1:A:256:TYR:CE2	1:A:1401:PHE:HE1	1.90	0.88
15:O:583:TRP:HH2	16:P:314:GLU:HG3	1.37	0.88
2:B:316:LYS:NZ	13:M:226:ARG:HH21	1.71	0.88
15:O:515:LYS:O	15:O:516:LEU:HG	1.73	0.87
1:A:235:LYS:CE	15:O:44:PRO:HB2	2.03	0.87
16:P:266:GLU:O	16:P:269:LEU:HG	1.74	0.87
1:A:89:PRO:HG3	1:A:228:LEU:HD21	1.54	0.87
1:A:178:ILE:HD11	1:A:222:LEU:HB2	1.54	0.86
18:R:83:ALA:O	18:R:87:LEU:CG	2.22	0.86
18:R:135:ARG:HH12	18:R:513:PRO:HG3	1.39	0.86
15:O:547:GLU:HG2	15:O:548:ILE:H	1.40	0.86
20:X:4:DT:H71	20:X:4:DT:OP2	1.75	0.86
1:A:1448:PHE:HZ	4:D:16:VAL:CG2	1.88	0.86
2:B:587:PHE:CE2	2:B:604:ASP:O	2.28	0.86
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.41	0.86
4:D:127:LEU:HD22	4:D:133:HIS:HD2	0.76	0.86
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.48	0.86
13:M:182:PHE:O	13:M:183:PHE:CD1	2.28	0.86
18:R:219:ARG:CA	18:R:514:GLU:HG3	2.05	0.85
21:Y:20:DT:H73	21:Y:21:DT:H73	1.55	0.85
15:O:200:LEU:HB3	15:O:280:LEU:HB3	1.57	0.85
15:O:125:GLU:CB	15:O:128:HIS:HB2	2.05	0.85
1:A:234:ILE:HD11	1:A:237:ALA:HB3	1.57	0.85
1:A:1366:GLY:HA3	5:E:179:GLN:HG3	1.59	0.85
2:B:521:THR:HG21	2:B:609:CYS:SG	2.17	0.84
14:N:306:VAL:HG23	14:N:415:LYS:HD3	1.56	0.84
15:O:467:PHE:HD2	15:O:468:LEU:HD13	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HZ3	15:O:44:PRO:CB	1.73	0.84
2:B:717:GLN:HE21	2:B:727:LEU:HD22	1.43	0.84
15:O:583:TRP:CH2	16:P:314:GLU:HG3	2.11	0.84
13:M:241:ALA:O	13:M:242:ASN:HB3	1.78	0.84
1:A:232:LYS:O	1:A:235:LYS:CE	2.25	0.84
3:C:85:PHE:HE2	3:C:94:ASP:O	1.60	0.84
2:B:587:PHE:CZ	2:B:607:ARG:HB3	2.13	0.83
13:M:245:LEU:HD22	14:N:405:SER:OG	1.78	0.83
11:K:111:THR:HG22	11:K:112:THR:N	1.87	0.83
15:O:73:ARG:HG2	15:O:121:TYR:CZ	2.14	0.83
15:O:123:ASN:O	15:O:124:GLU:O	1.97	0.82
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.60	0.82
1:A:476:ARG:HG2	1:A:477:GLN:HG3	1.59	0.82
1:A:200:GLU:HB3	15:O:516:LEU:HD21	0.84	0.82
1:A:234:ILE:HD11	1:A:237:ALA:CB	2.09	0.82
1:A:598:MET:O	1:A:599:LYS:CB	2.26	0.82
2:B:587:PHE:HE2	2:B:604:ASP:O	1.60	0.82
4:D:110:LEU:HB3	4:D:120:LYS:HE3	1.62	0.82
1:A:723:LEU:O	1:A:727:LYS:HB2	1.78	0.82
1:A:200:GLU:CB	15:O:516:LEU:CD2	2.45	0.82
1:A:601:TYR:CD1	3:C:23:PHE:HE2	1.97	0.82
3:C:105:PRO:HG3	10:J:6:ARG:HH21	1.42	0.82
1:A:256:TYR:CZ	1:A:1401:PHE:CE1	2.68	0.81
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.45	0.81
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.63	0.81
2:B:230:LYS:HE2	2:B:334:HIS:HE1	1.43	0.81
2:B:316:LYS:HZ2	13:M:226:ARG:NH2	1.79	0.81
7:G:5:SER:O	7:G:73:ARG:HA	1.79	0.81
1:A:980:SER:HA	5:E:163:GLU:HG2	1.63	0.81
1:A:1378:LYS:HG3	1:A:1379:MET:H	1.46	0.81
16:P:33:GLN:NE2	16:P:49:MET:SD	2.54	0.81
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.64	0.80
3:C:231:PRO:HA	3:C:293:ARG:HG2	1.62	0.80
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.63	0.80
15:O:48:LEU:HD22	15:O:581:LEU:HD11	1.62	0.80
2:B:521:THR:HG23	2:B:609:CYS:SG	2.20	0.80
2:B:141:ILE:HG23	2:B:142:ILE:H	1.44	0.80
14:N:290:ILE:O	14:N:294:LEU:CB	2.30	0.80
7:G:126:SER:CB	7:G:139:TYR:CB	2.55	0.80
18:R:218:ARG:O	18:R:514:GLU:HG2	1.82	0.80
2:B:464:ILE:HD11	2:B:746:TYR:HE1	1.46	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:CYS:HB2	7:G:128:TRP:HB3	1.64	0.79
1:A:597:ILE:HD11	1:A:603:LEU:HD12	1.65	0.79
4:D:145:PHE:HB2	4:D:149:THR:HG21	1.64	0.79
13:M:89:GLN:HE21	13:M:178:GLN:HE22	1.29	0.79
20:X:4:DT:H2'	20:X:5:DC:C6	2.18	0.79
15:O:297:ILE:O	15:O:301:LYS:HB2	1.83	0.79
21:Y:20:DT:H71	21:Y:21:DT:H73	1.63	0.79
1:A:574:ALA:HA	11:K:81:MET:HE3	1.65	0.79
2:B:228:LYS:HD2	2:B:333:ALA:HA	1.64	0.79
4:D:14:TYR:HD1	4:D:15:GLU:HG2	1.44	0.79
14:N:290:ILE:O	14:N:294:LEU:HB2	1.83	0.79
14:N:287:HIS:O	14:N:291:LEU:HB2	1.82	0.78
15:O:509:ARG:O	15:O:512:ARG:HB3	1.83	0.78
15:O:515:LYS:C	15:O:516:LEU:HG	2.08	0.78
1:A:235:LYS:CE	15:O:44:PRO:CG	2.61	0.78
1:A:235:LYS:O	1:A:236:SER:HB3	1.80	0.78
5:E:29:PHE:HB2	5:E:65:THR:HB	1.65	0.78
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.65	0.78
1:A:1178:LYS:HB2	1:A:1181:LEU:HD12	1.65	0.78
1:A:1213:SER:HB2	1:A:1217:ILE:HB	1.63	0.78
17:Q:54:LEU:O	17:Q:58:TYR:HB2	1.83	0.78
21:Y:20:DT:C5	21:Y:21:DT:H73	2.17	0.78
2:B:587:PHE:HZ	2:B:607:ARG:CG	1.95	0.78
1:A:400:LYS:HA	1:A:465:HIS:HD2	1.49	0.78
2:B:403:ILE:HD11	2:B:418:ALA:HB1	1.65	0.78
2:B:496:MET:HE2	2:B:608:ILE:HG22	1.65	0.77
1:A:1151:GLU:HG3	1:A:1152:ARG:HG3	1.66	0.77
16:P:33:GLN:NE2	19:S:372:MET:SD	2.58	0.77
1:A:212:GLU:CD	1:A:213:ARG:H	1.93	0.77
15:O:123:ASN:O	15:O:124:GLU:C	2.27	0.77
2:B:1006:SER:HB2	2:B:1013:LEU:HD21	1.67	0.77
19:S:494:THR:HB	19:S:497:ASP:HB2	1.67	0.77
20:X:53:DT:H2''	20:X:54:DG:H8	1.49	0.77
1:A:121:ARG:HG3	15:O:73:ARG:CD	2.15	0.77
1:A:395:PRO:HB3	1:A:496:ARG:HA	1.66	0.76
2:B:122:ASP:HA	2:B:189:GLY:HA3	1.65	0.76
2:B:332:ILE:HG13	2:B:333:ALA:H	1.50	0.76
2:B:766:ASP:OD1	2:B:945:ASN:HB2	1.86	0.76
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.67	0.76
1:A:179:ILE:CD1	15:O:557:ARG:NH2	2.48	0.76
3:C:94:ASP:O	12:L:67:PHE:CE2	2.38	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:LEU:HD12	7:G:139:TYR:O	1.85	0.76
13:M:112:TYR:HD1	13:M:119:TRP:HE1	1.31	0.76
18:R:219:ARG:CA	18:R:514:GLU:CG	2.63	0.76
2:B:427:ASN:OD1	2:B:431:SER:HB3	1.85	0.76
21:Y:20:DT:C4	21:Y:21:DT:C4	2.73	0.76
1:A:1380:ARG:HH11	1:A:1385:GLN:HE22	1.32	0.76
18:R:219:ARG:HA	18:R:514:GLU:HG2	1.64	0.76
20:X:53:DT:H2''	20:X:54:DG:C8	2.21	0.76
16:P:176:ASN:HA	16:P:179:LEU:HB2	1.66	0.76
1:A:431:ASN:OD1	1:A:432:TYR:N	2.19	0.76
2:B:230:LYS:CE	2:B:334:HIS:HE1	1.98	0.76
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.67	0.76
3:C:113:LEU:HD11	3:C:132:ILE:HD11	1.68	0.76
1:A:598:MET:C	1:A:599:LYS:HG2	2.11	0.76
2:B:735:MET:HB2	2:B:754:ASN:HD21	1.51	0.76
1:A:642:PRO:HB2	1:A:644:GLU:OE1	1.86	0.75
2:B:137:ARG:HG2	2:B:141:ILE:HG12	1.66	0.75
15:O:105:LYS:HB2	15:O:121:TYR:HB2	1.66	0.75
4:D:127:LEU:HD21	7:G:147:ARG:HD2	1.68	0.75
1:A:308:SER:HA	15:O:534:ARG:HD2	1.68	0.75
2:B:135:TYR:OH	2:B:419:LEU:HB2	1.86	0.75
18:R:515:LEU:O	18:R:516:PHE:HB2	1.86	0.75
1:A:1448:PHE:HZ	4:D:16:VAL:HG23	1.52	0.75
1:A:790:ALA:HB1	1:A:794:MET:HE2	1.69	0.75
2:B:68:PHE:CE1	2:B:385:SER:OG	2.40	0.75
1:A:117:GLU:HG2	1:A:119:ASP:H	1.52	0.74
1:A:330:ASP:OD1	1:A:331:SER:N	2.19	0.74
1:A:955:LEU:HB2	1:A:958:ALA:HB3	1.69	0.74
20:X:8:DC:O2	21:Y:62:DG:N2	2.13	0.74
1:A:153:ARG:NH2	15:O:337:GLN:O	2.20	0.74
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.69	0.74
5:E:123:LEU:HD21	5:E:126:SER:HB2	1.68	0.74
1:A:429:GLY:C	1:A:465:HIS:HD1	1.95	0.74
3:C:33:VAL:O	3:C:34:GLU:HB2	1.85	0.74
8:H:105:GLU:HG2	8:H:106:GLU:N	2.01	0.74
12:L:61:THR:HG23	12:L:63:ARG:H	1.53	0.74
15:O:584:ASN:O	15:O:588:LEU:CB	2.33	0.74
15:O:584:ASN:HB3	15:O:588:LEU:HB2	1.69	0.74
2:B:364:LYS:HG3	2:B:365:MET:H	1.53	0.74
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.69	0.74
8:H:21:ASN:OD1	8:H:22:LYS:N	2.19	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:51:CYS:SG	12:L:53:HIS:HB3	2.28	0.74
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.68	0.74
2:B:135:TYR:CE1	2:B:419:LEU:CB	2.70	0.74
15:O:196:GLU:HG3	15:O:197:MET:H	1.53	0.74
1:A:946:THR:HG21	1:A:1066:SER:HA	1.70	0.74
3:C:256:ILE:HA	3:C:268:LYS:H	1.53	0.74
18:R:245:VAL:HA	18:R:248:SER:HB3	1.70	0.74
15:O:200:LEU:HA	15:O:281:THR:O	1.87	0.73
15:O:480:TYR:HA	15:O:483:LEU:HB3	1.69	0.73
18:R:202:ALA:O	18:R:205:LEU:HB3	1.87	0.73
1:A:565:SER:HB2	1:A:664:MET:HE2	1.68	0.73
10:J:9:SER:OG	10:J:45:CYS:SG	2.44	0.73
20:X:26:DT:H2'	20:X:27:DT:C6	2.23	0.73
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.20	0.73
1:A:476:ARG:HD2	1:A:508:TYR:HB3	1.70	0.73
1:A:599:LYS:HG3	8:H:96:VAL:HG13	1.70	0.73
20:X:5:DC:O2	21:Y:65:DG:N2	2.17	0.73
2:B:416:TYR:CE1	18:R:151:GLN:HB2	2.23	0.73
7:G:92:CYS:SG	7:G:98:LYS:N	2.57	0.73
15:O:183:MET:O	15:O:187:ILE:HG13	1.89	0.73
1:A:276:ASP:O	1:A:277:SER:HB2	1.88	0.73
2:B:412:ARG:HG2	2:B:413:ALA:H	1.53	0.73
15:O:37:LEU:HD23	15:O:40:ARG:HD2	1.70	0.73
2:B:296:TYR:HB2	2:B:300:GLN:HE22	1.53	0.73
18:R:220:PRO:HD3	18:R:514:GLU:HG2	1.71	0.73
2:B:831:GLU:N	2:B:831:GLU:OE1	2.21	0.73
2:B:758:ALA:HA	2:B:1019:PHE:HB3	1.69	0.73
1:A:1184:ILE:HB	1:A:1232:ILE:HB	1.69	0.72
1:A:1395:HIS:O	1:A:1399:ALA:HB2	1.88	0.72
2:B:321:GLN:H	2:B:324:ILE:HB	1.54	0.72
2:B:754:ASN:O	10:J:48:ARG:NH1	2.22	0.72
15:O:585:MET:HE1	15:O:648:TRP:HB2	1.71	0.72
18:R:468:ILE:HG13	18:R:610:LEU:HD11	1.71	0.72
2:B:316:LYS:NZ	13:M:226:ARG:NH2	2.36	0.72
2:B:415:GLU:HG3	2:B:416:TYR:H	1.55	0.72
3:C:239:ILE:HG22	3:C:288:LYS:HD2	1.70	0.72
1:A:123:PHE:CG	1:A:144:ILE:HD13	2.25	0.72
1:A:777:VAL:HG12	1:A:811:ALA:HB1	1.71	0.72
14:N:384:LYS:HA	14:N:416:ILE:HD11	1.70	0.72
16:P:11:LEU:O	16:P:15:ALA:HB2	1.90	0.72
7:G:105:PHE:HD1	7:G:107:ASP:H	1.36	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:49:MET:HE2	19:S:364:LEU:HD11	1.70	0.72
1:A:599:LYS:CB	1:A:600:PRO:HD2	2.02	0.72
14:N:380:MET:SD	14:N:421:GLN:NE2	2.62	0.72
16:P:75:VAL:HG22	16:P:77:GLU:H	1.55	0.72
1:A:367:ASN:OD1	2:B:1049:GLN:NE2	2.23	0.72
2:B:797:ARG:HG2	2:B:803:GLN:HG2	1.68	0.72
2:B:822:GLN:O	2:B:824:LEU:N	2.22	0.72
13:M:112:TYR:O	13:M:243:ILE:CG2	2.37	0.72
1:A:598:MET:O	8:H:96:VAL:HG22	1.90	0.72
1:A:124:LEU:HB3	1:A:128:ARG:HH12	1.54	0.72
1:A:174:ALA:HB2	15:O:557:ARG:CB	2.19	0.72
1:A:1121:LEU:O	1:A:1346:HIS:NE2	2.22	0.72
3:C:93:GLN:HB3	3:C:95:GLU:CG	2.18	0.72
3:C:228:ARG:HH21	3:C:299:ILE:HD13	1.54	0.72
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.70	0.72
3:C:100:ARG:NH2	3:C:192:LEU:O	2.23	0.72
13:M:164:LYS:HG3	14:N:300:LYS:HD3	1.71	0.72
16:P:170:LEU:HD23	16:P:172:ILE:H	1.55	0.72
21:Y:20:DT:O4	21:Y:21:DT:O4	2.07	0.72
2:B:501:ASP:HB3	2:B:703:CYS:CB	2.20	0.71
9:I:24:LEU:HD23	9:I:33:PHE:CE1	2.25	0.71
2:B:295:ILE:O	2:B:300:GLN:NE2	2.23	0.71
2:B:554:GLY:HA2	2:B:564:SER:HA	1.71	0.71
4:D:17:LEU:HD11	4:D:63:VAL:HG23	1.72	0.71
15:O:495:VAL:O	15:O:496:ILE:HG13	1.91	0.71
1:A:328:ASN:OD1	1:A:329:SER:N	2.22	0.71
16:P:69:GLU:HG3	16:P:70:LEU:H	1.55	0.71
20:X:12:DT:H2''	20:X:13:DA:N7	2.05	0.71
20:X:4:DT:C2'	20:X:5:DC:O5'	2.36	0.71
2:B:428:ASN:OD1	2:B:429:ILE:N	2.23	0.71
2:B:694:ASN:HD21	2:B:916:HIS:CE1	2.08	0.71
15:O:183:MET:O	15:O:187:ILE:CG1	2.38	0.71
15:O:289:LYS:HE2	15:O:323:SER:HB3	1.72	0.71
19:S:470:GLU:O	19:S:474:ARG:CB	2.36	0.71
3:C:152:ASP:OD2	3:C:154:LYS:NZ	2.20	0.71
2:B:68:PHE:CD1	2:B:385:SER:OG	2.43	0.71
4:D:11:LEU:HD21	4:D:16:VAL:CG2	2.20	0.71
21:Y:20:DT:C4	21:Y:21:DT:O4	2.44	0.71
1:A:228:LEU:HB3	1:A:257:ILE:CD1	2.20	0.71
1:A:432:TYR:OH	18:R:20:ASN:ND2	2.24	0.71
15:O:45:ASP:N	15:O:582:GLU:OE2	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:267:ALA:HA	18:R:270:LEU:HB3	1.73	0.71
21:Y:47:DG:H2'	21:Y:48:DT:H71	1.73	0.71
6:F:79:ARG:NH1	6:F:145:ASP:O	2.24	0.70
15:O:35:SER:HB2	15:O:40:ARG:HH21	1.56	0.70
2:B:261:GLY:O	13:M:180:LYS:NZ	2.23	0.70
19:S:483:GLU:O	19:S:487:GLU:CB	2.39	0.70
2:B:227:ARG:HD3	2:B:449:MET:HG3	1.73	0.70
2:B:566:ARG:HD3	14:N:386:ALA:O	1.92	0.70
2:B:785:CYS:SG	2:B:1026:LYS:NZ	2.57	0.70
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.71	0.70
2:B:934:ASN:HB3	2:B:1004:LEU:HD23	1.72	0.70
9:I:32:GLU:HB2	13:M:130:PHE:HB3	1.73	0.70
2:B:137:ARG:H	2:B:141:ILE:HG21	1.56	0.70
2:B:315:GLN:O	2:B:316:LYS:CB	2.40	0.70
2:B:417:ASP:HB3	2:B:419:LEU:CG	2.20	0.70
1:A:92:HIS:CD2	1:A:94:GLY:H	2.09	0.70
15:O:493:GLU:O	15:O:494:TYR:O	2.09	0.70
1:A:228:LEU:HD12	1:A:228:LEU:C	2.17	0.70
2:B:265:ASP:O	2:B:268:ILE:N	2.22	0.70
16:P:310:VAL:HG11	17:Q:43:ILE:HD11	1.74	0.70
18:R:239:ARG:NH1	19:S:291:UNK:O	2.24	0.70
18:R:515:LEU:O	18:R:516:PHE:CB	2.40	0.70
1:A:999:ASP:OD1	1:A:1002:ARG:NH1	2.24	0.70
18:R:467:ARG:HG3	18:R:610:LEU:HD22	1.74	0.70
7:G:39:ILE:HD12	7:G:40:PRO:HD2	1.73	0.70
16:P:172:ILE:HG22	16:P:173:GLU:H	1.57	0.70
2:B:738:THR:HB	2:B:741:ILE:HD12	1.74	0.70
1:A:338:PRO:HG2	1:A:342:ASN:HB2	1.74	0.69
1:A:1305:CYS:SG	5:E:11:ARG:NH1	2.65	0.69
2:B:221:THR:HG21	2:B:334:HIS:HA	1.72	0.69
18:R:463:ARG:NH1	18:R:601:ASN:O	2.25	0.69
18:R:528:ILE:HG12	18:R:543:ALA:HB2	1.73	0.69
1:A:1448:PHE:CE1	4:D:12:SER:O	2.45	0.69
2:B:259:ALA:HB1	2:B:302:LEU:HD23	1.74	0.69
15:O:591:LYS:O	15:O:633:ARG:NH2	2.25	0.69
18:R:219:ARG:HD3	18:R:514:GLU:CG	2.21	0.69
18:R:436:LYS:NZ	19:S:462:GLU:OE2	2.25	0.69
3:C:215:ASP:OD2	12:L:70:ARG:NH2	2.25	0.69
5:E:83:CYS:SG	5:E:84:ASP:N	2.66	0.69
18:R:218:ARG:HH12	18:R:258:ARG:HB2	1.57	0.69
15:O:516:LEU:HD12	15:O:516:LEU:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:TYR:CD1	3:C:23:PHE:CE2	2.81	0.69
2:B:758:ALA:HB3	2:B:943:ILE:HD13	1.73	0.69
1:A:228:LEU:O	1:A:232:LYS:HG3	1.92	0.69
1:A:1448:PHE:CZ	4:D:16:VAL:CG2	2.73	0.69
2:B:195:LEU:HD11	2:B:472:ARG:HB3	1.73	0.69
2:B:1036:HIS:NE2	2:B:1058:GLY:HA2	2.07	0.69
8:H:105:GLU:CG	8:H:106:GLU:H	2.03	0.69
13:M:149:LYS:HB3	13:M:182:PHE:HE1	1.56	0.69
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.74	0.69
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.58	0.69
2:B:775:LYS:HG3	2:B:925:ILE:HG22	1.73	0.69
2:B:584:VAL:HB	2:B:588:ILE:HD12	1.75	0.69
3:C:132:ILE:O	3:C:208:CYS:HB3	1.93	0.69
2:B:760:MET:HB3	2:B:943:ILE:HD11	1.75	0.69
5:E:172:GLU:HG2	5:E:173:SER:H	1.57	0.69
16:P:191:PHE:HB2	16:P:192:PRO:HD2	1.75	0.69
2:B:197:GLN:NE2	2:B:476:GLN:OE1	2.25	0.68
3:C:33:VAL:HG12	3:C:34:GLU:H	1.58	0.68
1:A:89:PRO:HG3	1:A:228:LEU:CD2	2.23	0.68
1:A:543:THR:HG22	1:A:548:GLU:H	1.57	0.68
1:A:1447:LEU:HD23	1:A:1450:SER:HB3	1.74	0.68
2:B:253:ILE:HG22	2:B:286:ASN:HD21	1.58	0.68
14:N:364:ARG:NH1	14:N:365:VAL:O	2.26	0.68
15:O:292:ARG:HH12	15:O:650:VAL:HA	1.57	0.68
5:E:82:PHE:HD1	5:E:111:VAL:HB	1.58	0.68
15:O:75:SER:HB2	15:O:119:TYR:CE1	2.29	0.68
1:A:1448:PHE:CE1	4:D:14:TYR:CE2	2.82	0.68
16:P:266:GLU:HB3	16:P:269:LEU:CD2	2.24	0.68
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.28	0.68
1:A:1177:TYR:HE2	9:I:14:ILE:HG13	1.59	0.68
2:B:412:ARG:NH1	2:B:415:GLU:OE2	2.27	0.68
18:R:213:TRP:HE1	18:R:495:PRO:HB3	1.58	0.68
2:B:335:LEU:HD12	2:B:335:LEU:O	1.94	0.68
2:B:882:ASP:OD1	2:B:883:GLN:N	2.27	0.68
8:H:24:CYS:SG	8:H:25:ARG:N	2.66	0.68
1:A:58:MET:HE2	1:A:82:GLY:HA3	1.75	0.68
2:B:335:LEU:HD12	2:B:335:LEU:C	2.19	0.68
10:J:52:THR:HG22	10:J:53:HIS:H	1.58	0.68
13:M:112:TYR:O	13:M:243:ILE:HG22	1.93	0.68
1:A:89:PRO:HG2	1:A:225:LEU:HA	1.74	0.68
3:C:71:MET:HE2	3:C:314:PHE:HA	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:LEU:CD2	4:D:16:VAL:HG21	2.22	0.68
4:D:14:TYR:CE1	4:D:15:GLU:HB2	2.28	0.68
15:O:73:ARG:CG	15:O:121:TYR:CE1	2.75	0.67
15:O:595:LEU:HD21	15:O:630:VAL:HG23	1.76	0.67
20:X:57:DT:O2	21:Y:14:DG:N2	2.27	0.67
1:A:1136:ILE:HG21	1:A:1318:HIS:HB3	1.76	0.67
15:O:80:VAL:HG11	15:O:87:ASP:HB2	1.76	0.67
15:O:288:MET:SD	15:O:291:ARG:NH2	2.66	0.67
2:B:1101:MET:SD	2:B:1126:LYS:HG3	2.33	0.67
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.28	0.67
7:G:129:ILE:HG12	7:G:139:TYR:HB3	1.76	0.67
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.77	0.67
1:A:179:ILE:HD11	15:O:557:ARG:HH21	1.58	0.67
1:A:716:ASP:OD2	1:A:790:ALA:N	2.27	0.67
2:B:501:ASP:HB3	2:B:703:CYS:HB2	1.77	0.67
3:C:283:GLU:O	3:C:286:ALA:N	2.27	0.67
14:N:395:ILE:HA	14:N:411:ARG:HA	1.76	0.67
20:X:2:DT:O4	21:Y:67:DA:N6	2.27	0.67
11:K:68:GLU:HG3	11:K:69:ASP:H	1.59	0.67
3:C:238:PRO:O	3:C:239:ILE:HG13	1.95	0.67
1:A:927:GLU:HG2	1:A:928:GLY:H	1.58	0.67
7:G:126:SER:O	7:G:128:TRP:N	2.26	0.67
2:B:241:TYR:HB3	2:B:250:GLU:HB2	1.76	0.67
1:A:121:ARG:HG3	15:O:73:ARG:HD2	1.76	0.67
13:M:103:GLU:OE1	13:M:103:GLU:O	2.13	0.67
15:O:353:GLU:H	15:O:481:SER:HB2	1.60	0.67
18:R:420:TYR:O	18:R:627:TRP:NE1	2.28	0.66
1:A:1425:THR:HG23	6:F:92:ARG:HB2	1.77	0.66
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.76	0.66
12:L:31:CYS:SG	12:L:48:CYS:HB2	2.35	0.66
13:M:160:ALA:HA	14:N:306:VAL:HG12	1.77	0.66
13:M:245:LEU:HD13	14:N:405:SER:OG	1.95	0.66
19:S:480:ASN:OD1	19:S:481:PHE:N	2.25	0.66
1:A:209:PRO:O	1:A:212:GLU:HB2	1.95	0.66
2:B:247:ILE:HG12	2:B:251:ILE:HD11	1.77	0.66
4:D:7:ARG:HE	4:D:10:PHE:HZ	1.41	0.66
16:P:11:LEU:O	16:P:15:ALA:CB	2.43	0.66
16:P:137:VAL:HG21	16:P:149:MET:HE3	1.78	0.66
1:A:26:ILE:HD13	1:A:262:PRO:HG3	1.78	0.66
1:A:70:CYS:SG	1:A:80:HIS:HE1	2.18	0.66
2:B:461:LEU:HD21	2:B:1028:LYS:HD3	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:CYS:HB3	13:M:183:PHE:HE2	1.56	0.66
18:R:558:PRO:O	18:R:562:GLU:CB	2.43	0.66
1:A:303:LEU:HG	15:O:538:ALA:HB1	1.77	0.66
2:B:722:ASP:OD1	2:B:723:THR:N	2.27	0.66
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.77	0.66
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.78	0.66
18:R:213:TRP:CD1	18:R:287:PRO:HD3	2.30	0.66
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.78	0.66
1:A:1125:ARG:NH2	1:A:1338:GLU:OE2	2.27	0.66
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.25	0.66
5:E:117:THR:HG23	5:E:120:ALA:H	1.60	0.66
8:H:131:ASN:O	8:H:134:ASN:N	2.27	0.66
18:R:581:ASN:ND2	18:R:583:HIS:O	2.29	0.66
2:B:914:SER:O	2:B:915:ARG:HG2	1.96	0.66
4:D:122:GLN:HE22	7:G:83:GLU:HG3	1.61	0.66
16:P:269:LEU:HB3	16:P:297:PHE:CE1	2.30	0.66
18:R:123:GLN:HG2	18:R:150:LEU:HD21	1.78	0.66
1:A:572:ASP:OD1	1:A:573:ARG:N	2.28	0.66
2:B:416:TYR:CE1	18:R:151:GLN:CB	2.78	0.66
3:C:231:PRO:HB3	3:C:275:VAL:HG22	1.77	0.66
13:M:253:GLU:O	13:M:257:ASP:N	2.28	0.66
15:O:168:SER:HB3	15:O:279:SER:HB3	1.76	0.66
1:A:735:TYR:O	1:A:739:ASP:HB2	1.96	0.66
2:B:297:THR:HA	2:B:301:ALA:HB3	1.78	0.66
2:B:483:VAL:HG12	2:B:485:GLY:H	1.60	0.66
2:B:723:THR:HG23	2:B:724:LEU:H	1.61	0.66
2:B:1038:ARG:HE	2:B:1041:GLY:H	1.43	0.66
5:E:141:VAL:HG23	5:E:142:VAL:H	1.61	0.66
18:R:208:ARG:O	18:R:212:ASP:N	2.28	0.66
1:A:31:GLU:HG3	1:A:69:THR:HG21	1.77	0.66
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.31	0.66
2:B:762:TYR:O	2:B:764:GLY:N	2.29	0.66
5:E:101:GLN:O	5:E:104:ASN:ND2	2.29	0.66
16:P:190:THR:HA	16:P:215:TYR:CE1	2.31	0.66
8:H:123:MET:HE2	8:H:125:LEU:HD23	1.78	0.65
18:R:639:GLU:HG3	18:R:642:ARG:HE	1.61	0.65
1:A:49:LYS:HG3	1:A:56:PRO:HD3	1.78	0.65
2:B:49:PRO:HG3	2:B:743:LEU:HD21	1.78	0.65
15:O:144:MET:HE3	15:O:149:GLU:H	1.62	0.65
19:S:426:ILE:HA	19:S:429:TYR:HD2	1.61	0.65
1:A:274:MET:HA	1:A:280:SER:HB3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:ASP:HB2	1:A:1411:VAL:HG12	1.79	0.65
1:A:1161:VAL:HG22	1:A:1275:LEU:HD13	1.77	0.65
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.60	0.65
5:E:1:MET:HG3	5:E:3:GLN:H	1.60	0.65
18:R:190:ASP:O	18:R:195:LYS:NZ	2.25	0.65
18:R:209:MET:HA	18:R:212:ASP:HB2	1.78	0.65
19:S:432:LEU:O	19:S:476:LYS:NZ	2.29	0.65
2:B:542:THR:O	13:M:178:GLN:NE2	2.28	0.65
1:A:1256:VAL:O	1:A:1260:MET:HB2	1.96	0.65
2:B:763:SER:OG	2:B:764:GLY:N	2.30	0.65
5:E:18:THR:HG23	5:E:143:ASN:HB3	1.77	0.65
15:O:643:ARG:NH1	16:P:292:SER:OG	2.29	0.65
13:M:226:ARG:HG3	13:M:227:LEU:H	1.62	0.65
1:A:1026:ARG:NH2	8:H:129:TYR:OH	2.30	0.65
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	1.78	0.65
2:B:427:ASN:O	2:B:430:THR:N	2.29	0.65
18:R:12:PHE:HB3	18:R:23:LEU:HD11	1.78	0.65
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.78	0.65
18:R:640:SER:OG	19:S:506:GLN:NE2	2.30	0.65
1:A:589:HIS:HA	11:K:104:ARG:HH21	1.62	0.65
15:O:338:ASP:HB3	15:O:341:GLU:HB3	1.79	0.65
2:B:242:LEU:HD12	2:B:256:VAL:HG21	1.78	0.65
2:B:901:ARG:HH11	3:C:93:GLN:NE2	1.94	0.65
7:G:104:ILE:HG23	7:G:105:PHE:H	1.61	0.65
15:O:316:LEU:O	15:O:320:GLU:N	2.29	0.65
7:G:104:ILE:HG12	7:G:105:PHE:CD2	2.31	0.64
15:O:91:VAL:O	15:O:95:LEU:HB3	1.95	0.64
1:A:234:ILE:O	1:A:234:ILE:HG23	1.96	0.64
1:A:425:ASN:OD1	1:A:426:VAL:N	2.29	0.64
2:B:49:PRO:O	2:B:53:LYS:N	2.30	0.64
2:B:552:ASN:ND2	2:B:565:ILE:O	2.29	0.64
2:B:587:PHE:CZ	2:B:607:ARG:CB	2.78	0.64
2:B:832:VAL:O	12:L:60:ARG:NH1	2.30	0.64
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.62	0.64
14:N:302:GLU:HB3	14:N:410:GLY:HA2	1.78	0.64
15:O:644:LEU:O	15:O:647:LEU:N	2.30	0.64
16:P:296:TYR:CD1	16:P:297:PHE:N	2.64	0.64
20:X:16:DA:H61	21:Y:55:DA:H61	1.44	0.64
1:A:153:ARG:HH11	15:O:339:LEU:HG	1.62	0.64
1:A:741:LEU:HD13	1:A:765:LYS:HD3	1.79	0.64
2:B:77:ILE:HD13	2:B:98:ILE:HG12	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:SER:O	2:B:428:ASN:N	2.27	0.64
16:P:64:VAL:HB	16:P:71:LYS:HB2	1.78	0.64
1:A:599:LYS:NZ	8:H:91:ASP:HA	2.12	0.64
2:B:235:THR:HG22	2:B:236:LYS:HG3	1.78	0.64
4:D:1:MET:HG3	4:D:2:LYS:H	1.61	0.64
15:O:648:TRP:NE1	15:O:652:GLN:OE1	2.30	0.64
14:N:395:ILE:HD12	14:N:411:ARG:HA	1.80	0.64
1:A:746:ASN:OD1	1:A:747:LYS:N	2.31	0.64
2:B:723:THR:HA	2:B:790:LYS:HG2	1.80	0.64
6:F:80:ALA:O	6:F:81:THR:OG1	2.11	0.64
15:O:128:HIS:HE1	15:O:652:GLN:HE22	1.44	0.64
18:R:131:TYR:OH	18:R:135:ARG:NH1	2.30	0.64
18:R:513:PRO:O	18:R:515:LEU:N	2.30	0.64
18:R:636:LEU:HD13	19:S:502:LEU:HD21	1.80	0.64
1:A:353:PHE:O	1:A:356:ARG:HG2	1.97	0.64
1:A:843:GLN:H	1:A:847:PHE:HB3	1.63	0.64
5:E:80:VAL:HG23	5:E:109:ILE:HD11	1.80	0.64
14:N:287:HIS:CD2	14:N:384:LYS:HE2	2.31	0.64
1:A:1451:LEU:O	4:D:111:ASN:ND2	2.30	0.64
2:B:131:VAL:HG23	2:B:133:ILE:HD11	1.78	0.64
2:B:416:TYR:O	2:B:418:ALA:N	2.30	0.64
2:B:613:ILE:HA	2:B:646:VAL:HG12	1.80	0.64
2:B:974:GLU:HG2	2:B:987:MET:HE1	1.80	0.64
14:N:290:ILE:HD13	14:N:384:LYS:HZ2	1.61	0.64
1:A:1384:LEU:HB2	1:A:1413:GLU:OE1	1.98	0.64
2:B:932:PRO:HG2	2:B:940:PRO:HG3	1.78	0.64
16:P:21:GLN:O	16:P:26:GLY:N	2.30	0.64
18:R:464:LYS:NZ	18:R:605:VAL:O	2.25	0.64
18:R:514:GLU:OE1	18:R:514:GLU:HA	1.97	0.64
19:S:413:ARG:NH1	20:X:12:DT:OP2	2.30	0.64
1:A:602:TYR:HB2	3:C:23:PHE:O	1.98	0.64
2:B:801:HIS:ND1	18:R:137:GLU:OE2	2.29	0.64
1:A:332:VAL:HG13	1:A:333:ASN:H	1.62	0.63
1:A:489:TYR:CE1	1:A:532:ILE:HG12	2.33	0.63
1:A:873:VAL:HG21	2:B:487:ARG:HG2	1.78	0.63
18:R:463:ARG:NH1	18:R:598:ASP:O	2.29	0.63
18:R:619:ALA:O	18:R:623:LYS:HB3	1.98	0.63
1:A:892:SER:O	1:A:1380:ARG:NH2	2.32	0.63
1:A:1395:HIS:O	1:A:1399:ALA:CB	2.46	0.63
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.80	0.63
2:B:202:LYS:HD3	2:B:222:SER:HB2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:149:LYS:HB3	13:M:182:PHE:CE1	2.32	0.63
18:R:7:CYS:HB3	18:R:28:CYS:SG	2.39	0.63
18:R:485:ASN:OD1	18:R:486:ILE:N	2.31	0.63
1:A:33:GLU:HG3	1:A:83:HIS:NE2	2.13	0.63
1:A:100:ILE:O	1:A:104:GLN:CB	2.44	0.63
1:A:443:ASN:OD1	1:A:444:LEU:N	2.32	0.63
2:B:230:LYS:CE	2:B:334:HIS:CE1	2.81	0.63
13:M:95:ARG:HB3	13:M:101:PRO:HB3	1.81	0.63
1:A:373:VAL:HG12	1:A:374:ASP:H	1.62	0.63
1:A:476:ARG:CZ	1:A:510:ALA:HA	2.28	0.63
2:B:295:ILE:HG23	2:B:296:TYR:HD2	1.63	0.63
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.32	0.63
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.61	0.63
2:B:1038:ARG:NH1	2:B:1050:PRO:HB3	2.13	0.63
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.64	0.63
7:G:45:CYS:SG	7:G:46:ILE:N	2.71	0.63
7:G:52:LEU:HD12	7:G:53:THR:HG22	1.79	0.63
1:A:493:ARG:HB2	1:A:499:ARG:HH21	1.62	0.63
15:O:186:THR:O	15:O:187:ILE:C	2.42	0.63
1:A:276:ASP:O	1:A:277:SER:CB	2.47	0.63
7:G:83:GLU:H	7:G:150:ILE:H	1.47	0.63
13:M:112:TYR:HD1	13:M:119:TRP:NE1	1.96	0.63
15:O:326:ILE:HD12	15:O:653:MET:HB3	1.81	0.63
16:P:202:PRO:O	16:P:204:LYS:N	2.29	0.63
21:Y:20:DT:C7	21:Y:21:DT:C7	2.67	0.63
1:A:235:LYS:O	1:A:236:SER:CB	2.47	0.63
2:B:230:LYS:HE2	2:B:334:HIS:CE1	2.30	0.63
2:B:713:ILE:HG13	2:B:725:LEU:HD11	1.81	0.63
2:B:805:ILE:HG22	2:B:807:GLY:H	1.62	0.63
1:A:224:PRO:HD2	1:A:316:TRP:HH2	1.62	0.63
7:G:6:LYS:HA	7:G:72:PHE:O	1.99	0.63
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.81	0.63
16:P:106:TRP:CH2	16:P:108:LYS:HB3	2.32	0.63
18:R:419:GLU:O	18:R:428:VAL:HA	1.97	0.63
2:B:137:ARG:HG3	2:B:138:GLY:N	2.13	0.63
2:B:273:CYS:O	2:B:354:ARG:NH1	2.31	0.63
3:C:240:LYS:HB3	3:C:264:GLU:HB3	1.80	0.63
6:F:76:LYS:HD2	6:F:79:ARG:HH21	1.64	0.63
1:A:67:CYS:HB3	1:A:71:HIS:HA	1.80	0.62
1:A:153:ARG:HA	1:A:160:LEU:HA	1.81	0.62
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:ILE:H	1:A:1229:ARG:HE	1.46	0.62
2:B:930:ASP:O	2:B:931:MET:HG2	1.99	0.62
11:K:89:CYS:HA	11:K:104:ARG:O	1.99	0.62
15:O:102:ARG:NH2	15:O:282:ILE:O	2.31	0.62
15:O:495:VAL:C	15:O:496:ILE:HG12	2.23	0.62
1:A:86:LEU:HD21	1:A:319:LEU:HD21	1.81	0.62
2:B:201:SER:OG	2:B:376:ARG:NH1	2.32	0.62
18:R:195:LYS:O	18:R:199:VAL:N	2.26	0.62
2:B:626:HIS:HE1	2:B:640:PHE:CE1	2.18	0.62
2:B:1038:ARG:HB2	2:B:1058:GLY:HA3	1.81	0.62
5:E:185:ALA:O	5:E:189:GLY:N	2.32	0.62
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.80	0.62
2:B:658:TYR:CE2	2:B:670:MET:HG2	2.35	0.62
3:C:95:GLU:HG3	3:C:96:VAL:H	1.64	0.62
15:O:285:ASP:OD1	15:O:286:ARG:N	2.32	0.62
15:O:519:GLU:HA	15:O:522:ILE:HB	1.81	0.62
4:D:128:PRO:O	4:D:129:ALA:C	2.41	0.62
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.81	0.62
16:P:45:LEU:HA	19:S:372:MET:HE2	1.80	0.62
18:R:619:ALA:O	18:R:623:LYS:CB	2.47	0.62
1:A:41:ASP:OD2	1:A:50:ALA:N	2.31	0.62
1:A:128:ARG:NH2	1:A:240:GLU:OE2	2.32	0.62
1:A:1265:ARG:HH21	2:B:285:VAL:HG22	1.65	0.62
1:A:1448:PHE:CZ	4:D:14:TYR:CE2	2.88	0.62
2:B:279:TYR:HE1	2:B:358:MET:HA	1.65	0.62
2:B:299:GLN:HE22	13:M:190:ASN:HB2	1.63	0.62
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.65	0.62
5:E:32:GLN:HA	5:E:35:VAL:HG12	1.82	0.62
7:G:204:GLY:HA2	7:G:210:TRP:HB2	1.80	0.62
13:M:90:TYR:HB3	13:M:179:LEU:HB3	1.82	0.62
18:R:4:CYS:HB3	18:R:7:CYS:SG	2.40	0.62
1:A:921:LEU:HD23	1:A:932:PRO:HG3	1.82	0.62
1:A:1272:VAL:HG13	1:A:1273:LYS:H	1.64	0.62
1:A:1367:GLU:HG3	1:A:1369:LEU:HD23	1.81	0.62
2:B:416:TYR:O	2:B:417:ASP:C	2.41	0.62
2:B:612:LEU:HD13	2:B:672:HIS:HB3	1.81	0.62
7:G:112:GLN:HE22	7:G:128:TRP:CD1	2.18	0.62
18:R:455:GLU:HG2	18:R:588:THR:HG23	1.81	0.62
19:S:506:GLN:O	19:S:510:LYS:HB2	1.99	0.62
21:Y:20:DT:C5	21:Y:21:DT:C7	2.82	0.62
1:A:974:LEU:HD21	1:A:998:TYR:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:VAL:O	3:C:268:LYS:HB2	2.00	0.62
4:D:58:ILE:O	4:D:61:ASN:HB2	2.00	0.62
9:I:34:PRO:O	9:I:35:ILE:HG13	1.99	0.62
12:L:31:CYS:SG	12:L:34:CYS:HB2	2.39	0.62
2:B:415:GLU:O	2:B:416:TYR:O	2.18	0.62
2:B:767:ILE:HG22	2:B:768:GLU:N	2.15	0.62
15:O:455:SER:HA	15:O:458:LYS:HD3	1.81	0.62
16:P:128:LEU:HA	16:P:131:GLN:HB2	1.82	0.62
18:R:219:ARG:CD	18:R:514:GLU:HG3	2.26	0.62
18:R:138:LYS:NZ	18:R:173:LEU:O	2.29	0.61
2:B:901:ARG:HH11	3:C:93:GLN:HE22	1.46	0.61
1:A:520:HIS:HE1	2:B:1062:LEU:HD21	1.65	0.61
1:A:1163:LYS:HG3	1:A:1164:THR:H	1.64	0.61
1:A:1447:LEU:HD23	1:A:1450:SER:CB	2.28	0.61
2:B:137:ARG:HG2	2:B:141:ILE:HG21	1.81	0.61
2:B:566:ARG:HH22	14:N:282:LEU:HD23	1.63	0.61
2:B:1012:CYS:SG	3:C:293:ARG:NH2	2.69	0.61
16:P:62:LYS:HB2	16:P:73:GLN:O	2.00	0.61
1:A:378:ARG:HH11	1:A:518:ASN:HD21	1.48	0.61
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.81	0.61
1:A:577:THR:HG23	11:K:88:PHE:CD1	2.35	0.61
3:C:116:VAL:HB	3:C:209:ILE:HD11	1.82	0.61
18:R:116:PHE:CZ	18:R:120:ARG:NH1	2.68	0.61
18:R:419:GLU:HB2	18:R:429:ILE:HB	1.82	0.61
1:A:1048:VAL:HG11	1:A:1053:LYS:HG3	1.81	0.61
2:B:926:VAL:CG1	2:B:930:ASP:HB2	2.31	0.61
11:K:111:THR:CG2	11:K:112:THR:N	2.51	0.61
18:R:214:MET:O	18:R:258:ARG:NH1	2.29	0.61
21:Y:20:DT:H73	21:Y:21:DT:C7	2.29	0.61
1:A:225:LEU:O	1:A:228:LEU:HG	2.01	0.61
7:G:138:LEU:CD1	7:G:139:TYR:O	2.47	0.61
13:M:117:HIS:HD1	13:M:119:TRP:CD1	2.18	0.61
2:B:1054:ARG:HG2	2:B:1055:SER:H	1.66	0.61
3:C:255:VAL:HG13	3:C:256:ILE:N	2.16	0.61
4:D:135:TYR:HA	4:D:141:CYS:SG	2.41	0.61
11:K:69:ASP:OD1	11:K:70:HIS:N	2.31	0.61
15:O:40:ARG:O	15:O:40:ARG:HG2	2.00	0.61
20:X:3:DT:C2'	20:X:4:DT:C7	2.70	0.61
1:A:11:LYS:HD3	2:B:1145:ASP:HA	1.83	0.61
1:A:429:GLY:O	1:A:465:HIS:ND1	2.30	0.61
2:B:126:SER:OG	2:B:151:ARG:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:NH2	2:B:419:LEU:CD2	2.64	0.61
2:B:524:ASP:OD2	2:B:588:ILE:HD11	2.00	0.61
2:B:786:GLU:OE2	3:C:93:GLN:HG3	2.01	0.61
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.01	0.61
4:D:24:GLU:HG3	4:D:29:TRP:HA	1.82	0.61
8:H:115:TYR:HE1	8:H:124:ARG:HG3	1.65	0.61
14:N:287:HIS:HD2	14:N:384:LYS:HE2	1.64	0.61
1:A:141:LEU:HA	1:A:144:ILE:HG22	1.82	0.61
1:A:913:GLN:NE2	1:A:917:GLY:H	1.99	0.61
1:A:1202:ILE:HD13	1:A:1224:ILE:HB	1.82	0.61
15:O:171:VAL:O	15:O:175:LEU:HB3	2.00	0.61
18:R:219:ARG:N	21:Y:60:DA:OP1	2.30	0.61
21:Y:11:DG:H2''	21:Y:12:DG:C8	2.35	0.61
1:A:235:LYS:HE2	15:O:44:PRO:HG3	1.82	0.61
1:A:1384:LEU:O	1:A:1388:SER:N	2.34	0.61
11:K:95:HIS:HD2	11:K:96:PRO:HD2	1.66	0.61
18:R:289:SER:HB2	18:R:535:SER:HB2	1.81	0.61
5:E:9:ILE:HG22	5:E:53:PRO:HG3	1.82	0.60
9:I:22:TYR:O	9:I:23:THR:C	2.42	0.60
15:O:144:MET:HE1	15:O:153:LYS:HD2	1.83	0.60
18:R:13:GLU:CD	18:R:26:LYS:HG3	2.26	0.60
19:S:387:ALA:O	19:S:391:ASN:N	2.30	0.60
1:A:373:VAL:HG12	1:A:374:ASP:N	2.16	0.60
1:A:645:MET:HE2	8:H:122:LEU:HB3	1.83	0.60
18:R:467:ARG:HB3	18:R:610:LEU:HD13	1.82	0.60
20:X:54:DG:H2'	20:X:55:DA:C8	2.36	0.60
8:H:93:TYR:CD1	8:H:145:ARG:HD3	2.36	0.60
15:O:175:LEU:HD11	15:O:184:LYS:HB3	1.83	0.60
18:R:80:LEU:O	18:R:83:ALA:N	2.34	0.60
1:A:115:LEU:CD2	1:A:123:PHE:CE2	2.84	0.60
1:A:995:VAL:HG23	1:A:996:ASP:H	1.66	0.60
1:A:552:ALA:HB3	1:A:671:ASP:HB2	1.82	0.60
10:J:7:CYS:HA	10:J:49:MET:SD	2.41	0.60
15:O:91:VAL:O	15:O:95:LEU:CB	2.49	0.60
18:R:234:MET:HE1	18:R:274:LYS:HA	1.83	0.60
18:R:434:GLU:HA	18:R:436:LYS:H	1.66	0.60
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.81	0.60
18:R:439:ALA:HA	18:R:450:THR:H	1.66	0.60
1:A:388:SER:OG	1:A:695:ASN:ND2	2.34	0.60
1:A:622:VAL:HA	1:A:685:TYR:CE2	2.37	0.60
9:I:24:LEU:C	9:I:24:LEU:HD12	2.27	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:121:ILE:N	13:M:148:LEU:O	2.34	0.60
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.84	0.60
15:O:495:VAL:O	15:O:495:VAL:HG23	2.00	0.60
18:R:516:PHE:CD1	18:R:517:PRO:HD2	2.37	0.60
1:A:1217:ILE:HG22	1:A:1218:GLN:H	1.67	0.60
2:B:210:ASP:OD1	2:B:211:GLU:N	2.34	0.60
4:D:1:MET:HG2	7:G:9:ASP:HA	1.84	0.60
4:D:125:ASN:OD1	4:D:126:GLN:N	2.30	0.60
9:I:8:CYS:SG	9:I:29:CYS:HB2	2.41	0.60
14:N:290:ILE:O	14:N:294:LEU:HB3	2.00	0.60
15:O:166:LEU:HB3	15:O:169:LEU:HD11	1.84	0.60
15:O:197:MET:HB2	15:O:286:ARG:HD2	1.83	0.60
18:R:191:LEU:HD21	18:R:239:ARG:HE	1.67	0.60
1:A:302:GLY:C	1:A:304:ASP:H	2.09	0.60
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.83	0.60
8:H:101:ALA:HB2	8:H:116:TYR:HE1	1.66	0.60
15:O:184:LYS:HA	15:O:187:ILE:CG1	2.32	0.60
18:R:186:ALA:HA	18:R:189:LEU:HD12	1.83	0.60
18:R:546:ARG:HA	18:R:549:ILE:HD12	1.83	0.60
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.82	0.60
1:A:91:PHE:HD1	1:A:224:PRO:HB3	1.65	0.60
1:A:476:ARG:NH2	1:A:515:ASP:OD2	2.35	0.60
2:B:801:HIS:O	2:B:863:GLN:NE2	2.34	0.60
3:C:30:GLU:HG3	11:K:84:PRO:HG3	1.84	0.60
4:D:127:LEU:CD2	7:G:147:ARG:HD2	2.32	0.60
19:S:507:ASN:HA	19:S:510:LYS:HB3	1.84	0.60
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.01	0.59
17:Q:54:LEU:O	17:Q:58:TYR:CB	2.50	0.59
1:A:204:VAL:HG23	15:O:516:LEU:HD12	1.84	0.59
1:A:599:LYS:CB	1:A:600:PRO:HD3	2.29	0.59
2:B:658:TYR:O	2:B:671:THR:OG1	2.21	0.59
16:P:236:THR:HG23	16:P:239:ASN:H	1.66	0.59
1:A:1028:MET:SD	1:A:1048:VAL:HG22	2.43	0.59
1:A:1382:SER:HB2	1:A:1385:GLN:HG2	1.83	0.59
3:C:19:ASP:O	3:C:29:ASN:ND2	2.35	0.59
3:C:195:LYS:HD2	10:J:57:ILE:HG21	1.84	0.59
3:C:209:ILE:HG13	3:C:210:LEU:H	1.67	0.59
5:E:21:GLU:OE2	5:E:143:ASN:ND2	2.36	0.59
5:E:87:SER:HA	5:E:115:ASN:HB3	1.83	0.59
13:M:77:LYS:HZ3	13:M:262:GLU:HB2	1.67	0.59
2:B:316:LYS:CE	13:M:226:ARG:HE	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:ASP:HB3	2:B:419:LEU:CD2	2.32	0.59
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.83	0.59
15:O:364:ILE:HA	15:O:476:TYR:CZ	2.37	0.59
1:A:921:LEU:HA	1:A:1082:ARG:HA	1.85	0.59
1:A:1145:LEU:H	1:A:1292:GLU:HG2	1.68	0.59
15:O:339:LEU:O	15:O:343:LYS:NZ	2.36	0.59
16:P:14:ASN:HB3	16:P:51:ILE:HD13	1.84	0.59
18:R:470:GLN:OE1	18:R:602:LEU:HD22	2.02	0.59
21:Y:2:DC:H2''	21:Y:3:DT:H71	1.85	0.59
1:A:235:LYS:HB3	1:A:252:ARG:NE	2.17	0.59
2:B:811:VAL:HA	2:B:817:PRO:HA	1.84	0.59
3:C:134:LEU:HD23	3:C:167:LEU:HD23	1.84	0.59
13:M:92:ASN:ND2	13:M:148:LEU:HD21	2.18	0.59
14:N:287:HIS:O	14:N:291:LEU:CB	2.50	0.59
15:O:52:LEU:HD11	15:O:131:LEU:HD12	1.84	0.59
20:X:3:DT:H2''	20:X:4:DT:C5	2.38	0.59
20:X:25:DT:H2'	20:X:26:DT:H71	1.84	0.59
1:A:716:ASP:CG	1:A:791:PRO:HD2	2.27	0.59
1:A:957:TYR:CE2	1:A:1035:PRO:HD3	2.38	0.59
2:B:500:ALA:O	2:B:700:THR:HA	2.02	0.59
8:H:47:PHE:HZ	8:H:146:ARG:HG3	1.67	0.59
15:O:75:SER:HB2	15:O:119:TYR:CD1	2.38	0.59
15:O:128:HIS:O	15:O:132:TYR:HD1	1.86	0.59
1:A:786:ASP:OD1	1:A:787:ASN:N	2.36	0.59
1:A:974:LEU:HD11	1:A:998:TYR:CD1	2.38	0.59
1:A:1161:VAL:HG13	1:A:1275:LEU:HB2	1.84	0.59
13:M:72:GLU:H	14:N:364:ARG:HE	1.48	0.59
14:N:387:GLU:OE2	14:N:415:LYS:NZ	2.34	0.59
1:A:32:VAL:HG11	1:A:57:LYS:HD2	1.84	0.59
1:A:235:LYS:CE	15:O:44:PRO:HG3	2.32	0.59
2:B:60:GLN:H	2:B:60:GLN:CD	2.10	0.59
2:B:914:SER:C	2:B:916:HIS:H	2.10	0.59
2:B:1002:ASP:N	2:B:1017:ILE:O	2.30	0.59
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.38	0.59
11:K:85:ASP:OD1	11:K:86:VAL:N	2.35	0.59
13:M:94:PRO:HB3	14:N:391:LEU:HA	1.83	0.59
16:P:53:GLN:NE2	19:S:363:GLN:HA	2.18	0.59
16:P:153:LEU:HB3	16:P:155:PRO:HD3	1.83	0.59
1:A:37:ARG:HG2	1:A:38:ASP:H	1.67	0.59
1:A:653:ILE:HD11	1:A:655:ARG:NH2	2.18	0.59
2:B:817:PRO:HG2	2:B:822:GLN:OE1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:112:TYR:O	13:M:243:ILE:HG21	2.03	0.59
15:O:597:GLN:HA	15:O:600:SER:HB2	1.84	0.59
1:A:123:PHE:CD2	1:A:144:ILE:HD13	2.38	0.58
2:B:832:VAL:HG12	12:L:60:ARG:HD2	1.83	0.58
3:C:103:LEU:HD21	10:J:6:ARG:HG3	1.83	0.58
7:G:115:LEU:HG	7:G:130:TRP:HZ2	1.68	0.58
8:H:8:ASP:OD1	8:H:9:ILE:N	2.35	0.58
15:O:233:SER:O	15:O:236:LYS:HG2	2.03	0.58
15:O:480:TYR:O	15:O:484:MET:N	2.35	0.58
21:Y:23:DT:H2''	21:Y:24:DC:H6	1.68	0.58
3:C:19:ASP:HB2	3:C:29:ASN:HD21	1.68	0.58
5:E:153:HIS:CD2	5:E:198:ILE:HG12	2.38	0.58
7:G:83:GLU:O	7:G:149:ARG:HA	2.03	0.58
13:M:83:GLU:O	13:M:84:SER:HB2	2.02	0.58
16:P:75:VAL:HG21	16:P:80:ALA:HB2	1.84	0.58
16:P:135:LYS:NZ	16:P:153:LEU:O	2.34	0.58
18:R:219:ARG:HD3	18:R:514:GLU:HB3	1.84	0.58
18:R:469:ILE:O	18:R:473:GLY:N	2.36	0.58
1:A:99:THR:HA	1:A:102:ILE:HG22	1.85	0.58
1:A:598:MET:O	1:A:599:LYS:HB2	2.04	0.58
1:A:703:ARG:NH2	11:K:93:ILE:O	2.36	0.58
2:B:538:VAL:HG12	2:B:565:ILE:HB	1.85	0.58
2:B:802:THR:OG1	2:B:863:GLN:NE2	2.25	0.58
2:B:1040:ARG:HD3	18:R:35:ASN:HD21	1.69	0.58
3:C:20:PHE:CZ	3:C:23:PHE:HB3	2.37	0.58
15:O:141:ILE:HA	15:O:144:MET:HB2	1.85	0.58
1:A:666:LYS:HG2	1:A:667:SER:H	1.66	0.58
2:B:926:VAL:HG12	2:B:930:ASP:HB2	1.85	0.58
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.84	0.58
15:O:51:GLU:O	15:O:55:ALA:N	2.30	0.58
1:A:27:VAL:HG11	15:O:37:LEU:HD13	1.85	0.58
1:A:339:GLY:O	1:A:342:ASN:HB3	2.04	0.58
1:A:702:ALA:HB1	2:B:764:GLY:HA3	1.84	0.58
1:A:1125:ARG:NH2	1:A:1317:ASN:HB3	2.18	0.58
7:G:9:ASP:OD1	7:G:10:LEU:N	2.35	0.58
9:I:33:PHE:CD1	9:I:34:PRO:HD2	2.37	0.58
15:O:581:LEU:O	15:O:585:MET:HB2	2.03	0.58
18:R:467:ARG:O	18:R:471:LYS:CB	2.51	0.58
1:A:1026:ARG:HH12	8:H:110:ASP:HA	1.68	0.58
2:B:427:ASN:C	2:B:430:THR:H	2.12	0.58
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:HE1	5:E:135:PHE:CZ	2.38	0.58
16:P:54:GLU:O	16:P:58:LYS:N	2.34	0.58
17:Q:64:THR:O	17:Q:68:GLY:N	2.37	0.58
1:A:418:GLU:O	1:A:421:VAL:HG12	2.03	0.58
1:A:436:ARG:HH11	1:A:459:GLY:HA3	1.69	0.58
1:A:599:LYS:O	1:A:601:TYR:N	2.32	0.58
2:B:517:MET:HE2	2:B:611:PRO:HG2	1.84	0.58
2:B:760:MET:HE1	2:B:932:PRO:HD3	1.85	0.58
13:M:85:LEU:CD2	13:M:86:HIS:O	2.51	0.58
15:O:134:GLY:HA2	15:O:137:ILE:HD12	1.85	0.58
2:B:766:ASP:CG	2:B:945:ASN:HB2	2.28	0.58
1:A:108:LYS:HG2	1:A:180:HIS:CD2	2.38	0.58
1:A:600:PRO:O	1:A:601:TYR:HB2	2.04	0.58
1:A:1127:LYS:O	1:A:1131:ASN:HB2	2.04	0.58
1:A:1152:ARG:O	1:A:1156:VAL:N	2.33	0.58
1:A:1431:VAL:HG13	7:G:57:GLY:O	2.03	0.58
2:B:137:ARG:HG3	2:B:138:GLY:H	1.69	0.58
2:B:626:HIS:CE1	2:B:635:LEU:HD21	2.38	0.58
3:C:137:ASN:HA	3:C:202:ILE:O	2.03	0.58
7:G:96:GLY:HA2	7:G:112:GLN:HG3	1.84	0.58
1:A:413:ARG:NH1	1:A:456:LEU:O	2.37	0.58
2:B:166:ALA:HB1	2:B:170:LYS:HB2	1.84	0.58
2:B:223:SER:N	2:B:335:LEU:HD21	2.19	0.58
3:C:275:VAL:HG21	3:C:293:ARG:HD3	1.86	0.58
18:R:470:GLN:NE2	18:R:476:ALA:O	2.37	0.58
1:A:174:ALA:HB2	15:O:557:ARG:HB3	1.86	0.57
1:A:1202:ILE:O	1:A:1205:ILE:HG13	2.04	0.57
4:D:14:TYR:CE1	4:D:15:GLU:HG2	2.38	0.57
6:F:135:ARG:NH1	7:G:58:GLN:HE21	2.02	0.57
7:G:149:ARG:NH1	7:G:151:GLU:OE1	2.31	0.57
18:R:523:MET:O	18:R:527:LYS:HA	2.04	0.57
1:A:123:PHE:O	1:A:127:LEU:HD13	2.04	0.57
1:A:308:SER:N	1:A:311:ASN:OD1	2.37	0.57
1:A:890:MET:O	1:A:894:GLU:N	2.36	0.57
2:B:763:SER:OG	2:B:765:TYR:N	2.37	0.57
2:B:1057:ASP:OD1	2:B:1058:GLY:N	2.36	0.57
10:J:1:MET:O	10:J:53:HIS:NE2	2.37	0.57
13:M:106:PHE:CD2	13:M:107:ILE:HB	2.39	0.57
15:O:36:SER:O	15:O:40:ARG:CB	2.42	0.57
16:P:190:THR:HA	16:P:215:TYR:CZ	2.39	0.57
2:B:223:SER:H	2:B:335:LEU:HD21	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:MET:O	2:B:273:CYS:HB3	2.03	0.57
2:B:1048:ARG:HD2	2:B:1123:TYR:CZ	2.39	0.57
13:M:86:HIS:HD2	13:M:175:ARG:O	1.88	0.57
15:O:90:SER:O	15:O:94:THR:N	2.35	0.57
16:P:31:PHE:O	16:P:71:LYS:HA	2.05	0.57
1:A:556:ASP:OD1	2:B:947:HIS:NE2	2.37	0.57
1:A:584:SER:O	1:A:586:GLY:N	2.36	0.57
2:B:378:GLU:OE2	2:B:382:GLN:HB2	2.04	0.57
15:O:132:TYR:CE2	15:O:645:LEU:HD21	2.39	0.57
15:O:195:CYS:SG	15:O:196:GLU:N	2.78	0.57
16:P:296:TYR:CZ	16:P:297:PHE:HD1	2.23	0.57
18:R:94:LEU:HD23	18:R:149:ARG:HH21	1.69	0.57
1:A:482:ARG:HD3	1:A:544:PRO:HB3	1.85	0.57
2:B:314:ARG:O	2:B:317:LEU:HD23	2.05	0.57
13:M:117:HIS:HB2	13:M:119:TRP:HE1	1.68	0.57
15:O:307:VAL:HG13	15:O:308:THR:H	1.69	0.57
15:O:624:LEU:HA	15:O:627:LEU:HD12	1.84	0.57
18:R:271:SER:HB2	18:R:277:GLU:HG3	1.87	0.57
18:R:420:TYR:HB2	18:R:428:VAL:HG22	1.86	0.57
18:R:587:THR:O	18:R:590:THR:OG1	2.21	0.57
1:A:475:ASN:OD1	1:A:476:ARG:N	2.38	0.57
1:A:599:LYS:HB2	1:A:600:PRO:HD3	1.76	0.57
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.86	0.57
3:C:59:ILE:HD13	3:C:63:ILE:HD11	1.86	0.57
15:O:102:ARG:O	15:O:123:ASN:ND2	2.38	0.57
21:Y:53:DC:H2'	21:Y:54:DT:C5	2.39	0.57
2:B:738:THR:HG22	2:B:740:THR:H	1.69	0.57
5:E:26:ARG:HH22	5:E:189:GLY:HA3	1.69	0.57
16:P:62:LYS:O	16:P:72:PHE:HA	2.04	0.57
20:X:6:DA:H4'	20:X:7:DA:H5'	1.86	0.57
21:Y:42:DA:H1'	21:Y:43:DA:H5'	1.85	0.57
2:B:97:ASP:OD1	2:B:98:ILE:N	2.38	0.57
2:B:475:SER:HB3	2:B:510:LEU:HB3	1.86	0.57
2:B:961:LEU:HD11	2:B:1019:PHE:HA	1.87	0.57
15:O:128:HIS:CE1	15:O:652:GLN:HE22	2.23	0.57
15:O:171:VAL:O	15:O:175:LEU:CB	2.53	0.57
15:O:353:GLU:N	15:O:481:SER:HB2	2.20	0.57
18:R:388:GLY:HA3	18:R:576:SER:HB2	1.86	0.57
1:A:389:ILE:HG22	1:A:390:ASP:H	1.70	0.57
1:A:978:ASP:HB2	1:A:984:VAL:HB	1.87	0.57
1:A:1305:CYS:HB2	5:E:141:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:687:LEU:HA	2:B:741:ILE:HD11	1.87	0.57
2:B:998:TYR:CD1	3:C:281:ARG:HD2	2.40	0.57
13:M:96:LEU:HB2	13:M:101:PRO:HA	1.86	0.57
15:O:496:ILE:O	15:O:496:ILE:HG22	2.05	0.57
18:R:623:LYS:HE2	19:S:435:TRP:HD1	1.69	0.57
1:A:890:MET:O	1:A:893:LEU:N	2.38	0.57
2:B:325:GLU:HG3	2:B:328:ALA:HB3	1.86	0.57
2:B:780:ARG:HE	3:C:217:ALA:HB1	1.70	0.57
2:B:1002:ASP:OD1	2:B:1003:MET:N	2.37	0.57
7:G:55:GLU:N	7:G:55:GLU:OE1	2.38	0.57
13:M:255:PHE:O	13:M:258:THR:OG1	2.22	0.57
16:P:118:GLN:HE22	21:Y:41:DG:H3'	1.70	0.57
18:R:218:ARG:NH1	18:R:258:ARG:HB2	2.19	0.57
1:A:113:ILE:HB	1:A:238:ASP:OD2	2.05	0.56
2:B:613:ILE:HG13	2:B:675:ILE:HG22	1.85	0.56
2:B:758:ALA:HA	2:B:1019:PHE:CB	2.34	0.56
2:B:800:ASN:ND2	2:B:851:SER:O	2.37	0.56
6:F:86:THR:HG1	6:F:89:GLU:H	1.53	0.56
9:I:32:GLU:CG	13:M:132:ASN:HB2	2.34	0.56
13:M:255:PHE:O	13:M:259:ILE:HG12	2.05	0.56
21:Y:49:DA:H5'	21:Y:49:DA:C8	2.39	0.56
1:A:167:ALA:HB1	15:O:557:ARG:HD3	1.88	0.56
1:A:330:ASP:CG	1:A:331:SER:H	2.12	0.56
1:A:997:GLN:C	1:A:999:ASP:H	2.13	0.56
1:A:1448:PHE:CE1	4:D:14:TYR:CD2	2.93	0.56
3:C:96:VAL:O	3:C:99:HIS:N	2.38	0.56
7:G:151:GLU:N	7:G:197:LEU:O	2.28	0.56
9:I:3:SER:HB2	9:I:12:LEU:HD12	1.87	0.56
13:M:251:THR:OG1	14:N:302:GLU:OE2	2.24	0.56
1:A:716:ASP:CG	1:A:789:ASN:HB2	2.30	0.56
1:A:735:TYR:O	1:A:739:ASP:CB	2.54	0.56
1:A:1399:ALA:HA	1:A:1404:LYS:HE2	1.88	0.56
2:B:38:ILE:HG13	2:B:43:ASP:HB3	1.86	0.56
2:B:177:CYS:SG	2:B:714:ALA:HB1	2.45	0.56
2:B:593:ASN:OD1	2:B:594:SER:N	2.38	0.56
5:E:85:GLU:HG3	5:E:87:SER:H	1.70	0.56
7:G:88:TRP:CD1	7:G:143:ASN:H	2.22	0.56
7:G:203:ASP:HB3	7:G:211:TRP:HE1	1.69	0.56
15:O:220:GLU:HG2	15:O:221:LYS:H	1.70	0.56
15:O:370:LEU:HD22	15:O:453:ILE:HD11	1.87	0.56
19:S:430:LYS:O	19:S:434:MET:HG2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:51:DT:H2''	21:Y:52:DA:H8	1.70	0.56
1:A:327:ILE:O	1:A:354:CYS:HB2	2.06	0.56
2:B:281:ASP:OD1	2:B:282:ILE:N	2.38	0.56
2:B:541:ILE:HA	2:B:544:ILE:HD12	1.86	0.56
3:C:85:PHE:CE2	3:C:94:ASP:O	2.49	0.56
10:J:53:HIS:ND1	10:J:53:HIS:O	2.38	0.56
15:O:471:THR:OG1	15:O:477:TYR:HB3	2.06	0.56
16:P:216:SER:HB2	16:P:261:TYR:H	1.70	0.56
19:S:460:ASN:ND2	20:X:9:DA:OP2	2.38	0.56
1:A:133:ASP:OD1	1:A:134:ASN:N	2.36	0.56
1:A:1177:TYR:CE2	9:I:14:ILE:HG13	2.41	0.56
2:B:640:PHE:HB3	2:B:645:LEU:HB2	1.88	0.56
15:O:362:ASN:HD21	15:O:478:VAL:HG23	1.70	0.56
18:R:172:GLU:OE1	18:R:172:GLU:N	2.34	0.56
1:A:722:ASP:O	1:A:725:GLN:N	2.38	0.56
1:A:733:ILE:HD12	1:A:736:HIS:NE2	2.21	0.56
2:B:316:LYS:HZ3	13:M:226:ARG:NE	2.04	0.56
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.88	0.56
7:G:2:PHE:N	7:G:76:VAL:O	2.38	0.56
13:M:107:ILE:HG21	13:M:124:PRO:HD3	1.86	0.56
14:N:361:GLY:HA3	14:N:374:LYS:O	2.05	0.56
15:O:183:MET:O	15:O:187:ILE:HG12	2.06	0.56
15:O:316:LEU:HA	15:O:319:THR:HG22	1.88	0.56
1:A:322:THR:O	1:A:325:MET:N	2.39	0.56
15:O:288:MET:O	15:O:291:ARG:HG2	2.06	0.56
1:A:26:ILE:CD1	1:A:262:PRO:HG3	2.36	0.56
1:A:978:ASP:N	1:A:982:CYS:O	2.35	0.56
3:C:33:VAL:HG12	3:C:34:GLU:N	2.21	0.56
5:E:127:ILE:HG22	5:E:130:ALA:H	1.69	0.56
6:F:116:ASP:OD2	6:F:119:ARG:NH1	2.39	0.56
9:I:5:CYS:HB3	9:I:10:ASN:H	1.71	0.56
18:R:418:ALA:HA	18:R:429:ILE:O	2.06	0.56
2:B:334:HIS:HB2	2:B:345:LYS:NZ	2.21	0.56
9:I:29:CYS:HB3	13:M:183:PHE:CZ	2.41	0.56
13:M:86:HIS:CD2	13:M:175:ARG:HB2	2.40	0.56
15:O:137:ILE:O	15:O:140:ILE:HG12	2.06	0.56
16:P:269:LEU:HD22	16:P:296:TYR:OH	2.05	0.56
21:Y:26:DT:H1'	21:Y:27:DG:C5	2.41	0.56
4:D:119:GLU:HA	4:D:122:GLN:HB3	1.88	0.56
7:G:122:THR:O	7:G:124:GLU:N	2.39	0.56
10:J:10:CYS:SG	10:J:43:ARG:NE	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:361:PHE:HB2	15:O:477:TYR:HE1	1.71	0.56
18:R:195:LYS:HA	18:R:198:VAL:HB	1.88	0.56
18:R:395:ASN:H	18:R:487:VAL:HB	1.71	0.56
18:R:519:LEU:HB3	18:R:532:ILE:HB	1.88	0.56
19:S:399:GLU:O	19:S:400:ASN:C	2.43	0.56
21:Y:17:DA:H2''	21:Y:18:DT:C5	2.41	0.56
1:A:409:THR:O	1:A:411:TYR:N	2.33	0.55
1:A:476:ARG:CD	1:A:508:TYR:HB3	2.36	0.55
1:A:723:LEU:O	1:A:727:LYS:CB	2.52	0.55
2:B:58:VAL:HG12	2:B:58:VAL:O	2.06	0.55
2:B:1105:GLY:O	2:B:1116:ILE:HD12	2.05	0.55
5:E:121:MET:HA	5:E:124:VAL:HB	1.88	0.55
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.88	0.55
15:O:553:ARG:HB3	15:O:562:ALA:HA	1.87	0.55
20:X:67:DA:H2''	20:X:68:DG:C8	2.42	0.55
1:A:1186:VAL:H	1:A:1230:ILE:HG12	1.70	0.55
2:B:775:LYS:HB2	2:B:927:LYS:HA	1.88	0.55
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.41	0.55
12:L:26:THR:HA	12:L:62:LYS:HE3	1.87	0.55
12:L:31:CYS:SG	12:L:48:CYS:CB	2.93	0.55
16:P:10:GLN:HB3	16:P:13:ASP:HB3	1.88	0.55
16:P:95:SER:HA	16:P:98:GLU:HG2	1.88	0.55
1:A:1299:GLY:C	1:A:1301:ARG:H	2.14	0.55
16:P:314:GLU:HB3	17:Q:37:PRO:HB3	1.88	0.55
1:A:1079:ARG:HG2	6:F:84:TYR:HE2	1.71	0.55
2:B:517:MET:SD	2:B:675:ILE:HD11	2.46	0.55
2:B:1079:LEU:O	2:B:1082:ARG:N	2.39	0.55
2:B:1106:TRP:NE1	7:G:163:PRO:HD3	2.22	0.55
14:N:364:ARG:HH11	14:N:365:VAL:H	1.54	0.55
18:R:219:ARG:HG2	21:Y:60:DA:OP1	2.05	0.55
18:R:485:ASN:ND2	20:X:15:DT:O4'	2.39	0.55
1:A:363:ARG:NH1	2:B:1131:GLU:OE2	2.39	0.55
1:A:502:GLU:CD	2:B:767:ILE:HG13	2.31	0.55
1:A:919:ASP:OD2	1:A:921:LEU:HB2	2.07	0.55
2:B:767:ILE:O	2:B:945:ASN:ND2	2.39	0.55
8:H:99:GLY:HA3	8:H:118:PHE:CD1	2.42	0.55
13:M:253:GLU:HB2	13:M:257:ASP:HB2	1.88	0.55
14:N:286:ASP:O	14:N:289:HIS:N	2.39	0.55
1:A:235:LYS:HZ2	15:O:44:PRO:CB	1.88	0.55
1:A:252:ARG:HH21	15:O:44:PRO:HD2	1.70	0.55
1:A:937:ARG:HG3	1:A:938:SER:N	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:VAL:HA	1:A:1186:VAL:HG12	1.88	0.55
2:B:68:PHE:HE1	2:B:385:SER:OG	1.86	0.55
2:B:762:TYR:OH	2:B:930:ASP:HB3	2.05	0.55
3:C:197:ARG:HG3	10:J:61:LEU:HD13	1.89	0.55
4:D:14:TYR:CE1	4:D:15:GLU:CG	2.89	0.55
6:F:101:ILE:HG21	6:F:120:ILE:HD11	1.88	0.55
12:L:27:LEU:HD11	12:L:37:LYS:HB2	1.89	0.55
15:O:353:GLU:HA	15:O:357:PRO:HG2	1.89	0.55
18:R:470:GLN:HG3	18:R:476:ALA:HB3	1.89	0.55
19:S:310:UNK:O	19:S:314:UNK:N	2.40	0.55
1:A:389:ILE:HG22	1:A:390:ASP:N	2.21	0.55
2:B:61:HIS:O	2:B:155:MET:HE1	2.06	0.55
2:B:536:LEU:HD23	2:B:536:LEU:O	2.07	0.55
2:B:1038:ARG:CZ	2:B:1050:PRO:HB3	2.36	0.55
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.40	0.55
4:D:127:LEU:CD2	7:G:147:ARG:CD	2.85	0.55
4:D:130:ASN:HA	4:D:154:LEU:HD11	1.88	0.55
15:O:592:LYS:NZ	15:O:593:GLU:OE2	2.39	0.55
16:P:90:GLU:HA	16:P:93:VAL:HB	1.88	0.55
16:P:209:ALA:C	16:P:211:ASN:H	2.15	0.55
18:R:468:ILE:O	18:R:472:ILE:N	2.39	0.55
1:A:818:ILE:HD11	1:A:824:PRO:HD2	1.89	0.55
2:B:64:SER:HB3	2:B:381:GLY:HA3	1.89	0.55
3:C:127:THR:H	3:C:130:ASN:HB3	1.71	0.55
3:C:259:ASP:HB2	3:C:266:TYR:CD1	2.42	0.55
5:E:1:MET:HB3	5:E:4:GLU:HG2	1.88	0.55
6:F:135:ARG:HH12	7:G:58:GLN:HE21	1.54	0.55
16:P:86:MET:HE1	16:P:131:GLN:HE21	1.71	0.55
18:R:106:GLN:O	18:R:109:LYS:HB3	2.07	0.55
18:R:610:LEU:HA	18:R:613:HIS:HB2	1.88	0.55
19:S:429:TYR:HA	19:S:432:LEU:HD12	1.88	0.55
2:B:821:HIS:NE2	2:B:824:LEU:HD12	2.21	0.55
2:B:926:VAL:HG12	2:B:927:LYS:H	1.71	0.55
3:C:31:TRP:CZ2	11:K:123:ASP:HB3	2.42	0.55
4:D:14:TYR:CD1	4:D:15:GLU:CG	2.87	0.55
5:E:112:TYR:N	5:E:135:PHE:O	2.27	0.55
15:O:80:VAL:HG21	15:O:87:ASP:HA	1.89	0.55
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.39	0.55
6:F:101:ILE:HD12	6:F:107:VAL:HG12	1.88	0.55
13:M:163:VAL:HG22	13:M:168:VAL:HG22	1.88	0.55
15:O:35:SER:CB	15:O:40:ARG:HH21	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:516:LEU:HA	15:O:566:PHE:O	2.06	0.55
2:B:128:PRO:HA	2:B:151:ARG:HG2	1.87	0.54
2:B:192:LYS:NZ	2:B:438:SER:O	2.27	0.54
2:B:525:GLU:HG3	2:B:528:PRO:HD2	1.90	0.54
2:B:778:ILE:HG13	2:B:906:PRO:HG2	1.89	0.54
9:I:24:LEU:HG	9:I:24:LEU:O	2.06	0.54
1:A:66:GLU:HB3	1:A:71:HIS:HB2	1.89	0.54
1:A:102:ILE:CD1	1:A:242:LEU:HD12	2.31	0.54
1:A:643:ASN:HB2	1:A:651:PHE:CZ	2.42	0.54
1:A:1120:THR:H	1:A:1138:THR:HG21	1.71	0.54
1:A:1130:ILE:HG23	1:A:1371:ILE:HG13	1.90	0.54
1:A:1448:PHE:CZ	4:D:11:LEU:HG	2.42	0.54
2:B:317:LEU:O	2:B:319:ILE:N	2.41	0.54
2:B:362:ASN:ND2	2:B:365:MET:SD	2.72	0.54
15:O:47:PHE:CE2	15:O:586:ALA:HB1	2.41	0.54
15:O:105:LYS:N	15:O:121:TYR:O	2.35	0.54
15:O:292:ARG:NH2	15:O:653:MET:O	2.39	0.54
15:O:581:LEU:HB2	15:O:648:TRP:CH2	2.42	0.54
18:R:274:LYS:H	19:S:277:UNK:H	1.56	0.54
19:S:523:ALA:HA	19:S:526:GLU:HB3	1.90	0.54
2:B:208:GLU:O	2:B:215:ILE:HA	2.06	0.54
2:B:252:PRO:HD2	2:B:255:ILE:HD12	1.88	0.54
2:B:587:PHE:CD2	2:B:604:ASP:O	2.61	0.54
2:B:592:SER:N	2:B:656:ASP:OD2	2.38	0.54
5:E:22:MET:HE1	5:E:135:PHE:HZ	1.72	0.54
5:E:117:THR:HG23	5:E:120:ALA:N	2.23	0.54
7:G:59:LEU:C	7:G:59:LEU:HD12	2.33	0.54
15:O:480:TYR:CD1	15:O:484:MET:HE2	2.42	0.54
16:P:203:LYS:HD2	16:P:206:VAL:HG23	1.89	0.54
18:R:105:PHE:O	18:R:108:TYR:HB3	2.07	0.54
1:A:44:LYS:HG3	1:A:45:ASP:H	1.72	0.54
1:A:916:TYR:CE1	1:A:1089:ILE:HG21	2.43	0.54
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.88	0.54
2:B:944:MET:HE1	2:B:957:LYS:HE2	1.89	0.54
3:C:66:ALA:O	3:C:70:ILE:HG22	2.07	0.54
15:O:168:SER:OG	15:O:281:THR:OG1	2.25	0.54
16:P:45:LEU:HD21	19:S:366:LEU:HB3	1.90	0.54
1:A:1174:GLN:CB	1:A:1185:GLN:O	2.43	0.54
1:A:1448:PHE:CE1	4:D:14:TYR:HE2	2.25	0.54
3:C:31:TRP:CG	3:C:32:ASN:N	2.72	0.54
4:D:127:LEU:HD21	7:G:147:ARG:CD	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:O	1:A:40:PHE:N	2.36	0.54
1:A:120:LYS:HG3	1:A:241:LEU:CD1	2.37	0.54
2:B:167:ASP:O	2:B:169:SER:N	2.41	0.54
2:B:1003:MET:SD	3:C:293:ARG:NH2	2.80	0.54
2:B:1038:ARG:NE	2:B:1041:GLY:H	2.05	0.54
11:K:136:THR:HA	11:K:139:ILE:HG22	1.90	0.54
18:R:213:TRP:HD1	18:R:287:PRO:HD3	1.73	0.54
18:R:395:ASN:ND2	21:Y:54:DT:O2	2.40	0.54
21:Y:23:DT:H2''	21:Y:24:DC:H5'	1.90	0.54
1:A:949:ASN:OD1	1:A:950:GLN:N	2.40	0.54
1:A:1059:LEU:HD11	8:H:106:GLU:HB3	1.90	0.54
1:A:1160:ARG:HA	1:A:1273:LYS:HE3	1.88	0.54
2:B:556:TYR:HD2	2:B:600:HIS:CE1	2.26	0.54
8:H:81:PRO:HD2	11:K:108:TYR:OH	2.08	0.54
15:O:578:ARG:HE	15:O:652:GLN:HA	1.73	0.54
19:S:439:PHE:HD1	19:S:454:VAL:HG12	1.71	0.54
1:A:233:GLN:HE21	15:O:575:ASN:ND2	2.06	0.54
1:A:277:SER:HB3	1:A:278:PRO:HD2	1.88	0.54
1:A:408:VAL:O	1:A:458:ILE:O	2.26	0.54
1:A:528:ARG:O	1:A:531:ALA:N	2.34	0.54
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.90	0.54
2:B:141:ILE:HG23	2:B:142:ILE:N	2.21	0.54
2:B:427:ASN:C	2:B:429:ILE:N	2.60	0.54
2:B:476:GLN:HG2	2:B:477:PHE:H	1.73	0.54
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.41	0.54
7:G:152:ARG:HB3	7:G:197:LEU:HD11	1.90	0.54
8:H:76:THR:C	8:H:78:SER:H	2.16	0.54
13:M:117:HIS:HB2	13:M:119:TRP:NE1	2.23	0.54
13:M:135:LYS:HE3	13:M:140:TRP:HE1	1.73	0.54
15:O:73:ARG:CG	15:O:121:TYR:HE1	2.19	0.54
16:P:217:THR:HA	16:P:220:GLU:HB3	1.90	0.54
18:R:83:ALA:O	18:R:87:LEU:CD1	2.55	0.54
18:R:406:LEU:HD13	18:R:411:VAL:HG21	1.89	0.54
1:A:45:ASP:OD1	1:A:46:ARG:N	2.41	0.54
2:B:554:GLY:HA2	2:B:564:SER:CA	2.38	0.54
2:B:565:ILE:HG12	2:B:566:ARG:N	2.22	0.54
3:C:75:VAL:HG23	3:C:221:PRO:HG3	1.89	0.54
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.43	0.54
4:D:64:ASN:ND2	7:G:102:LEU:HD22	2.23	0.54
7:G:121:TYR:HD2	7:G:127:ALA:O	1.90	0.54
13:M:93:ARG:HH21	13:M:105:PRO:HB3	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:55:LEU:HD22	16:P:60:LEU:HD12	1.90	0.54
16:P:63:LEU:HD11	16:P:70:LEU:HD13	1.89	0.54
1:A:407:LYS:HG2	1:A:461:VAL:HG22	1.90	0.54
1:A:416:LEU:HD11	1:A:464:ARG:HH21	1.72	0.54
1:A:501:ASN:O	1:A:504:VAL:HG22	2.07	0.54
1:A:931:GLN:O	1:A:933:VAL:N	2.35	0.54
1:A:1166:LEU:O	1:A:1170:ALA:N	2.41	0.54
2:B:347:LEU:HD13	2:B:541:ILE:HD11	1.89	0.54
5:E:31:THR:HG23	5:E:34:GLU:H	1.74	0.54
8:H:7:ASP:OD1	8:H:7:ASP:O	2.26	0.54
13:M:113:LYS:HG3	13:M:116:SER:O	2.08	0.54
15:O:347:ASP:OD1	15:O:348:GLU:N	2.41	0.54
15:O:581:LEU:HB2	15:O:648:TRP:CZ3	2.43	0.54
18:R:219:ARG:CA	18:R:514:GLU:HG2	2.36	0.54
1:A:573:ARG:NH2	11:K:87:GLU:OE1	2.40	0.53
1:A:599:LYS:HG2	8:H:96:VAL:HG22	1.90	0.53
2:B:55:LYS:CG	2:B:59:LYS:HD3	2.38	0.53
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.43	0.53
3:C:85:PHE:HE1	3:C:204:LEU:HD22	1.72	0.53
1:A:232:LYS:HD3	16:P:315:TRP:CH2	2.44	0.53
1:A:599:LYS:HZ1	8:H:91:ASP:HA	1.72	0.53
2:B:306:GLY:O	2:B:309:VAL:HG12	2.08	0.53
7:G:45:CYS:HA	7:G:76:VAL:HA	1.91	0.53
10:J:16:ASP:CG	10:J:17:LYS:HG3	2.33	0.53
18:R:96:ILE:HG22	18:R:141:HIS:CE1	2.43	0.53
20:X:66:DA:N1	21:Y:4:DT:N3	2.56	0.53
21:Y:10:DT:H2"	21:Y:11:DG:C8	2.43	0.53
1:A:92:HIS:CD2	1:A:258:TRP:HE1	2.26	0.53
1:A:1300:LEU:HD22	1:A:1316:THR:HG21	1.90	0.53
2:B:330:THR:HA	2:B:345:LYS:HE3	1.90	0.53
2:B:337:VAL:HG23	2:B:338:GLU:H	1.72	0.53
2:B:846:SER:OG	2:B:866:TYR:HB3	2.08	0.53
3:C:211:GLY:HA3	3:C:219:PHE:CE2	2.43	0.53
3:C:285:PHE:HA	3:C:288:LYS:NZ	2.23	0.53
4:D:14:TYR:CE1	4:D:15:GLU:CB	2.91	0.53
8:H:38:LEU:HD21	8:H:40:LEU:HB2	1.89	0.53
9:I:29:CYS:CB	13:M:183:PHE:CE2	2.88	0.53
13:M:159:TYR:HD1	13:M:172:PRO:HA	1.71	0.53
18:R:2:PRO:HG2	18:R:12:PHE:HE2	1.73	0.53
18:R:478:PHE:HB3	18:R:599:PRO:HA	1.90	0.53
1:A:196:ILE:O	1:A:200:GLU:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:CG	8:H:96:VAL:HG13	2.38	0.53
2:B:143:MET:CG	19:S:399:GLU:HB2	2.38	0.53
2:B:351:MET:HE1	2:B:549:LEU:HD21	1.90	0.53
2:B:855:PRO:HD2	18:R:106:GLN:CD	2.34	0.53
3:C:1:MET:HB3	3:C:14:ASN:HD21	1.74	0.53
3:C:260:GLU:O	3:C:264:GLU:N	2.42	0.53
11:K:63:PHE:HD2	11:K:117:LEU:HD13	1.74	0.53
15:O:537:LEU:HD11	15:O:566:PHE:CE2	2.43	0.53
18:R:18:ASN:HD21	18:R:20:ASN:ND2	2.07	0.53
1:A:185:TRP:C	1:A:187:GLY:H	2.17	0.53
1:A:816:GLN:HG2	1:A:864:HIS:HA	1.91	0.53
2:B:328:ALA:O	2:B:332:ILE:HG23	2.08	0.53
2:B:395:PHE:HA	2:B:428:ASN:HD21	1.73	0.53
7:G:88:TRP:HA	7:G:146:ILE:HD12	1.90	0.53
13:M:88:PHE:HB2	14:N:395:ILE:CG2	2.38	0.53
16:P:215:TYR:OH	16:P:262:ARG:NE	2.42	0.53
1:A:1222:VAL:HA	1:A:1231:ALA:O	2.09	0.53
2:B:263:LEU:HD12	2:B:297:THR:HG22	1.91	0.53
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.90	0.53
7:G:49:TYR:HB2	7:G:75:VAL:HG23	1.89	0.53
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.90	0.53
13:M:113:LYS:HE2	13:M:118:LEU:HB2	1.90	0.53
13:M:134:ASP:O	13:M:138:SER:N	2.42	0.53
16:P:131:GLN:HB3	16:P:133:TYR:CD2	2.44	0.53
1:A:34:VAL:HG13	1:A:35:SER:H	1.72	0.53
2:B:727:LEU:HD21	2:B:788:ARG:HE	1.74	0.53
2:B:1043:ARG:HH12	18:R:35:ASN:ND2	2.07	0.53
9:I:24:LEU:HD23	9:I:33:PHE:CG	2.44	0.53
15:O:168:SER:HG	15:O:281:THR:HG1	1.56	0.53
18:R:215:PHE:HD1	18:R:223:ILE:HD13	1.72	0.53
18:R:219:ARG:HD3	18:R:514:GLU:CB	2.39	0.53
20:X:66:DA:H2''	20:X:67:DA:C8	2.44	0.53
1:A:380:VAL:O	1:A:497:THR:OG1	2.25	0.53
1:A:557:PHE:HA	1:A:701:CYS:SG	2.48	0.53
1:A:600:PRO:O	1:A:601:TYR:CB	2.57	0.53
2:B:416:TYR:C	2:B:418:ALA:N	2.65	0.53
2:B:714:ALA:O	2:B:717:GLN:HB2	2.09	0.53
8:H:76:THR:O	8:H:78:SER:N	2.42	0.53
10:J:8:PHE:CG	10:J:49:MET:HE1	2.44	0.53
13:M:251:THR:OG1	13:M:254:GLN:NE2	2.42	0.53
16:P:217:THR:HB	16:P:221:ILE:HB	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:CB	1:A:253:PRO:CD	2.70	0.53
1:A:986:ARG:H	1:A:989:LEU:HD11	1.73	0.53
1:A:1229:ARG:HH12	1:A:1231:ALA:HB2	1.74	0.53
2:B:657:SER:OG	2:B:658:TYR:N	2.42	0.53
3:C:197:ARG:HB3	3:C:198:PRO:HD2	1.90	0.53
18:R:136:LYS:HE2	18:R:173:LEU:HD13	1.91	0.53
21:Y:9:DA:H2'	21:Y:10:DT:H71	1.91	0.53
21:Y:44:DA:H1'	21:Y:45:DA:H5'	1.91	0.53
1:A:124:LEU:HB3	1:A:128:ARG:NH1	2.22	0.53
1:A:200:GLU:CA	15:O:516:LEU:HD21	2.35	0.53
1:A:957:TYR:HD1	1:A:1031:LEU:HG	1.74	0.53
2:B:244:HIS:O	2:B:247:ILE:HG22	2.09	0.53
2:B:539:GLU:OE1	2:B:539:GLU:N	2.42	0.53
2:B:647:GLU:OE1	2:B:647:GLU:N	2.42	0.53
7:G:21:ASP:OD1	7:G:22:THR:N	2.42	0.53
8:H:128:ASN:CG	8:H:129:TYR:H	2.16	0.53
15:O:254:ASN:HA	15:O:257:ASN:HB2	1.91	0.53
15:O:640:ARG:NH1	17:Q:44:ASN:OD1	2.41	0.53
19:S:434:MET:HE3	19:S:479:PRO:HB3	1.90	0.53
21:Y:24:DC:H6	21:Y:24:DC:H5'	1.74	0.53
21:Y:25:DT:H2'	21:Y:26:DT:C4	2.43	0.53
1:A:673:LYS:O	1:A:676:SER:OG	2.23	0.52
1:A:926:MET:HA	1:A:932:PRO:HB3	1.90	0.52
1:A:1411:VAL:HG23	1:A:1421:MET:HE2	1.92	0.52
2:B:135:TYR:CZ	2:B:419:LEU:CB	2.91	0.52
2:B:416:TYR:CZ	18:R:151:GLN:HB2	2.44	0.52
2:B:419:LEU:HD12	2:B:419:LEU:C	2.33	0.52
2:B:526:GLU:O	2:B:529:ILE:HG22	2.09	0.52
2:B:901:ARG:NH1	3:C:93:GLN:NE2	2.56	0.52
2:B:1147:PHE:HD2	7:G:10:LEU:HD11	1.73	0.52
4:D:130:ASN:OD1	4:D:133:HIS:ND1	2.42	0.52
15:O:457:LEU:HD21	15:O:476:TYR:CZ	2.44	0.52
1:A:504:VAL:O	1:A:507:PRO:HD2	2.09	0.52
1:A:516:GLU:OE2	2:B:1034:LYS:HD3	2.09	0.52
1:A:1022:LEU:HD22	1:A:1060:TYR:HE2	1.74	0.52
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.90	0.52
2:B:531:LYS:O	2:B:535:VAL:HG23	2.09	0.52
2:B:763:SER:HB2	2:B:765:TYR:HD1	1.75	0.52
2:B:832:VAL:CG1	12:L:60:ARG:HD2	2.37	0.52
12:L:29:TYR:HB3	12:L:58:LYS:HA	1.91	0.52
13:M:182:PHE:C	13:M:183:PHE:CD1	2.86	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:484:MET:HB2	15:O:485:PRO:HD3	1.91	0.52
16:P:90:GLU:O	16:P:94:TYR:N	2.42	0.52
18:R:213:TRP:CD1	18:R:285:ALA:HB1	2.44	0.52
18:R:218:ARG:HD3	21:Y:60:DA:OP1	2.09	0.52
18:R:397:VAL:HA	18:R:449:VAL:O	2.09	0.52
1:A:188:LYS:NZ	21:Y:7:DC:H3'	2.24	0.52
1:A:449:ARG:O	1:A:452:LEU:N	2.25	0.52
1:A:1448:PHE:CE2	4:D:11:LEU:HG	2.43	0.52
3:C:32:ASN:CG	3:C:33:VAL:H	2.17	0.52
5:E:26:ARG:NH2	5:E:133:GLU:OE2	2.43	0.52
5:E:96:PHE:HZ	5:E:108:GLY:HA3	1.74	0.52
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.91	0.52
13:M:184:LYS:O	13:M:187:ASP:HB3	2.08	0.52
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.90	0.52
16:P:269:LEU:C	16:P:269:LEU:HD12	2.34	0.52
18:R:116:PHE:CE1	18:R:120:ARG:NH1	2.78	0.52
1:A:91:PHE:HE2	1:A:96:PHE:HD1	1.56	0.52
3:C:255:VAL:HG13	3:C:256:ILE:H	1.73	0.52
7:G:46:ILE:N	7:G:75:VAL:O	2.41	0.52
13:M:77:LYS:HA	14:N:360:VAL:HG22	1.90	0.52
16:P:106:TRP:HE1	16:P:145:ARG:HA	1.75	0.52
20:X:5:DC:N3	21:Y:65:DG:N1	2.40	0.52
5:E:23:VAL:HG22	5:E:28:TYR:HB2	1.90	0.52
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.26	0.52
10:J:48:ARG:O	10:J:52:THR:N	2.22	0.52
13:M:135:LYS:HZ1	13:M:140:TRP:HZ2	1.55	0.52
15:O:73:ARG:HG2	15:O:121:TYR:OH	2.10	0.52
18:R:83:ALA:O	18:R:87:LEU:CB	2.56	0.52
1:A:517:MET:O	1:A:518:ASN:ND2	2.43	0.52
1:A:774:ARG:HH21	1:A:808:GLN:HE21	1.55	0.52
2:B:400:LYS:O	2:B:403:ILE:N	2.42	0.52
4:D:102:SER:HA	4:D:105:GLU:HB2	1.91	0.52
15:O:95:LEU:HD21	15:O:120:TYR:CZ	2.44	0.52
1:A:67:CYS:HB3	1:A:70:CYS:O	2.10	0.52
1:A:115:LEU:HD21	1:A:123:PHE:HE2	1.75	0.52
1:A:154:CYS:SG	1:A:155:LEU:N	2.83	0.52
1:A:235:LYS:CG	15:O:44:PRO:HG2	2.40	0.52
1:A:676:SER:HB2	1:A:679:TYR:HB3	1.91	0.52
1:A:830:ARG:NH2	1:A:833:PRO:O	2.43	0.52
2:B:658:TYR:CD2	2:B:670:MET:HG2	2.45	0.52
3:C:33:VAL:C	3:C:35:LYS:H	2.18	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:PHE:HE1	5:E:112:TYR:O	1.92	0.52
1:A:897:SER:HB2	1:A:1423:ILE:HG22	1.92	0.52
1:A:1421:MET:HE1	2:B:1079:LEU:HD12	1.90	0.52
2:B:120:LEU:HD23	2:B:885:MET:SD	2.49	0.52
2:B:132:ASP:OD1	2:B:146:ASP:HA	2.10	0.52
2:B:588:ILE:O	2:B:588:ILE:HG22	2.10	0.52
3:C:255:VAL:HG22	3:C:256:ILE:H	1.75	0.52
14:N:395:ILE:HD11	14:N:408:LEU:HD21	1.91	0.52
15:O:544:ASN:HB3	15:O:576:PHE:CZ	2.44	0.52
16:P:221:ILE:O	16:P:225:ILE:HG12	2.09	0.52
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.74	0.52
5:E:77:SER:O	5:E:105:PHE:HB3	2.09	0.52
5:E:83:CYS:SG	5:E:92:THR:OG1	2.68	0.52
5:E:93:MET:SD	5:E:120:ALA:HA	2.50	0.52
7:G:87:GLY:HA3	7:G:148:PHE:HE1	1.74	0.52
15:O:634:GLU:O	15:O:637:VAL:HG12	2.10	0.52
16:P:55:LEU:HB3	16:P:60:LEU:HB2	1.91	0.52
18:R:140:HIS:ND1	18:R:140:HIS:O	2.43	0.52
18:R:191:LEU:HB2	18:R:195:LYS:HD3	1.91	0.52
20:X:4:DT:H2'	20:X:5:DC:C5'	2.32	0.52
20:X:24:DT:H2'	20:X:25:DT:C6	2.43	0.52
2:B:137:ARG:HH22	2:B:419:LEU:CD2	2.23	0.52
7:G:104:ILE:HG23	7:G:105:PHE:N	2.25	0.52
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.91	0.52
15:O:507:LEU:O	15:O:511:ILE:HG12	2.09	0.52
16:P:184:ARG:O	16:P:187:SER:OG	2.21	0.52
20:X:61:DT:H2''	20:X:62:DG:C8	2.45	0.52
21:Y:12:DG:H2''	21:Y:13:DA:C8	2.45	0.52
1:A:1171:PHE:HB3	1:A:1187:ARG:O	2.10	0.51
2:B:934:ASN:OD1	2:B:935:ASP:N	2.44	0.51
5:E:90:VAL:O	5:E:94:LYS:N	2.39	0.51
7:G:57:GLY:HA3	7:G:68:ILE:HG12	1.92	0.51
7:G:149:ARG:HD3	7:G:201:GLN:HE22	1.75	0.51
13:M:106:PHE:O	13:M:107:ILE:HG22	2.10	0.51
18:R:232:CYS:HB3	18:R:237:LEU:HD11	1.91	0.51
18:R:498:LEU:HD22	18:R:519:LEU:HD13	1.92	0.51
20:X:17:DG:H1	21:Y:53:DC:H42	1.58	0.51
1:A:223:ASN:O	1:A:226:LYS:N	2.42	0.51
1:A:645:MET:HE1	8:H:124:ARG:HB2	1.92	0.51
9:I:24:LEU:CD2	9:I:33:PHE:CD1	2.86	0.51
13:M:243:ILE:HG13	13:M:244:GLU:N	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:364:LEU:HA	19:S:375:ASP:HB3	1.92	0.51
19:S:421:THR:HG23	19:S:424:GLU:H	1.73	0.51
1:A:174:ALA:HB2	15:O:557:ARG:HB2	1.91	0.51
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.91	0.51
2:B:400:LYS:O	2:B:403:ILE:HG22	2.10	0.51
2:B:587:PHE:CZ	2:B:607:ARG:CG	2.81	0.51
2:B:771:LEU:O	2:B:923:GLY:N	2.43	0.51
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.92	0.51
2:B:961:LEU:HD21	2:B:1019:PHE:C	2.35	0.51
3:C:278:GLU:N	3:C:278:GLU:OE1	2.43	0.51
13:M:151:VAL:HG12	13:M:152:GLY:H	1.74	0.51
20:X:17:DG:O6	21:Y:52:DA:N6	2.42	0.51
21:Y:24:DC:H5'	21:Y:24:DC:C6	2.45	0.51
1:A:385:PRO:HD2	2:B:765:TYR:CE2	2.46	0.51
1:A:477:GLN:NE2	1:A:515:ASP:OD2	2.43	0.51
1:A:1160:ARG:NH1	1:A:1307:ASP:OD2	2.44	0.51
1:A:1187:ARG:HA	1:A:1228:ASP:O	2.10	0.51
1:A:1317:ASN:O	1:A:1318:HIS:ND1	2.44	0.51
1:A:1456:ALA:O	1:A:1460:ASN:ND2	2.43	0.51
2:B:81:GLN:N	2:B:81:GLN:OE1	2.43	0.51
2:B:295:ILE:HG12	2:B:296:TYR:H	1.75	0.51
2:B:316:LYS:NZ	13:M:226:ARG:HE	2.08	0.51
2:B:398:ASP:C	2:B:425:HIS:HE1	2.19	0.51
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.92	0.51
18:R:440:LEU:O	18:R:447:MET:HB2	2.10	0.51
1:A:179:ILE:HD12	15:O:557:ARG:NH2	2.26	0.51
1:A:1285:ILE:HA	1:A:1291:ARG:HG2	1.93	0.51
2:B:490:GLN:H	2:B:490:GLN:CD	2.19	0.51
3:C:57:ILE:HD13	3:C:297:HIS:CD2	2.44	0.51
3:C:230:LEU:HD13	3:C:297:HIS:ND1	2.25	0.51
7:G:114:MET:HB2	7:G:199:SER:HB2	1.90	0.51
13:M:230:SER:O	13:M:234:HIS:N	2.44	0.51
15:O:242:LYS:O	15:O:246:LYS:N	2.32	0.51
15:O:356:THR:HB	15:O:357:PRO:HD3	1.92	0.51
18:R:485:ASN:HD21	18:R:542:GLY:H	1.57	0.51
1:A:204:VAL:CG2	15:O:516:LEU:HD12	2.40	0.51
1:A:247:THR:CG2	1:A:249:PRO:HD3	2.41	0.51
1:A:314:GLU:N	1:A:314:GLU:OE1	2.43	0.51
1:A:379:THR:HG21	1:A:497:THR:HA	1.93	0.51
1:A:1318:HIS:CD2	1:A:1321:GLU:HB3	2.46	0.51
2:B:198:GLU:HA	2:B:377:LEU:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:ASP:O	2:B:501:ASP:OD1	2.28	0.51
2:B:904:ARG:NH2	2:B:1033:ASP:OD1	2.44	0.51
2:B:929:GLU:OE1	3:C:69:ARG:NH2	2.44	0.51
2:B:1094:VAL:O	2:B:1116:ILE:HA	2.11	0.51
3:C:34:GLU:C	3:C:36:PHE:N	2.65	0.51
3:C:164:ALA:O	3:C:186:PRO:HG3	2.11	0.51
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.45	0.51
8:H:98:TYR:HD1	8:H:141:TYR:CE2	2.29	0.51
16:P:180:THR:O	16:P:184:ARG:HG2	2.10	0.51
16:P:187:SER:HA	16:P:263:VAL:HG21	1.91	0.51
19:S:425:MET:O	19:S:428:PHE:HB3	2.11	0.51
21:Y:59:DT:H2'	21:Y:60:DA:H8	1.75	0.51
1:A:595:PRO:HB3	1:A:604:TRP:CE2	2.46	0.51
1:A:788:TRP:HA	1:A:793:ILE:HD11	1.92	0.51
1:A:955:LEU:HD12	1:A:959:ILE:HG13	1.92	0.51
2:B:250:GLU:H	2:B:308:LYS:NZ	2.09	0.51
2:B:766:ASP:O	2:B:770:ALA:HB3	2.10	0.51
2:B:1105:GLY:O	2:B:1113:ALA:HA	2.11	0.51
3:C:55:ASP:OD2	3:C:297:HIS:NE2	2.42	0.51
5:E:136:ASN:HB3	5:E:139:ALA:HB2	1.93	0.51
7:G:190:LYS:C	7:G:192:PRO:HD3	2.35	0.51
15:O:159:ILE:O	15:O:163:VAL:HG23	2.10	0.51
15:O:312:TYR:HE1	15:O:468:LEU:HD11	1.74	0.51
16:P:117:HIS:HB2	16:P:120:VAL:HG22	1.93	0.51
16:P:235:LEU:HD21	16:P:239:ASN:HB3	1.93	0.51
18:R:467:ARG:O	18:R:471:LYS:HB2	2.11	0.51
1:A:273:MET:O	1:A:275:GLN:CG	2.59	0.51
1:A:559:THR:HG21	2:B:947:HIS:HE1	1.76	0.51
1:A:976:ARG:HD3	1:A:989:LEU:HD22	1.92	0.51
2:B:227:ARG:HH11	2:B:449:MET:HE3	1.76	0.51
2:B:760:MET:HE3	2:B:762:TYR:HB2	1.93	0.51
2:B:1106:TRP:NE1	7:G:161:LYS:O	2.44	0.51
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.92	0.51
4:D:133:HIS:CE1	7:G:211:TRP:HB3	2.46	0.51
5:E:112:TYR:CD1	5:E:116:ILE:HG12	2.45	0.51
6:F:135:ARG:NH2	7:G:56:GLU:OE1	2.44	0.51
15:O:47:PHE:CD2	15:O:586:ALA:HB1	2.46	0.51
15:O:222:HIS:CE1	15:O:244:ASN:HB3	2.45	0.51
16:P:31:PHE:HD2	16:P:72:PHE:HB2	1.76	0.51
18:R:147:SER:OG	18:R:154:VAL:HG22	2.11	0.51
19:S:427:LYS:HB2	19:S:446:TYR:OH	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:3:DT:H1'	21:Y:4:DT:H5'	1.93	0.51
1:A:587:ILE:HA	11:K:53:ALA:HB2	1.93	0.51
1:A:633:PHE:CZ	1:A:643:ASN:HB3	2.46	0.51
1:A:653:ILE:HD11	1:A:655:ARG:HH21	1.75	0.51
1:A:1448:PHE:CZ	4:D:14:TYR:HE2	2.29	0.51
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.46	0.51
9:I:29:CYS:CB	13:M:183:PHE:HE2	2.23	0.51
1:A:625:ASN:HD21	1:A:941:HIS:HA	1.75	0.51
1:A:1454:GLU:HG2	1:A:1457:LEU:HD12	1.93	0.51
2:B:767:ILE:HG22	2:B:768:GLU:H	1.75	0.51
4:D:17:LEU:HD22	4:D:66:LEU:HB3	1.93	0.51
8:H:26:ILE:HG23	8:H:40:LEU:HB3	1.93	0.51
13:M:139:GLU:HB3	13:M:140:TRP:CE3	2.46	0.51
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.92	0.51
2:B:404:ASP:O	2:B:408:LYS:HG3	2.12	0.50
2:B:501:ASP:HB3	2:B:703:CYS:HB3	1.92	0.50
2:B:510:LEU:HD21	2:B:512:LYS:HE3	1.93	0.50
4:D:15:GLU:O	4:D:19:PHE:N	2.40	0.50
5:E:22:MET:HE3	5:E:187:TYR:O	2.10	0.50
5:E:64:PRO:HD3	5:E:77:SER:HA	1.93	0.50
15:O:132:TYR:HD2	15:O:135:LEU:HD23	1.75	0.50
16:P:55:LEU:O	16:P:60:LEU:N	2.32	0.50
18:R:510:SER:O	18:R:520:ILE:HG13	2.10	0.50
1:A:38:ASP:C	1:A:40:PHE:H	2.20	0.50
1:A:185:TRP:O	1:A:186:VAL:HG22	2.10	0.50
1:A:408:VAL:O	1:A:408:VAL:HG13	2.11	0.50
1:A:624:ILE:HG22	1:A:625:ASN:N	2.26	0.50
1:A:911:ILE:HG23	5:E:176:PRO:HD3	1.93	0.50
1:A:1182:SER:OG	1:A:1260:MET:HE1	2.11	0.50
1:A:1332:ARG:O	1:A:1335:ILE:HG22	2.11	0.50
2:B:94:LYS:HB3	2:B:134:GLU:HB3	1.93	0.50
2:B:997:ASN:OD1	2:B:998:TYR:N	2.44	0.50
13:M:230:SER:C	13:M:234:HIS:HD1	2.18	0.50
15:O:133:SER:O	15:O:136:ILE:N	2.44	0.50
15:O:297:ILE:HD13	15:O:313:LYS:HG3	1.93	0.50
15:O:515:LYS:O	15:O:516:LEU:C	2.53	0.50
18:R:218:ARG:C	18:R:514:GLU:HG2	2.36	0.50
21:Y:50:DT:H2''	21:Y:51:DT:C6	2.46	0.50
1:A:103:LEU:HD11	1:A:222:LEU:HD22	1.93	0.50
1:A:111:SER:HB2	1:A:233:GLN:HG2	1.94	0.50
1:A:273:MET:O	1:A:275:GLN:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:GLN:HG2	1:A:915:THR:O	2.11	0.50
1:A:1449:GLU:O	4:D:117:LYS:NZ	2.45	0.50
2:B:44:LYS:HZ1	2:B:663:GLU:HB2	1.77	0.50
2:B:137:ARG:NH2	2:B:419:LEU:HD23	2.25	0.50
2:B:611:PRO:HG3	2:B:648:TYR:HE1	1.77	0.50
2:B:756:THR:N	10:J:48:ARG:HH12	2.09	0.50
3:C:321:LEU:HD21	11:K:124:LEU:HD21	1.93	0.50
6:F:84:TYR:HD1	6:F:152:ILE:HG23	1.77	0.50
8:H:97:MET:HG3	8:H:142:LEU:HD23	1.93	0.50
11:K:99:ASN:O	11:K:100:LEU:HD12	2.11	0.50
12:L:28:LYS:NZ	12:L:40:LEU:O	2.33	0.50
13:M:93:ARG:NH2	13:M:105:PRO:HB3	2.26	0.50
15:O:74:LEU:HG	15:O:79:LEU:HD12	1.93	0.50
15:O:589:LEU:O	15:O:592:LYS:HB3	2.11	0.50
18:R:11:GLU:N	18:R:11:GLU:OE1	2.43	0.50
18:R:431:ARG:HA	18:R:438:THR:HA	1.94	0.50
18:R:467:ARG:HA	18:R:602:LEU:HD21	1.93	0.50
19:S:432:LEU:HB3	19:S:472:ALA:HB1	1.94	0.50
20:X:57:DT:H2"	20:X:58:DC:C6	2.47	0.50
7:G:141:ASP:OD1	7:G:142:VAL:N	2.43	0.50
13:M:148:LEU:HD23	13:M:179:LEU:HG	1.93	0.50
15:O:324:PRO:HD3	15:O:353:GLU:CD	2.36	0.50
1:A:431:ASN:O	1:A:444:LEU:HD13	2.11	0.50
1:A:809:MET:O	1:A:851:SER:HB3	2.11	0.50
2:B:56:GLY:O	2:B:59:LYS:HG2	2.12	0.50
2:B:68:PHE:HD1	2:B:385:SER:OG	1.93	0.50
2:B:540:ASP:OD1	2:B:541:ILE:N	2.44	0.50
2:B:772:VAL:HG23	2:B:924:ILE:O	2.12	0.50
2:B:906:PRO:HB3	2:B:1026:LYS:HE3	1.93	0.50
4:D:14:TYR:CG	4:D:15:GLU:N	2.56	0.50
5:E:20:LYS:O	5:E:23:VAL:HG12	2.12	0.50
6:F:104:ASN:OD1	6:F:104:ASN:O	2.30	0.50
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.93	0.50
15:O:634:GLU:HA	15:O:637:VAL:HG12	1.94	0.50
19:S:422:VAL:O	19:S:426:ILE:N	2.44	0.50
1:A:186:VAL:HG23	1:A:188:LYS:HG2	1.94	0.50
1:A:265:PRO:O	1:A:269:ARG:HG2	2.12	0.50
1:A:351:ARG:HD2	1:A:355:GLN:CD	2.37	0.50
1:A:392:VAL:HG23	1:A:488:HIS:CG	2.47	0.50
1:A:1145:LEU:HB2	1:A:1292:GLU:CG	2.42	0.50
2:B:135:TYR:CZ	2:B:419:LEU:HB2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG11	2:B:608:ILE:HD12	1.93	0.50
6:F:143:PHE:O	6:F:144:GLU:HB2	2.11	0.50
12:L:29:TYR:CB	12:L:58:LYS:HA	2.40	0.50
15:O:53:VAL:HG21	15:O:65:ILE:HD12	1.93	0.50
15:O:506:ARG:HB3	16:P:250:ASP:OD1	2.11	0.50
17:Q:1079:UNK:O	17:Q:1083:UNK:N	2.44	0.50
18:R:144:ILE:O	18:R:147:SER:OG	2.27	0.50
18:R:512:GLU:OE1	18:R:512:GLU:N	2.42	0.50
20:X:3:DT:O4	21:Y:66:DA:N6	2.45	0.50
1:A:33:GLU:HB3	1:A:35:SER:OG	2.11	0.50
1:A:445:ARG:HG2	18:R:24:VAL:HG11	1.93	0.50
1:A:1431:VAL:HG21	6:F:135:ARG:CZ	2.42	0.50
2:B:736:VAL:HG21	2:B:960:GLU:HG3	1.93	0.50
2:B:1009:THR:O	3:C:65:ASN:ND2	2.44	0.50
4:D:13:ASP:OD1	4:D:17:LEU:N	2.44	0.50
7:G:158:VAL:C	7:G:160:PRO:HD3	2.37	0.50
8:H:106:GLU:N	8:H:106:GLU:OE1	2.45	0.50
15:O:248:ASP:O	15:O:252:ILE:HG12	2.11	0.50
15:O:317:ARG:HA	15:O:320:GLU:CD	2.36	0.50
16:P:27:ILE:HB	16:P:31:PHE:HB2	1.94	0.50
16:P:172:ILE:O	16:P:175:ILE:HD11	2.12	0.50
18:R:428:VAL:O	18:R:441:ILE:HG22	2.12	0.50
21:Y:46:DA:C6	21:Y:47:DG:C6	3.00	0.50
1:A:835:PHE:CE2	1:A:844:SER:HA	2.47	0.50
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.12	0.50
2:B:732:GLN:HB3	10:J:52:THR:CG2	2.42	0.50
2:B:957:LYS:HZ2	2:B:1022:ILE:HD13	1.76	0.50
3:C:284:GLU:O	3:C:288:LYS:NZ	2.45	0.50
7:G:95:GLU:HG3	7:G:96:GLY:H	1.77	0.50
14:N:286:ASP:CG	14:N:385:GLY:H	2.20	0.50
1:A:716:ASP:OD2	1:A:791:PRO:HD2	2.12	0.50
1:A:1123:VAL:N	1:A:1124:PRO:HD2	2.26	0.50
1:A:1305:CYS:SG	5:E:141:VAL:HG11	2.52	0.50
2:B:780:ARG:NH1	10:J:9:SER:O	2.44	0.50
13:M:87:VAL:HG23	14:N:395:ILE:O	2.12	0.50
16:P:106:TRP:HB2	16:P:147:ILE:HG22	1.94	0.50
16:P:241:ARG:O	16:P:245:GLU:HG2	2.12	0.50
18:R:621:LYS:O	18:R:625:ARG:N	2.43	0.50
1:A:120:LYS:CG	1:A:241:LEU:HD11	2.41	0.49
1:A:485:ILE:O	1:A:486:LEU:HD12	2.12	0.49
1:A:1064:GLU:O	1:A:1067:VAL:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:VAL:HG22	1:A:1230:ILE:HG12	1.94	0.49
1:A:1343:MET:HE1	1:A:1355:ILE:HD11	1.93	0.49
3:C:103:LEU:HD22	10:J:5:VAL:HG23	1.92	0.49
13:M:113:LYS:HG2	13:M:117:HIS:O	2.12	0.49
13:M:183:PHE:HB3	13:M:185:TYR:HB2	1.94	0.49
15:O:202:GLN:N	15:O:280:LEU:HG	2.26	0.49
18:R:144:ILE:HD12	18:R:154:VAL:HG21	1.94	0.49
18:R:607:ASP:C	18:R:609:GLU:H	2.18	0.49
1:A:424:PRO:HB3	1:A:431:ASN:HB3	1.94	0.49
1:A:518:ASN:ND2	2:B:1060:LEU:HD13	2.26	0.49
2:B:316:LYS:HE2	13:M:226:ARG:HE	1.76	0.49
2:B:949:PHE:HB2	2:B:950:PRO:HD3	1.94	0.49
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.49
4:D:122:GLN:NE2	7:G:83:GLU:HG3	2.27	0.49
9:I:22:TYR:C	9:I:23:THR:HG22	2.37	0.49
13:M:88:PHE:HZ	13:M:119:TRP:HE3	1.59	0.49
13:M:104:HIS:CG	13:M:105:PRO:HD2	2.47	0.49
14:N:287:HIS:ND1	14:N:369:GLY:O	2.35	0.49
15:O:182:SER:OG	15:O:187:ILE:HG21	2.12	0.49
18:R:287:PRO:O	18:R:289:SER:N	2.43	0.49
18:R:417:ASN:HA	19:S:437:THR:HG22	1.94	0.49
18:R:467:ARG:HG2	18:R:606:ASP:OD1	2.12	0.49
1:A:533:ASN:HD21	6:F:90:ARG:HG2	1.76	0.49
1:A:1458:LYS:NZ	4:D:112:SER:HA	2.27	0.49
2:B:649:LEU:HD22	2:B:653:GLU:OE1	2.12	0.49
3:C:69:ARG:HE	11:K:71:THR:HG22	1.78	0.49
7:G:119:CYS:HB3	7:G:130:TRP:HD1	1.77	0.49
8:H:15:VAL:HG13	8:H:24:CYS:SG	2.52	0.49
9:I:20:GLY:C	9:I:22:TYR:H	2.21	0.49
15:O:37:LEU:HD23	15:O:40:ARG:CD	2.41	0.49
18:R:468:ILE:HG23	18:R:472:ILE:HD12	1.93	0.49
21:Y:41:DG:H1'	21:Y:42:DA:H5'	1.95	0.49
1:A:309:ILE:HG12	15:O:566:PHE:CE1	2.47	0.49
2:B:876:PRO:HG2	2:B:1032:LEU:HD21	1.94	0.49
3:C:211:GLY:HA3	3:C:219:PHE:CD2	2.46	0.49
16:P:36:LEU:O	16:P:40:MET:N	2.46	0.49
16:P:154:GLN:HG2	19:S:520:LYS:HE2	1.95	0.49
18:R:396:ILE:N	18:R:452:ALA:O	2.41	0.49
18:R:626:ILE:HD11	19:S:487:GLU:HG3	1.93	0.49
21:Y:55:DA:H1'	21:Y:56:DA:C4	2.46	0.49
1:A:69:THR:OG1	1:A:80:HIS:NE2	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:123:PHE:CE2	2.47	0.49
1:A:235:LYS:CA	1:A:252:ARG:CD	2.72	0.49
1:A:373:VAL:HG11	2:B:1082:ARG:HD2	1.93	0.49
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.94	0.49
1:A:541:LEU:HG	1:A:551:ILE:CD1	2.43	0.49
2:B:545:ASP:OD2	2:B:547:ALA:HB3	2.12	0.49
2:B:798:TYR:CG	2:B:851:SER:HB2	2.48	0.49
2:B:957:LYS:NZ	2:B:1022:ILE:HG21	2.28	0.49
7:G:50:ASP:OD1	7:G:73:ARG:N	2.40	0.49
14:N:299:ASN:CG	14:N:301:PRO:HD3	2.37	0.49
21:Y:28:DT:H2''	21:Y:29:DG:H8	1.78	0.49
1:A:273:MET:HB3	18:R:39:SER:OG	2.12	0.49
1:A:1165:LEU:HD22	1:A:1198:LEU:HD21	1.94	0.49
1:A:1408:VAL:HG23	1:A:1413:GLU:CG	2.42	0.49
2:B:296:TYR:HE1	13:M:182:PHE:HA	1.78	0.49
4:D:1:MET:HG3	4:D:2:LYS:N	2.27	0.49
4:D:24:GLU:HG2	4:D:30:ASP:CG	2.38	0.49
12:L:40:LEU:HD11	12:L:44:ASP:HB3	1.95	0.49
13:M:159:TYR:CD1	13:M:172:PRO:HA	2.47	0.49
15:O:39:GLN:O	15:O:40:ARG:HB2	2.12	0.49
15:O:92:LYS:O	15:O:96:VAL:HG22	2.13	0.49
16:P:31:PHE:CD2	16:P:72:PHE:HB2	2.48	0.49
20:X:2:DT:H1'	20:X:3:DT:H5'	1.95	0.49
21:Y:65:DG:H4'	21:Y:66:DA:H5'	1.94	0.49
1:A:14:LYS:HD3	2:B:1144:GLU:CD	2.37	0.49
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.93	0.49
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.41	0.49
2:B:55:LYS:HZ2	2:B:59:LYS:HE3	1.75	0.49
2:B:316:LYS:HE2	13:M:226:ARG:HB2	1.94	0.49
18:R:220:PRO:HD3	18:R:514:GLU:CG	2.41	0.49
1:A:181:ASP:HB2	1:A:219:MET:HG3	1.94	0.49
1:A:226:LYS:HD3	15:O:547:GLU:HG3	1.95	0.49
1:A:610:PHE:O	1:A:613:LEU:HB3	2.12	0.49
1:A:1217:ILE:H	1:A:1217:ILE:HD12	1.78	0.49
2:B:232:TYR:HD1	2:B:242:LEU:HD23	1.76	0.49
2:B:944:MET:SD	2:B:1024:TYR:OH	2.71	0.49
4:D:126:GLN:HE21	7:G:85:VAL:HA	1.77	0.49
5:E:191:LYS:H	5:E:194:GLU:CD	2.20	0.49
13:M:247:TRP:CH2	13:M:249:GLU:HB2	2.48	0.49
16:P:221:ILE:O	16:P:225:ILE:N	2.40	0.49
18:R:83:ALA:O	18:R:87:LEU:HD12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:140:HIS:ND1	18:R:184:HIS:HB2	2.28	0.49
20:X:3:DT:H2''	20:X:4:DT:H73	1.86	0.49
1:A:381:ILE:HG22	1:A:382:SER:H	1.78	0.49
1:A:611:SER:OG	1:A:658:GLN:HA	2.13	0.49
1:A:1127:LYS:O	1:A:1131:ASN:CB	2.60	0.49
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.94	0.49
2:B:265:ASP:O	2:B:267:GLU:N	2.46	0.49
2:B:338:GLU:CD	2:B:339:ALA:H	2.20	0.49
2:B:464:ILE:HD11	2:B:746:TYR:CE1	2.37	0.49
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.78	0.49
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.28	0.49
12:L:41:SER:HB3	12:L:44:ASP:HB2	1.93	0.49
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.42	0.49
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.46	0.49
15:O:467:PHE:CD2	15:O:468:LEU:HD13	2.34	0.49
15:O:468:LEU:HD12	15:O:483:LEU:HD21	1.95	0.49
15:O:567:ARG:HG2	15:O:568:CYS:H	1.78	0.49
16:P:296:TYR:CG	16:P:297:PHE:N	2.81	0.49
16:P:308:GLU:OE1	16:P:308:GLU:N	2.46	0.49
1:A:36:THR:HG21	1:A:51:ASN:ND2	2.28	0.49
1:A:601:TYR:CE1	3:C:23:PHE:HE2	2.31	0.49
1:A:1152:ARG:O	1:A:1155:ARG:N	2.46	0.49
3:C:94:ASP:C	12:L:67:PHE:HE2	2.20	0.49
3:C:103:LEU:HD21	10:J:6:ARG:CD	2.43	0.49
4:D:61:ASN:HB3	7:G:103:GLY:O	2.13	0.49
7:G:147:ARG:NH2	7:G:204:GLY:O	2.45	0.49
11:K:85:ASP:OD1	11:K:86:VAL:HG23	2.12	0.49
15:O:73:ARG:HG2	15:O:121:TYR:HE1	1.64	0.49
15:O:302:THR:O	16:P:265:LEU:HD11	2.12	0.49
16:P:142:PHE:CZ	20:X:30:DT:H4'	2.47	0.49
16:P:263:VAL:HG12	16:P:265:LEU:H	1.77	0.49
18:R:583:HIS:NE2	18:R:585:LEU:O	2.46	0.49
1:A:238:ASP:OD1	1:A:238:ASP:N	2.45	0.48
1:A:476:ARG:HE	1:A:477:GLN:CD	2.21	0.48
1:A:482:ARG:HB3	1:A:544:PRO:HG3	1.96	0.48
1:A:753:GLN:O	1:A:755:GLY:N	2.36	0.48
1:A:818:ILE:HG22	1:A:867:SER:HA	1.94	0.48
1:A:912:VAL:HG12	1:A:1364:TYR:CD1	2.48	0.48
1:A:1099:GLU:OE1	1:A:1099:GLU:N	2.38	0.48
1:A:1205:ILE:O	1:A:1209:ILE:HG12	2.13	0.48
1:A:1448:PHE:CZ	4:D:16:VAL:HG23	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:GLU:O	2:B:563:GLY:HA2	2.13	0.48
2:B:1147:PHE:HB2	7:G:10:LEU:HD11	1.95	0.48
5:E:46:TYR:CZ	5:E:58:MET:HA	2.48	0.48
13:M:154:GLU:N	13:M:154:GLU:OE1	2.45	0.48
13:M:241:ALA:O	13:M:242:ASN:CB	2.51	0.48
18:R:198:VAL:O	18:R:201:ASP:HB2	2.13	0.48
1:A:172:GLY:HA3	1:A:331:SER:HB2	1.95	0.48
1:A:472:VAL:HG22	1:A:521:VAL:HG12	1.94	0.48
1:A:577:THR:HG21	11:K:89:CYS:H	1.78	0.48
1:A:919:ASP:OD1	1:A:921:LEU:HD13	2.13	0.48
2:B:112:LEU:HD23	2:B:113:THR:N	2.28	0.48
2:B:296:TYR:HB2	2:B:300:GLN:NE2	2.24	0.48
2:B:416:TYR:CZ	18:R:151:GLN:CB	2.96	0.48
2:B:693:HIS:HB3	2:B:955:VAL:HG23	1.95	0.48
2:B:1084:MET:HE1	2:B:1121:ILE:N	2.28	0.48
8:H:39:THR:HB	8:H:124:ARG:HB3	1.95	0.48
10:J:16:ASP:OD1	10:J:17:LYS:N	2.46	0.48
15:O:369:HIS:CG	15:O:370:LEU:H	2.30	0.48
15:O:472:LYS:HG2	15:O:473:PRO:HD2	1.94	0.48
18:R:213:TRP:CG	18:R:285:ALA:HB1	2.48	0.48
18:R:214:MET:SD	18:R:288:PRO:HD3	2.53	0.48
1:A:5:VAL:HG22	7:G:37:LYS:HB3	1.96	0.48
1:A:269:ARG:O	1:A:269:ARG:HG3	2.12	0.48
1:A:493:ARG:HB2	1:A:499:ARG:NH2	2.28	0.48
1:A:520:HIS:CE1	2:B:1062:LEU:HD21	2.45	0.48
1:A:988:ASP:CG	1:A:993:GLU:H	2.22	0.48
2:B:481:ARG:NH2	21:Y:21:DT:H2'	2.28	0.48
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.78	0.48
2:B:809:MET:HA	2:B:821:HIS:CD2	2.47	0.48
2:B:986:ASP:OD1	2:B:987:MET:N	2.46	0.48
3:C:70:ILE:HG13	3:C:74:GLU:HB2	1.95	0.48
8:H:3:ASN:HB2	8:H:61:SER:O	2.14	0.48
16:P:292:SER:OG	16:P:293:ILE:N	2.46	0.48
1:A:654:ILE:HG23	1:A:658:GLN:O	2.14	0.48
1:A:997:GLN:O	1:A:999:ASP:N	2.46	0.48
1:A:1128:GLU:OE1	1:A:1136:ILE:HG13	2.14	0.48
2:B:493:GLN:HG3	2:B:497:LEU:HB2	1.96	0.48
2:B:587:PHE:CD1	2:B:609:CYS:SG	3.06	0.48
2:B:623:LYS:O	2:B:625:ILE:N	2.41	0.48
2:B:926:VAL:HG12	2:B:927:LYS:N	2.28	0.48
10:J:55:ASP:OD1	10:J:57:ILE:HG22	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:LEU:HD23	14:N:363:ILE:HG13	1.95	0.48
13:M:92:ASN:HD21	13:M:148:LEU:HD21	1.76	0.48
14:N:365:VAL:HG13	14:N:370:LYS:O	2.13	0.48
1:A:173:SER:OG	15:O:557:ARG:O	2.31	0.48
1:A:233:GLN:NE2	15:O:575:ASN:ND2	2.62	0.48
1:A:607:LYS:O	1:A:611:SER:HB2	2.13	0.48
1:A:714:ILE:HD13	2:B:958:MET:HE3	1.95	0.48
2:B:434:ASN:HA	2:B:437:ILE:HG22	1.94	0.48
3:C:70:ILE:HD11	3:C:320:ILE:CG2	2.44	0.48
3:C:122:ASP:OD1	3:C:123:ASP:N	2.46	0.48
10:J:57:ILE:O	10:J:61:LEU:HG	2.12	0.48
13:M:72:GLU:OE1	14:N:364:ARG:NE	2.38	0.48
15:O:464:ASN:HA	15:O:469:ASN:CG	2.38	0.48
15:O:578:ARG:O	15:O:581:LEU:HB3	2.13	0.48
16:P:177:SER:O	16:P:180:THR:HG22	2.14	0.48
16:P:254:GLU:HB3	16:P:262:ARG:HB2	1.94	0.48
1:A:308:SER:HA	15:O:534:ARG:CD	2.42	0.48
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.95	0.48
8:H:107:VAL:O	8:H:111:LEU:HB2	2.14	0.48
18:R:121:ARG:HB2	18:R:124:ASN:HD22	1.78	0.48
18:R:467:ARG:O	18:R:471:LYS:HB3	2.12	0.48
19:S:409:GLY:N	21:Y:61:DT:H5"	2.28	0.48
1:A:1411:VAL:HG13	1:A:1412:SER:N	2.26	0.48
2:B:77:ILE:HG21	2:B:98:ILE:HD11	1.95	0.48
2:B:177:CYS:SG	2:B:179:LEU:N	2.87	0.48
2:B:327:ILE:HD13	13:M:231:LEU:HD13	1.95	0.48
2:B:733:GLN:HG3	10:J:54:VAL:HG13	1.95	0.48
5:E:112:TYR:CE1	5:E:116:ILE:HG12	2.49	0.48
6:F:89:GLU:OE1	6:F:90:ARG:N	2.47	0.48
6:F:147:SER:HB3	6:F:150:GLU:HG3	1.96	0.48
9:I:6:PRO:C	9:I:7:SER:HG	2.18	0.48
18:R:79:THR:HG21	20:X:26:DT:H5"	1.96	0.48
19:S:462:GLU:HA	19:S:469:ILE:HG13	1.95	0.48
21:Y:26:DT:C2	21:Y:27:DG:C6	3.00	0.48
1:A:1378:LYS:HG3	1:A:1379:MET:N	2.22	0.48
2:B:103:LYS:HB3	2:B:130:TYR:CE2	2.49	0.48
2:B:721:ILE:HG12	2:B:899:LEU:HD23	1.94	0.48
2:B:1126:LYS:O	2:B:1129:PHE:N	2.46	0.48
3:C:31:TRP:HH2	11:K:127:LEU:HG	1.79	0.48
3:C:283:GLU:O	3:C:285:PHE:N	2.47	0.48
4:D:65:TYR:CE1	7:G:101:LEU:HD11	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:ASP:HA	13:M:146:GLN:O	2.14	0.48
13:M:144:ASN:CG	13:M:145:VAL:H	2.21	0.48
14:N:376:GLY:H	14:N:379:VAL:HG12	1.78	0.48
16:P:175:ILE:O	16:P:178:LEU:HG	2.13	0.48
18:R:7:CYS:SG	18:R:27:ALA:HB3	2.54	0.48
18:R:104:ALA:O	18:R:107:TRP:HB2	2.13	0.48
21:Y:65:DG:H1'	21:Y:66:DA:C8	2.49	0.48
1:A:742:ILE:HG12	1:A:840:LYS:HB2	1.95	0.48
1:A:903:THR:HA	1:A:914:PHE:O	2.14	0.48
1:A:1050:ASP:O	1:A:1053:LYS:N	2.45	0.48
1:A:1193:ILE:HG12	1:A:1200:LEU:HD11	1.96	0.48
1:A:1300:LEU:HB3	1:A:1321:GLU:OE2	2.14	0.48
1:A:1386:LEU:HB3	1:A:1395:HIS:CD2	2.49	0.48
1:A:1449:GLU:OE2	4:D:10:PHE:N	2.47	0.48
2:B:496:MET:CG	2:B:610:ARG:HD2	2.44	0.48
2:B:776:SER:HB3	3:C:217:ALA:HB2	1.95	0.48
3:C:276:SER:OG	3:C:278:GLU:OE2	2.22	0.48
6:F:81:THR:HG21	6:F:136:ARG:HH11	1.78	0.48
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.95	0.48
16:P:266:GLU:HA	16:P:268:ILE:HG13	1.96	0.48
18:R:499:GLU:OE1	18:R:499:GLU:N	2.42	0.48
1:A:287:VAL:O	1:A:290:THR:HG22	2.14	0.48
1:A:962:THR:O	1:A:965:GLU:HB3	2.14	0.48
2:B:1057:ASP:OD1	18:R:19:ALA:HB1	2.13	0.48
3:C:100:ARG:HH22	10:J:2:ILE:HG21	1.79	0.48
5:E:81:GLU:HB3	5:E:110:PHE:HB3	1.95	0.48
6:F:104:ASN:OD1	6:F:104:ASN:C	2.55	0.48
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.47	0.48
13:M:159:TYR:CG	13:M:170:LEU:HD21	2.49	0.48
18:R:213:TRP:CH2	18:R:497:ARG:HB3	2.49	0.48
19:S:424:GLU:OE2	19:S:449:ARG:NE	2.37	0.48
20:X:13:DA:P	20:X:13:DA:H8	2.37	0.48
1:A:186:VAL:HG22	1:A:189:LYS:HG2	1.96	0.47
1:A:316:TRP:O	1:A:319:LEU:HB3	2.14	0.47
1:A:665:ASP:CG	1:A:797:CYS:HB3	2.39	0.47
1:A:675:HIS:HA	1:A:937:ARG:HH22	1.78	0.47
1:A:1125:ARG:HH22	1:A:1317:ASN:HB3	1.79	0.47
2:B:1112:SER:OG	2:B:1113:ALA:N	2.46	0.47
3:C:258:ILE:HD13	3:C:265:ALA:HB2	1.97	0.47
5:E:85:GLU:CD	5:E:86:PRO:HD2	2.38	0.47
7:G:203:ASP:O	7:G:205:MET:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:63:PHE:CD2	11:K:117:LEU:HD13	2.48	0.47
15:O:39:GLN:HG3	15:O:47:PHE:CZ	2.49	0.47
15:O:262:ILE:O	15:O:274:VAL:HA	2.14	0.47
15:O:472:LYS:CG	15:O:473:PRO:HD2	2.44	0.47
1:A:385:PRO:HD2	2:B:765:TYR:CD2	2.48	0.47
1:A:386:ASN:ND2	1:A:703:ARG:HH21	2.12	0.47
1:A:502:GLU:H	1:A:502:GLU:HG3	1.49	0.47
1:A:568:ASP:OD1	8:H:22:LYS:HG2	2.14	0.47
1:A:1203:GLU:HA	1:A:1206:ALA:HB3	1.96	0.47
2:B:640:PHE:O	2:B:644:GLY:N	2.47	0.47
2:B:678:PHE:HB3	2:B:978:CYS:O	2.13	0.47
2:B:705:MET:O	2:B:708:GLN:N	2.25	0.47
2:B:884:VAL:HB	2:B:898:VAL:HG12	1.96	0.47
5:E:26:ARG:HH22	5:E:189:GLY:CA	2.26	0.47
9:I:22:TYR:O	9:I:23:THR:CG2	2.62	0.47
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.79	0.47
15:O:326:ILE:HG21	15:O:653:MET:SD	2.54	0.47
1:A:313:MET:O	1:A:316:TRP:N	2.47	0.47
1:A:363:ARG:NH1	2:B:1127:LEU:HG	2.28	0.47
1:A:372:ARG:HD2	2:B:1050:PRO:O	2.14	0.47
1:A:427:HIS:O	1:A:429:GLY:N	2.48	0.47
1:A:842:PRO:C	1:A:844:SER:H	2.22	0.47
2:B:632:ASP:OD1	2:B:633:GLY:N	2.48	0.47
2:B:834:MET:CE	12:L:63:ARG:HD2	2.44	0.47
3:C:59:ILE:HD12	3:C:60:ASP:O	2.14	0.47
15:O:51:GLU:HB2	15:O:590:PHE:CZ	2.49	0.47
18:R:122:SER:N	20:X:25:DT:OP1	2.44	0.47
18:R:414:HIS:HB2	18:R:472:ILE:HD13	1.95	0.47
19:S:425:MET:HG2	19:S:429:TYR:CE2	2.48	0.47
1:A:857:SER:N	1:A:860:GLU:OE2	2.36	0.47
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.97	0.47
2:B:248:ALA:HB3	2:B:308:LYS:HG2	1.96	0.47
2:B:389:GLU:O	2:B:393:LYS:HB2	2.14	0.47
6:F:136:ARG:O	6:F:144:GLU:HB3	2.13	0.47
15:O:483:LEU:O	15:O:487:LEU:N	2.47	0.47
16:P:151:TYR:OH	18:R:647:ALA:O	2.31	0.47
18:R:501:LEU:HA	18:R:563:PHE:CE2	2.48	0.47
1:A:224:PRO:HA	1:A:227:THR:HG22	1.95	0.47
1:A:323:VAL:O	1:A:326:TYR:HB3	2.14	0.47
1:A:633:PHE:HZ	1:A:643:ASN:HB3	1.79	0.47
1:A:675:HIS:HA	1:A:937:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:SER:OG	2:B:1016:TYR:O	2.30	0.47
1:A:856:LEU:HD13	2:B:692:HIS:O	2.15	0.47
1:A:998:TYR:HB2	1:A:1002:ARG:HH12	1.79	0.47
2:B:1057:ASP:CG	2:B:1058:GLY:H	2.21	0.47
9:I:4:PHE:O	9:I:6:PRO:HD3	2.15	0.47
15:O:140:ILE:O	15:O:144:MET:N	2.47	0.47
15:O:203:ILE:HB	15:O:207:HIS:CD2	2.48	0.47
16:P:78:SER:O	16:P:82:LYS:HB2	2.15	0.47
18:R:273:GLN:HB2	19:S:277:UNK:N	2.30	0.47
18:R:397:VAL:HG21	20:X:16:DA:H2	1.80	0.47
1:A:429:GLY:C	1:A:465:HIS:ND1	2.69	0.47
1:A:1302:ASP:N	1:A:1302:ASP:OD1	2.45	0.47
5:E:151:PRO:HB2	5:E:199:ILE:O	2.14	0.47
15:O:124:GLU:CG	15:O:125:GLU:H	2.27	0.47
15:O:292:ARG:NH1	15:O:650:VAL:HA	2.27	0.47
16:P:194:GLY:O	16:P:196:LYS:NZ	2.47	0.47
16:P:203:LYS:HB2	16:P:206:VAL:H	1.80	0.47
18:R:223:ILE:HD12	18:R:258:ARG:HH21	1.79	0.47
1:A:18:PHE:CE2	1:A:1383:VAL:HG21	2.49	0.47
1:A:46:ARG:CZ	1:A:278:PRO:HA	2.44	0.47
1:A:96:PHE:O	1:A:99:THR:N	2.47	0.47
1:A:436:ARG:N	1:A:460:ASP:OD1	2.35	0.47
1:A:624:ILE:HG22	1:A:625:ASN:H	1.78	0.47
1:A:858:PRO:HD2	2:B:661:LEU:HD13	1.96	0.47
2:B:217:GLN:CG	2:B:232:TYR:HB3	2.44	0.47
2:B:220:VAL:HG12	2:B:229:SER:HA	1.96	0.47
2:B:316:LYS:HZ3	13:M:226:ARG:CZ	2.28	0.47
2:B:426:SER:C	2:B:428:ASN:H	2.17	0.47
2:B:615:VAL:HG12	2:B:620:SER:HA	1.97	0.47
2:B:622:VAL:HG12	2:B:624:ASP:H	1.80	0.47
2:B:724:LEU:HD12	2:B:789:ARG:NH1	2.30	0.47
2:B:774:ASN:O	2:B:778:ILE:HG22	2.15	0.47
2:B:780:ARG:HH12	10:J:10:CYS:C	2.23	0.47
2:B:1054:ARG:O	2:B:1055:SER:OG	2.25	0.47
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.95	0.47
5:E:82:PHE:CD1	5:E:111:VAL:HB	2.45	0.47
7:G:152:ARG:O	7:G:197:LEU:HG	2.15	0.47
11:K:132:GLU:O	11:K:136:THR:HG22	2.15	0.47
13:M:72:GLU:OE1	13:M:72:GLU:N	2.48	0.47
13:M:85:LEU:HD23	13:M:85:LEU:C	2.39	0.47
13:M:184:LYS:HD2	13:M:184:LYS:HA	1.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:472:LYS:O	15:O:474:GLY:N	2.48	0.47
18:R:140:HIS:CE1	18:R:184:HIS:HB2	2.50	0.47
18:R:491:ASP:HB2	18:R:537:LYS:HD3	1.96	0.47
18:R:500:GLY:HA2	18:R:503:PHE:HB3	1.96	0.47
1:A:168:ALA:HB3	1:A:174:ALA:HB3	1.97	0.47
1:A:1163:LYS:HG3	1:A:1164:THR:N	2.30	0.47
2:B:556:TYR:HD1	2:B:561:LEU:HA	1.80	0.47
2:B:957:LYS:NZ	2:B:1022:ILE:HD13	2.30	0.47
3:C:96:VAL:O	3:C:99:HIS:HB3	2.15	0.47
5:E:188:LEU:HD23	5:E:190:LEU:HD11	1.96	0.47
7:G:119:CYS:CB	7:G:128:TRP:HB3	2.41	0.47
8:H:105:GLU:CG	8:H:106:GLU:N	2.69	0.47
13:M:151:VAL:HG12	13:M:152:GLY:N	2.29	0.47
15:O:130:LEU:O	15:O:133:SER:OG	2.31	0.47
16:P:51:ILE:O	16:P:55:LEU:HG	2.14	0.47
16:P:110:ILE:O	16:P:114:THR:HG22	2.15	0.47
16:P:304:LYS:HG3	16:P:305:HIS:CD2	2.50	0.47
18:R:610:LEU:HA	18:R:613:HIS:CD2	2.49	0.47
1:A:38:ASP:OD1	1:A:38:ASP:N	2.41	0.47
1:A:46:ARG:HD3	1:A:278:PRO:HA	1.97	0.47
1:A:223:ASN:ND2	1:A:225:LEU:HB3	2.30	0.47
1:A:450:MET:O	1:A:453:ALA:N	2.48	0.47
1:A:818:ILE:HG21	1:A:866:ILE:HG22	1.95	0.47
1:A:997:GLN:C	1:A:999:ASP:N	2.73	0.47
1:A:1278:ILE:HG23	1:A:1296:GLU:O	2.14	0.47
1:A:1451:LEU:HD23	4:D:107:MET:HB3	1.96	0.47
2:B:244:HIS:HE1	2:B:332:ILE:O	1.97	0.47
2:B:415:GLU:HG3	2:B:416:TYR:N	2.28	0.47
2:B:889:SER:OG	2:B:891:ASN:OD1	2.32	0.47
3:C:122:ASP:CG	3:C:123:ASP:H	2.23	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.14	0.47
18:R:229:LEU:HB2	18:R:244:ILE:HD13	1.96	0.47
21:Y:18:DT:C6	21:Y:18:DT:H5'	2.50	0.47
1:A:573:ARG:O	1:A:577:THR:OG1	2.22	0.47
1:A:903:THR:O	1:A:905:ARG:HG3	2.14	0.47
2:B:657:SER:OG	2:B:671:THR:OG1	2.33	0.47
3:C:173:GLY:C	3:C:175:GLN:H	2.23	0.47
3:C:227:TYR:HB3	3:C:300:PHE:HD1	1.80	0.47
7:G:149:ARG:HB3	7:G:199:SER:O	2.15	0.47
15:O:197:MET:HG3	15:O:286:ARG:HB3	1.96	0.47
15:O:216:GLN:O	15:O:219:TYR:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:127:SER:O	16:P:131:GLN:N	2.37	0.47
16:P:269:LEU:CB	16:P:297:PHE:CE1	2.97	0.47
18:R:191:LEU:CD2	18:R:239:ARG:HE	2.28	0.47
1:A:329:SER:OG	1:A:330:ASP:N	2.48	0.46
1:A:800:LYS:HB3	2:B:951:SER:OG	2.16	0.46
1:A:1202:ILE:HG21	1:A:1224:ILE:HG21	1.97	0.46
2:B:45:TRP:CD1	2:B:739:LYS:HD3	2.50	0.46
2:B:206:ILE:HD13	2:B:374:ASN:HD21	1.81	0.46
2:B:500:ALA:HB3	2:B:685:ALA:HB2	1.97	0.46
2:B:901:ARG:HH22	3:C:94:ASP:HB2	1.79	0.46
7:G:95:GLU:HG3	7:G:96:GLY:N	2.30	0.46
8:H:95:TYR:O	8:H:144:ILE:HB	2.15	0.46
15:O:64:VAL:HG13	15:O:65:ILE:H	1.80	0.46
18:R:623:LYS:HE2	19:S:435:TRP:CD1	2.49	0.46
20:X:16:DA:N6	21:Y:55:DA:H61	2.09	0.46
1:A:449:ARG:O	1:A:450:MET:C	2.56	0.46
1:A:608:GLN:O	1:A:611:SER:N	2.49	0.46
2:B:298:GLN:HG3	13:M:182:PHE:CD2	2.50	0.46
2:B:1040:ARG:HD3	18:R:35:ASN:ND2	2.30	0.46
3:C:1:MET:HB3	3:C:14:ASN:ND2	2.30	0.46
3:C:32:ASN:OD1	3:C:33:VAL:N	2.45	0.46
3:C:33:VAL:C	3:C:35:LYS:N	2.72	0.46
4:D:127:LEU:HD21	7:G:147:ARG:NH1	2.30	0.46
5:E:96:PHE:CZ	5:E:108:GLY:HA3	2.50	0.46
7:G:125:GLU:O	7:G:140:PHE:O	2.34	0.46
12:L:25:ALA:HB2	12:L:37:LYS:NZ	2.30	0.46
16:P:202:PRO:C	16:P:203:LYS:HG2	2.41	0.46
18:R:506:GLY:HA2	18:R:509:SER:O	2.15	0.46
1:A:891:LYS:NZ	2:B:1064:GLU:OE2	2.47	0.46
1:A:1145:LEU:HB2	1:A:1292:GLU:HG3	1.97	0.46
2:B:317:LEU:C	2:B:319:ILE:N	2.71	0.46
2:B:424:VAL:HG23	18:R:89:ALA:O	2.16	0.46
3:C:251:PHE:CD2	3:C:255:VAL:HG21	2.50	0.46
4:D:8:ASN:HB3	7:G:4:LEU:O	2.15	0.46
4:D:58:ILE:O	4:D:62:VAL:N	2.31	0.46
5:E:200:ARG:HD2	5:E:208:TYR:OH	2.14	0.46
8:H:99:GLY:HA3	8:H:118:PHE:HD1	1.80	0.46
12:L:29:TYR:CE1	12:L:56:LEU:HD13	2.50	0.46
13:M:89:GLN:NE2	13:M:178:GLN:HE22	2.06	0.46
15:O:264:THR:HA	15:O:272:ARG:HE	1.79	0.46
15:O:285:ASP:O	15:O:288:MET:HB3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:482:LYS:O	15:O:486:VAL:HG22	2.16	0.46
21:Y:40:DA:H1'	21:Y:41:DG:H5'	1.97	0.46
1:A:378:ARG:HG3	1:A:517:MET:O	2.16	0.46
2:B:58:VAL:HG11	2:B:470:MET:HE2	1.97	0.46
2:B:141:ILE:CG2	2:B:142:ILE:H	2.23	0.46
2:B:167:ASP:OD1	2:B:168:GLU:HG2	2.15	0.46
2:B:212:LYS:HG3	2:B:213:LYS:H	1.80	0.46
2:B:233:VAL:HG22	2:B:234:ILE:N	2.30	0.46
2:B:447:PHE:O	2:B:449:MET:HG2	2.15	0.46
2:B:817:PRO:CG	2:B:822:GLN:OE1	2.64	0.46
3:C:6:GLY:HA3	3:C:13:THR:HB	1.97	0.46
7:G:38:ILE:HB	7:G:44:LEU:HB3	1.97	0.46
7:G:121:TYR:CD2	7:G:127:ALA:O	2.68	0.46
15:O:41:THR:HG22	15:O:42:LEU:N	2.31	0.46
15:O:118:THR:O	15:O:119:TYR:CD2	2.68	0.46
15:O:468:LEU:HG	15:O:478:VAL:HG11	1.97	0.46
16:P:201:GLY:N	16:P:202:PRO:CD	2.78	0.46
19:S:413:ARG:NH1	20:X:11:DA:H3'	2.30	0.46
1:A:235:LYS:HB3	1:A:252:ARG:CZ	2.46	0.46
1:A:251:GLY:O	1:A:252:ARG:HB2	2.15	0.46
1:A:522:PRO:HA	2:B:1082:ARG:NH2	2.30	0.46
2:B:217:GLN:HG3	2:B:232:TYR:HB3	1.98	0.46
2:B:242:LEU:O	2:B:250:GLU:HA	2.16	0.46
15:O:364:ILE:HA	15:O:476:TYR:OH	2.15	0.46
19:S:428:PHE:O	19:S:432:LEU:HG	2.15	0.46
1:A:27:VAL:HG23	1:A:83:HIS:NE2	2.31	0.46
1:A:238:ASP:CG	1:A:239:CYS:H	2.24	0.46
1:A:882:THR:O	1:A:885:MET:HB3	2.16	0.46
1:A:896:LEU:HD11	1:A:912:VAL:HG21	1.98	0.46
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.97	0.46
2:B:295:ILE:HG12	2:B:296:TYR:N	2.30	0.46
2:B:609:CYS:HB3	2:B:648:TYR:HB3	1.98	0.46
2:B:914:SER:C	2:B:916:HIS:N	2.74	0.46
3:C:103:LEU:HD21	10:J:6:ARG:CG	2.45	0.46
4:D:146:ASP:O	4:D:150:ILE:HG12	2.16	0.46
5:E:143:ASN:OD1	5:E:143:ASN:N	2.49	0.46
7:G:4:LEU:HG	7:G:73:ARG:HB3	1.98	0.46
7:G:34:PHE:O	7:G:37:LYS:HB2	2.16	0.46
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.97	0.46
9:I:22:TYR:O	9:I:23:THR:O	2.34	0.46
16:P:218:THR:O	16:P:221:ILE:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:266:GLU:HB3	16:P:269:LEU:HD23	1.98	0.46
18:R:213:TRP:C	18:R:214:MET:HE2	2.40	0.46
18:R:414:HIS:HD2	18:R:615:LEU:O	1.98	0.46
1:A:9:THR:OG1	4:D:1:MET:HE1	2.16	0.46
1:A:88:LEU:HB3	1:A:316:TRP:HE1	1.81	0.46
1:A:373:VAL:CG1	1:A:374:ASP:H	2.26	0.46
1:A:573:ARG:O	1:A:577:THR:CB	2.63	0.46
1:A:1152:ARG:C	1:A:1156:VAL:HG23	2.41	0.46
1:A:1452:SER:HB2	4:D:117:LYS:HZ1	1.81	0.46
2:B:949:PHE:O	2:B:953:MET:N	2.48	0.46
2:B:1147:PHE:CZ	7:G:60:LYS:HB3	2.50	0.46
3:C:5:VAL:HG22	3:C:293:ARG:H	1.80	0.46
3:C:110:PRO:O	3:C:111:ASP:HB2	2.16	0.46
7:G:119:CYS:HB3	7:G:130:TRP:CD1	2.50	0.46
8:H:93:TYR:HB2	8:H:143:LEU:HD11	1.98	0.46
13:M:154:GLU:OE1	13:M:175:ARG:HG2	2.16	0.46
14:N:315:ALA:HB1	14:N:376:GLY:HA3	1.97	0.46
15:O:265:VAL:O	15:O:273:ILE:N	2.25	0.46
18:R:107:TRP:O	18:R:111:ALA:N	2.37	0.46
18:R:416:ARG:HG2	18:R:613:HIS:O	2.16	0.46
21:Y:23:DT:H2''	21:Y:24:DC:C6	2.49	0.46
1:A:124:LEU:HG	1:A:241:LEU:HD21	1.97	0.46
1:A:553:ALA:HB3	1:A:669:LEU:HD13	1.98	0.46
1:A:563:LEU:HD13	1:A:708:ARG:NH1	2.31	0.46
1:A:565:SER:OG	1:A:663:VAL:HA	2.16	0.46
1:A:572:ASP:O	1:A:576:LEU:N	2.35	0.46
1:A:893:LEU:HD13	1:A:1361:VAL:HG21	1.97	0.46
2:B:45:TRP:NE1	2:B:739:LYS:HD3	2.31	0.46
2:B:328:ALA:HA	2:B:331:VAL:O	2.15	0.46
2:B:583:LYS:HG2	2:B:584:VAL:HG13	1.98	0.46
5:E:190:LEU:HD23	5:E:214:CYS:HB2	1.97	0.46
9:I:7:SER:OG	9:I:8:CYS:N	2.45	0.46
9:I:32:GLU:HG2	13:M:132:ASN:HB2	1.98	0.46
15:O:250:ALA:O	15:O:253:ILE:HG13	2.15	0.46
15:O:260:SER:HB3	15:O:264:THR:HG1	1.81	0.46
15:O:295:GLN:HE22	15:O:650:VAL:HB	1.79	0.46
15:O:353:GLU:HB2	15:O:481:SER:HB2	1.98	0.46
15:O:499:THR:HG22	15:O:500:LEU:HD12	1.98	0.46
19:S:461:GLU:OE1	19:S:465:ARG:NH2	2.38	0.46
20:X:7:DA:H4'	20:X:8:DC:OP1	2.16	0.46
21:Y:55:DA:H1'	21:Y:56:DA:C5	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:HZ3	21:Y:7:DC:H3'	1.80	0.46
1:A:307:ILE:HB	1:A:311:ASN:OD1	2.15	0.46
1:A:667:SER:OG	1:A:668:VAL:N	2.48	0.46
1:A:668:VAL:O	1:A:677:VAL:N	2.37	0.46
1:A:1286:ARG:N	1:A:1290:LYS:O	2.41	0.46
1:A:1330:ALA:HB2	5:E:150:VAL:HG22	1.98	0.46
2:B:416:TYR:CE1	18:R:151:GLN:HB3	2.51	0.46
2:B:541:ILE:HA	2:B:544:ILE:CD1	2.46	0.46
2:B:713:ILE:O	2:B:749:LEU:HD13	2.15	0.46
2:B:723:THR:HG23	2:B:724:LEU:N	2.29	0.46
2:B:778:ILE:CD1	2:B:906:PRO:HG2	2.45	0.46
5:E:95:THR:O	5:E:99:HIS:ND1	2.38	0.46
9:I:21:VAL:C	9:I:23:THR:H	2.24	0.46
13:M:149:LYS:HE3	13:M:182:PHE:CZ	2.51	0.46
18:R:402:LEU:HA	18:R:477:LYS:O	2.16	0.46
18:R:478:PHE:O	18:R:599:PRO:HB3	2.16	0.46
21:Y:62:DG:C8	21:Y:63:DT:H72	2.51	0.46
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.97	0.46
1:A:682:LEU:HD13	1:A:687:PRO:HA	1.98	0.46
1:A:822:ARG:NH2	1:A:845:LYS:HB2	2.31	0.46
1:A:829:ASP:OD1	1:A:838:ASN:ND2	2.49	0.46
2:B:297:THR:CA	2:B:301:ALA:HB3	2.44	0.46
3:C:242:GLU:O	3:C:245:ARG:N	2.43	0.46
5:E:66:GLU:HG3	5:E:67:GLU:H	1.81	0.46
6:F:136:ARG:HB2	6:F:144:GLU:HB3	1.96	0.46
9:I:34:PRO:C	9:I:35:ILE:HG13	2.41	0.46
10:J:36:LEU:H	10:J:36:LEU:HD12	1.81	0.46
13:M:86:HIS:O	13:M:87:VAL:HB	2.16	0.46
15:O:128:HIS:CE1	15:O:132:TYR:CE1	3.04	0.46
15:O:307:VAL:HG13	15:O:308:THR:N	2.31	0.46
15:O:494:TYR:CD2	16:P:294:PHE:HE2	2.34	0.46
15:O:573:SER:HA	15:O:576:PHE:HE1	1.80	0.46
15:O:633:ARG:CZ	16:P:308:GLU:HG2	2.46	0.46
16:P:118:GLN:O	16:P:122:LEU:HG	2.16	0.46
18:R:155:TYR:O	18:R:159:ALA:N	2.37	0.46
18:R:402:LEU:HB3	18:R:476:ALA:HA	1.98	0.46
18:R:467:ARG:HB2	18:R:602:LEU:HD11	1.98	0.46
18:R:609:GLU:O	18:R:613:HIS:N	2.47	0.46
1:A:134:ASN:HD21	1:A:1404:LYS:NZ	2.14	0.45
2:B:143:MET:HG2	19:S:399:GLU:HB2	1.97	0.45
2:B:565:ILE:CG1	2:B:566:ARG:N	2.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:GLU:HG3	2:B:648:TYR:HD2	1.80	0.45
2:B:933:PHE:CE2	2:B:1005:TYR:HD2	2.34	0.45
4:D:27:HIS:NE2	4:D:53:PRO:HG3	2.31	0.45
15:O:68:LEU:HD21	15:O:121:TYR:C	2.41	0.45
15:O:623:GLU:O	15:O:627:LEU:HG	2.15	0.45
18:R:617:GLU:HG2	18:R:621:LYS:HE2	1.98	0.45
1:A:559:THR:HG21	2:B:947:HIS:CE1	2.50	0.45
1:A:560:GLY:HA3	1:A:701:CYS:SG	2.56	0.45
2:B:325:GLU:O	2:B:328:ALA:N	2.49	0.45
2:B:589:SER:OG	2:B:653:GLU:HB2	2.15	0.45
2:B:1106:TRP:HE1	7:G:163:PRO:HD3	1.81	0.45
5:E:82:PHE:HZ	5:E:113:GLN:HB2	1.82	0.45
7:G:10:LEU:HA	7:G:69:ASN:HA	1.98	0.45
10:J:2:ILE:H	10:J:2:ILE:HD12	1.81	0.45
11:K:107:THR:HG23	11:K:108:TYR:O	2.17	0.45
13:M:89:GLN:CB	14:N:394:VAL:HG22	2.45	0.45
13:M:148:LEU:HB3	13:M:179:LEU:HD11	1.97	0.45
14:N:389:THR:HG23	14:N:390:PHE:H	1.81	0.45
15:O:190:LEU:HD11	15:O:199:TYR:CE1	2.51	0.45
20:X:7:DA:C5	20:X:8:DC:C4	3.04	0.45
1:A:46:ARG:HH21	2:B:852:ALA:CB	2.29	0.45
1:A:539:ASN:OD1	1:A:687:PRO:HG3	2.16	0.45
1:A:570:PHE:CG	1:A:603:LEU:HD13	2.51	0.45
2:B:300:GLN:O	2:B:303:GLU:N	2.50	0.45
2:B:970:ASN:OD1	2:B:990:ILE:HD13	2.16	0.45
5:E:124:VAL:HG22	5:E:132:ILE:HG12	1.99	0.45
7:G:2:PHE:N	7:G:77:PHE:HA	2.32	0.45
8:H:13:SER:HB3	8:H:27:GLU:O	2.17	0.45
15:O:468:LEU:HG	15:O:478:VAL:CG1	2.46	0.45
15:O:585:MET:HE1	15:O:648:TRP:CB	2.44	0.45
16:P:202:PRO:C	16:P:204:LYS:H	2.22	0.45
18:R:290:PHE:CE2	18:R:495:PRO:HG3	2.52	0.45
20:X:3:DT:C2	20:X:4:DT:N3	2.84	0.45
1:A:508:TYR:O	1:A:509:ASN:OD1	2.34	0.45
1:A:955:LEU:O	1:A:959:ILE:HG13	2.17	0.45
1:A:1225:ILE:N	1:A:1229:ARG:HE	2.13	0.45
1:A:1332:ARG:O	1:A:1335:ILE:N	2.50	0.45
2:B:137:ARG:HG2	2:B:141:ILE:CG1	2.42	0.45
2:B:587:PHE:CE1	2:B:609:CYS:SG	3.09	0.45
2:B:1031:VAL:O	2:B:1034:LYS:N	2.47	0.45
5:E:55:ARG:HD2	5:E:82:PHE:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:60:SER:HA	11:K:106:GLN:HA	1.98	0.45
13:M:79:SER:OG	13:M:170:LEU:O	2.21	0.45
15:O:163:VAL:HG12	15:O:282:ILE:HD11	1.97	0.45
20:X:6:DA:C2	21:Y:65:DG:C2	3.04	0.45
1:A:99:THR:HA	1:A:102:ILE:CG2	2.47	0.45
1:A:302:GLY:C	1:A:304:ASP:N	2.74	0.45
1:A:415:LYS:O	1:A:419:LEU:N	2.49	0.45
1:A:880:ALA:O	21:Y:22:DA:H5'	2.17	0.45
1:A:884:TYR:CZ	1:A:888:ARG:HD3	2.51	0.45
2:B:193:VAL:HG21	2:B:458:LEU:HD12	1.98	0.45
2:B:724:LEU:HD21	2:B:726:TYR:CE2	2.51	0.45
2:B:842:TYR:HB2	2:B:881:ILE:HD11	1.98	0.45
2:B:932:PRO:HB2	2:B:1004:LEU:HD22	1.97	0.45
5:E:132:ILE:HD13	5:E:134:THR:HG23	1.98	0.45
15:O:211:ILE:O	15:O:214:LEU:HG	2.16	0.45
15:O:484:MET:O	15:O:488:LYS:HG2	2.16	0.45
16:P:195:PHE:HB3	16:P:201:GLY:HA3	1.97	0.45
18:R:268:ALA:O	18:R:272:VAL:HB	2.17	0.45
20:X:28:DT:H2''	20:X:29:DC:C6	2.51	0.45
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.97	0.45
1:A:89:PRO:CG	1:A:225:LEU:HA	2.46	0.45
1:A:114:LEU:HD22	1:A:161:ASN:HD21	1.82	0.45
1:A:205:LEU:HG	1:A:212:GLU:HA	1.97	0.45
2:B:832:VAL:HG13	2:B:882:ASP:O	2.17	0.45
2:B:841:ILE:HD13	2:B:872:ILE:HA	1.99	0.45
2:B:1147:PHE:CD2	7:G:10:LEU:HD11	2.52	0.45
5:E:90:VAL:O	5:E:94:LYS:HG2	2.17	0.45
13:M:85:LEU:HD23	13:M:86:HIS:N	2.32	0.45
13:M:155:ASN:OD1	13:M:155:ASN:N	2.49	0.45
14:N:361:GLY:HA3	14:N:375:ILE:HA	1.98	0.45
1:A:584:SER:C	1:A:586:GLY:H	2.25	0.45
1:A:894:GLU:OE2	1:A:1412:SER:HB3	2.17	0.45
1:A:1202:ILE:O	1:A:1205:ILE:N	2.50	0.45
2:B:167:ASP:C	2:B:169:SER:H	2.24	0.45
2:B:392:PHE:O	2:B:395:PHE:HB3	2.17	0.45
7:G:194:TYR:CZ	7:G:196:LEU:HD11	2.51	0.45
1:A:88:LEU:HD11	1:A:303:LEU:HD13	1.98	0.45
1:A:678:PHE:CE2	1:A:694:MET:HG2	2.52	0.45
1:A:856:LEU:HD23	1:A:861:PHE:HA	1.98	0.45
1:A:988:ASP:OD1	1:A:992:ALA:N	2.50	0.45
1:A:1125:ARG:HH12	1:A:1136:ILE:HD11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:ILE:HG22	1:A:1218:GLN:N	2.30	0.45
2:B:591:TYR:CD1	2:B:652:ASN:HB3	2.52	0.45
2:B:617:ASP:CG	2:B:618:GLY:H	2.25	0.45
3:C:157:TYR:HE2	3:C:197:ARG:NH1	2.15	0.45
5:E:100:ILE:HG21	5:E:127:ILE:HG13	1.99	0.45
9:I:13:LEU:HD21	9:I:27:ARG:HB2	1.99	0.45
14:N:395:ILE:HD12	14:N:411:ARG:CA	2.45	0.45
15:O:45:ASP:H	15:O:582:GLU:CD	2.17	0.45
15:O:185:TYR:O	15:O:189:SER:HA	2.17	0.45
16:P:175:ILE:HG22	16:P:179:LEU:HD13	1.98	0.45
1:A:89:PRO:CB	1:A:228:LEU:HD23	2.46	0.45
1:A:90:VAL:HG23	1:A:320:GLN:HB3	1.98	0.45
1:A:1023:ARG:HG2	1:A:1028:MET:HB2	1.97	0.45
3:C:25:LYS:HE2	8:H:82:PRO:HG2	1.98	0.45
3:C:88:ASN:OD1	3:C:89:THR:N	2.49	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
12:L:56:LEU:HD12	12:L:56:LEU:O	2.17	0.45
13:M:84:SER:HB3	13:M:85:LEU:H	1.60	0.45
14:N:385:GLY:O	14:N:416:ILE:HG13	2.17	0.45
15:O:37:LEU:HA	15:O:40:ARG:HB3	1.99	0.45
15:O:579:GLN:HG3	15:O:580:ASN:N	2.32	0.45
15:O:583:TRP:CZ3	16:P:315:TRP:HB2	2.51	0.45
16:P:82:LYS:O	16:P:86:MET:HG2	2.17	0.45
16:P:107:SER:O	16:P:110:ILE:HG22	2.17	0.45
16:P:269:LEU:HA	16:P:297:PHE:CE2	2.52	0.45
1:A:385:PRO:HG3	2:B:764:GLY:C	2.42	0.45
1:A:545:LYS:HA	1:A:1354:HIS:HE1	1.81	0.45
1:A:591:ASP:HB2	8:H:77:ARG:O	2.17	0.45
1:A:801:GLY:N	2:B:951:SER:OG	2.49	0.45
1:A:858:PRO:HA	2:B:979:PHE:CZ	2.52	0.45
1:A:862:LEU:O	1:A:866:ILE:HG12	2.17	0.45
1:A:873:VAL:CG2	2:B:487:ARG:HG2	2.46	0.45
1:A:884:TYR:CE2	1:A:888:ARG:HD3	2.52	0.45
1:A:957:TYR:OH	1:A:1040:GLN:NE2	2.50	0.45
1:A:1235:PHE:HB2	1:A:1236:PRO:HD2	1.98	0.45
2:B:256:VAL:O	2:B:260:CYS:N	2.43	0.45
2:B:316:LYS:NZ	13:M:226:ARG:NE	2.65	0.45
2:B:612:LEU:HD21	2:B:649:LEU:HD12	2.00	0.45
3:C:133:VAL:HG11	3:C:172:GLN:HE22	1.82	0.45
3:C:245:ARG:O	3:C:248:GLN:HG2	2.17	0.45
5:E:43:LYS:O	5:E:47:CYS:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:MET:O	6:F:104:ASN:HB3	2.17	0.45
10:J:8:PHE:N	10:J:49:MET:HE1	2.31	0.45
13:M:112:TYR:H	13:M:243:ILE:CG2	2.30	0.45
15:O:41:THR:C	15:O:43:ASN:H	2.25	0.45
15:O:318:LEU:HD21	15:O:368:ARG:CZ	2.47	0.45
15:O:353:GLU:H	15:O:481:SER:CB	2.29	0.45
15:O:495:VAL:CG1	15:O:647:LEU:HD11	2.47	0.45
18:R:214:MET:HE1	18:R:286:ARG:C	2.42	0.45
18:R:397:VAL:HG21	20:X:16:DA:C2	2.52	0.45
20:X:18:DT:H71	20:X:19:DA:H62	1.82	0.45
1:A:114:LEU:HD11	1:A:148:CYS:HB2	1.99	0.44
1:A:1165:LEU:O	1:A:1169:VAL:N	2.48	0.44
1:A:1224:ILE:HG12	1:A:1226:GLY:N	2.32	0.44
1:A:1365:LYS:HE3	1:A:1379:MET:HB2	1.98	0.44
2:B:55:LYS:HD2	2:B:519:HIS:CD2	2.52	0.44
2:B:100:VAL:HG12	2:B:129:ILE:HD13	1.98	0.44
2:B:378:GLU:OE1	2:B:383:LEU:HD13	2.17	0.44
2:B:715:TYR:HA	10:J:60:PHE:HE1	1.82	0.44
5:E:72:PHE:HE1	5:E:157:SER:HA	1.82	0.44
15:O:352:VAL:N	15:O:481:SER:OG	2.50	0.44
16:P:222:LEU:HA	16:P:225:ILE:HB	2.00	0.44
17:Q:55:ALA:O	17:Q:58:TYR:HB3	2.17	0.44
21:Y:25:DT:H2'	21:Y:26:DT:C5	2.51	0.44
1:A:49:LYS:CD	1:A:54:LEU:HB3	2.47	0.44
1:A:155:LEU:HD12	1:A:156:HIS:N	2.31	0.44
1:A:204:VAL:O	1:A:208:ASN:N	2.27	0.44
2:B:311:THR:HG23	2:B:313:ARG:H	1.82	0.44
2:B:1007:GLY:HA2	3:C:68:ARG:NH2	2.32	0.44
4:D:11:LEU:H	7:G:3:ILE:HG22	1.82	0.44
5:E:115:ASN:OD1	5:E:116:ILE:N	2.50	0.44
6:F:108:PHE:HE2	6:F:131:PRO:HG3	1.82	0.44
7:G:207:LEU:HB3	7:G:210:TRP:CE2	2.52	0.44
15:O:95:LEU:HD21	15:O:120:TYR:CE1	2.52	0.44
15:O:495:VAL:C	15:O:496:ILE:CG1	2.77	0.44
15:O:507:LEU:HD21	15:O:536:THR:HG23	1.99	0.44
15:O:650:VAL:HG13	15:O:651:PHE:H	1.82	0.44
16:P:102:ARG:O	16:P:155:PRO:HG2	2.17	0.44
16:P:106:TRP:O	16:P:109:THR:HG22	2.17	0.44
18:R:2:PRO:HG2	18:R:12:PHE:CE2	2.52	0.44
18:R:211:LYS:HE2	18:R:282:ASP:HB3	1.99	0.44
18:R:391:PRO:HA	18:R:490:CYS:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:23:DT:C2	21:Y:24:DC:H5	2.35	0.44
1:A:66:GLU:HB3	1:A:71:HIS:CB	2.48	0.44
1:A:92:HIS:CD2	1:A:258:TRP:NE1	2.85	0.44
1:A:234:ILE:O	1:A:234:ILE:CG2	2.64	0.44
1:A:342:ASN:ND2	21:Y:38:DA:H2''	2.33	0.44
1:A:481:HIS:HA	1:A:1095:GLN:OE1	2.17	0.44
1:A:881:GLU:OE2	1:A:1127:LYS:NZ	2.46	0.44
1:A:1199:GLU:HG2	5:E:3:GLN:HE22	1.81	0.44
2:B:467:LEU:HA	2:B:470:MET:HB3	1.98	0.44
2:B:884:VAL:HG22	12:L:58:LYS:HB3	1.99	0.44
2:B:991:LEU:O	2:B:994:GLN:N	2.50	0.44
3:C:77:SER:OG	3:C:221:PRO:HB3	2.17	0.44
5:E:143:ASN:CG	5:E:146:HIS:HB3	2.42	0.44
14:N:305:MET:HE3	14:N:414:GLY:HA3	1.99	0.44
21:Y:49:DA:H5'	21:Y:49:DA:H8	1.79	0.44
1:A:235:LYS:C	1:A:252:ARG:HD3	2.40	0.44
1:A:753:GLN:OE1	1:A:761:THR:HG23	2.17	0.44
1:A:1446:CYS:HB2	4:D:14:TYR:OH	2.17	0.44
2:B:410:PRO:HA	2:B:414:MET:SD	2.57	0.44
2:B:586:GLU:O	2:B:587:PHE:O	2.34	0.44
2:B:1138:ALA:O	2:B:1140:ARG:N	2.50	0.44
3:C:40:PHE:CD1	3:C:59:ILE:HG23	2.52	0.44
3:C:108:VAL:HB	3:C:184:VAL:HG12	1.99	0.44
5:E:42:PHE:CE1	5:E:46:TYR:HD2	2.36	0.44
5:E:200:ARG:HD2	5:E:208:TYR:CZ	2.52	0.44
8:H:6:PHE:HB3	8:H:59:ILE:HG13	1.99	0.44
9:I:29:CYS:C	13:M:135:LYS:HE2	2.43	0.44
15:O:273:ILE:HG23	15:O:274:VAL:O	2.17	0.44
15:O:506:ARG:NH2	15:O:527:LEU:O	2.50	0.44
15:O:507:LEU:HD12	15:O:508:SER:N	2.32	0.44
15:O:517:VAL:HG23	15:O:521:ILE:HD11	1.98	0.44
18:R:486:ILE:N	18:R:543:ALA:O	2.50	0.44
1:A:34:VAL:HG13	1:A:35:SER:N	2.32	0.44
1:A:363:ARG:O	1:A:367:ASN:HB3	2.16	0.44
1:A:624:ILE:N	1:A:657:SER:OG	2.48	0.44
2:B:123:MET:O	2:B:189:GLY:N	2.50	0.44
2:B:244:HIS:HE1	2:B:332:ILE:C	2.26	0.44
2:B:247:ILE:HG13	2:B:248:ALA:H	1.83	0.44
2:B:369:ARG:HG3	2:B:369:ARG:O	2.17	0.44
2:B:493:GLN:CG	2:B:497:LEU:HB2	2.48	0.44
2:B:773:LEU:HD21	2:B:912:PHE:HE2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:833:GLY:HA3	12:L:60:ARG:CZ	2.47	0.44
2:B:842:TYR:HD2	2:B:873:TYR:HB2	1.81	0.44
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.99	0.44
5:E:94:LYS:O	5:E:98:ILE:HG12	2.17	0.44
9:I:24:LEU:O	9:I:33:PHE:HB2	2.18	0.44
11:K:127:LEU:O	11:K:130:VAL:N	2.50	0.44
13:M:132:ASN:OD1	13:M:134:ASP:HB2	2.17	0.44
14:N:286:ASP:OD2	14:N:384:LYS:HB3	2.16	0.44
15:O:32:MET:O	15:O:34:ILE:N	2.51	0.44
15:O:118:THR:O	15:O:119:TYR:CG	2.70	0.44
15:O:292:ARG:HG2	15:O:325:LYS:HD2	1.98	0.44
15:O:578:ARG:HH21	15:O:652:GLN:HA	1.81	0.44
15:O:620:LEU:HD23	15:O:623:GLU:HB2	2.00	0.44
15:O:650:VAL:HG13	15:O:651:PHE:N	2.32	0.44
18:R:251:ALA:HB3	18:R:254:THR:OG1	2.18	0.44
20:X:9:DA:C5	20:X:10:DT:C4	3.05	0.44
20:X:14:DT:H2''	20:X:15:DT:H5'	1.99	0.44
1:A:614:ILE:O	1:A:622:VAL:HG21	2.18	0.44
1:A:940:ASP:O	1:A:943:TYR:N	2.50	0.44
1:A:943:TYR:O	1:A:947:PHE:N	2.50	0.44
1:A:1026:ARG:NH2	1:A:1055:SER:OG	2.51	0.44
2:B:553:TYR:HD1	2:B:597:MET:HB3	1.83	0.44
2:B:658:TYR:HE2	2:B:670:MET:HG2	1.78	0.44
2:B:860:VAL:HG13	2:B:861:ASN:N	2.33	0.44
2:B:1055:SER:OG	2:B:1056:ARG:N	2.51	0.44
2:B:1145:ASP:OD1	2:B:1145:ASP:N	2.49	0.44
3:C:256:ILE:HD13	3:C:265:ALA:HB1	1.99	0.44
7:G:157:ASP:CG	7:G:158:VAL:H	2.25	0.44
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.82	0.44
13:M:245:LEU:CD2	14:N:405:SER:OG	2.59	0.44
18:R:198:VAL:HA	18:R:201:ASP:HB2	1.99	0.44
18:R:213:TRP:NE1	18:R:495:PRO:HB3	2.30	0.44
18:R:220:PRO:HD3	18:R:514:GLU:HB2	2.00	0.44
18:R:511:TYR:HB2	18:R:519:LEU:CD1	2.48	0.44
18:R:604:ASP:OD1	18:R:605:VAL:N	2.51	0.44
1:A:153:ARG:CZ	15:O:338:ASP:HA	2.47	0.44
1:A:555:GLN:HG2	1:A:800:LYS:HD3	2.00	0.44
1:A:683:ARG:HH12	1:A:925:GLU:HB2	1.82	0.44
1:A:813:VAL:O	1:A:848:VAL:HG13	2.18	0.44
1:A:1083:LEU:HA	1:A:1083:LEU:HD23	1.63	0.44
1:A:1299:GLY:O	1:A:1301:ARG:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:ILE:O	1:A:1331:ALA:N	2.51	0.44
2:B:305:ILE:CG2	2:B:325:GLU:HG2	2.47	0.44
2:B:710:ILE:HG13	2:B:728:MET:HE3	1.99	0.44
2:B:738:THR:O	2:B:741:ILE:N	2.51	0.44
3:C:81:GLU:OE2	12:L:70:ARG:NH1	2.49	0.44
3:C:89:THR:CG2	3:C:201:GLU:H	2.31	0.44
3:C:113:LEU:HD21	3:C:132:ILE:HD12	1.99	0.44
4:D:11:LEU:HB3	7:G:3:ILE:HA	1.99	0.44
7:G:203:ASP:OD1	7:G:204:GLY:N	2.40	0.44
13:M:183:PHE:C	13:M:185:TYR:N	2.74	0.44
15:O:64:VAL:HG13	15:O:65:ILE:N	2.33	0.44
18:R:130:LEU:HD23	18:R:146:PHE:HE1	1.82	0.44
18:R:198:VAL:O	18:R:202:ALA:N	2.33	0.44
18:R:424:ARG:HH21	21:Y:51:DT:H5''	1.83	0.44
19:S:420:TRP:CD1	19:S:457:LYS:HD2	2.52	0.44
21:Y:18:DT:H6	21:Y:18:DT:H2'	1.58	0.44
1:A:234:ILE:CD1	1:A:237:ALA:HB3	2.40	0.44
1:A:360:LYS:NZ	21:Y:21:DT:OP2	2.51	0.44
1:A:361:GLN:N	1:A:361:GLN:OE1	2.51	0.44
1:A:1078:TYR:O	1:A:1081:ALA:N	2.51	0.44
1:A:1332:ARG:NH2	5:E:200:ARG:NE	2.66	0.44
2:B:317:LEU:O	2:B:318:THR:C	2.60	0.44
2:B:804:ASP:OD1	2:B:804:ASP:N	2.51	0.44
15:O:454:ASN:O	15:O:457:LEU:HB3	2.18	0.44
18:R:398:ALA:HB3	18:R:449:VAL:HB	2.00	0.44
19:S:382:ASP:C	19:S:384:HIS:H	2.26	0.44
19:S:502:LEU:HD12	19:S:505:LEU:HD23	1.99	0.44
19:S:509:HIS:HA	19:S:512:HIS:HB3	1.99	0.44
21:Y:44:DA:C6	21:Y:45:DA:C6	3.05	0.44
1:A:590:PHE:O	11:K:106:GLN:NE2	2.51	0.44
1:A:665:ASP:OD2	1:A:797:CYS:HB3	2.18	0.44
1:A:774:ARG:NH2	1:A:808:GLN:HE21	2.15	0.44
2:B:260:CYS:O	2:B:342:PHE:HB3	2.18	0.44
2:B:553:TYR:HA	2:B:597:MET:HB3	1.99	0.44
2:B:732:GLN:HB3	10:J:52:THR:HG22	1.99	0.44
2:B:824:LEU:O	2:B:831:GLU:HB3	2.18	0.44
3:C:95:GLU:HA	12:L:67:PHE:CE2	2.53	0.44
3:C:270:ALA:C	3:C:272:LYS:H	2.26	0.44
5:E:24:LYS:HB2	5:E:30:ILE:HD11	2.00	0.44
5:E:191:LYS:N	5:E:194:GLU:OE1	2.38	0.44
6:F:108:PHE:CE2	6:F:131:PRO:HG3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:151:LEU:HD23	6:F:152:ILE:N	2.32	0.44
7:G:101:LEU:HB3	7:G:104:ILE:CG2	2.48	0.44
16:P:59:ASN:CG	16:P:80:ALA:HB1	2.43	0.44
16:P:296:TYR:CZ	16:P:297:PHE:CD1	3.04	0.44
18:R:116:PHE:CE2	18:R:164:MET:HB3	2.53	0.44
19:S:414:GLY:HA3	20:X:11:DA:OP1	2.18	0.44
1:A:107:CYS:N	1:A:114:LEU:HD23	2.33	0.43
1:A:378:ARG:NH1	1:A:518:ASN:HD21	2.12	0.43
1:A:890:MET:HE3	1:A:890:MET:HB2	1.47	0.43
2:B:209:ALA:HA	2:B:215:ILE:HA	1.99	0.43
15:O:470:GLU:HB2	15:O:479:PRO:CG	2.36	0.43
15:O:495:VAL:HG11	15:O:647:LEU:HD11	2.00	0.43
15:O:583:TRP:CE3	15:O:583:TRP:HA	2.53	0.43
16:P:185:PHE:HE2	16:P:217:THR:HG22	1.83	0.43
18:R:191:LEU:HD21	18:R:237:LEU:HD13	2.00	0.43
18:R:417:ASN:O	18:R:430:MET:HG2	2.18	0.43
20:X:19:DA:H1'	20:X:20:DA:O4'	2.17	0.43
1:A:151:GLN:O	1:A:152:ARG:NH1	2.51	0.43
1:A:675:HIS:O	1:A:676:SER:OG	2.36	0.43
1:A:715:ASN:OD1	1:A:716:ASP:N	2.52	0.43
1:A:781:CYS:O	1:A:785:LEU:HB2	2.18	0.43
2:B:217:GLN:NE2	2:B:352:MET:HE3	2.33	0.43
2:B:954:THR:HG23	2:B:954:THR:O	2.18	0.43
3:C:95:GLU:HG3	3:C:96:VAL:N	2.33	0.43
7:G:38:ILE:HD11	7:G:43:GLY:HA2	2.00	0.43
13:M:74:PHE:HE2	14:N:364:ARG:HD2	1.83	0.43
15:O:362:ASN:O	15:O:477:TYR:HD1	2.00	0.43
15:O:505:MET:O	15:O:509:ARG:N	2.41	0.43
15:O:515:LYS:O	15:O:516:LEU:O	2.36	0.43
1:A:30:SER:OG	1:A:83:HIS:ND1	2.50	0.43
1:A:256:TYR:CD2	1:A:1401:PHE:HE1	2.34	0.43
1:A:506:THR:OG1	1:A:507:PRO:HD3	2.18	0.43
1:A:606:GLY:HA2	1:A:609:VAL:HG12	1.99	0.43
1:A:1165:LEU:HB3	1:A:1169:VAL:HG23	1.99	0.43
2:B:96:VAL:HG13	2:B:97:ASP:H	1.83	0.43
2:B:534:TYR:HA	2:B:538:VAL:HG22	1.99	0.43
2:B:544:ILE:HG22	2:B:546:SER:H	1.84	0.43
2:B:710:ILE:HG12	2:B:1026:LYS:O	2.16	0.43
2:B:795:LEU:HB2	2:B:894:ALA:HB3	2.00	0.43
3:C:15:THR:O	3:C:295:ARG:HD3	2.19	0.43
3:C:35:LYS:HD2	3:C:35:LYS:HA	1.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:TYR:HE2	3:C:197:ARG:HH11	1.66	0.43
3:C:209:ILE:HG13	3:C:210:LEU:N	2.33	0.43
4:D:61:ASN:O	4:D:64:ASN:HB3	2.18	0.43
5:E:171:LYS:H	5:E:174:GLN:NE2	2.15	0.43
15:O:264:THR:HA	15:O:272:ARG:NE	2.32	0.43
15:O:287:PHE:HE2	15:O:291:ARG:HH11	1.65	0.43
15:O:547:GLU:HG2	15:O:548:ILE:N	2.20	0.43
18:R:97:PRO:HD2	18:R:100:ILE:HD12	1.99	0.43
18:R:622:LEU:HD22	19:S:483:GLU:OE2	2.18	0.43
20:X:13:DA:H2'	20:X:14:DT:H71	2.00	0.43
1:A:51:ASN:OD1	1:A:52:GLY:N	2.51	0.43
1:A:167:ALA:HB1	15:O:557:ARG:CD	2.48	0.43
1:A:616:PRO:HG3	1:A:696:ARG:NH1	2.34	0.43
1:A:835:PHE:C	2:B:658:TYR:HE1	2.27	0.43
2:B:306:GLY:CA	2:B:325:GLU:HB2	2.49	0.43
2:B:427:ASN:O	2:B:431:SER:N	2.51	0.43
3:C:89:THR:HG21	3:C:200:GLN:HA	2.00	0.43
5:E:178:ILE:HG13	5:E:212:ARG:HD3	2.00	0.43
15:O:105:LYS:HE3	15:O:123:ASN:OD1	2.18	0.43
15:O:183:MET:C	15:O:187:ILE:HG12	2.43	0.43
15:O:310:GLN:NE2	15:O:313:LYS:HD3	2.33	0.43
15:O:573:SER:HA	15:O:576:PHE:CE1	2.54	0.43
15:O:623:GLU:OE1	15:O:624:LEU:HD12	2.19	0.43
16:P:296:TYR:CE1	16:P:297:PHE:HB3	2.53	0.43
18:R:516:PHE:CG	18:R:517:PRO:HD2	2.53	0.43
1:A:298:LEU:HD21	1:A:315:HIS:CE1	2.54	0.43
1:A:347:VAL:HG12	1:A:349:PRO:HD2	2.00	0.43
1:A:351:ARG:HD2	1:A:355:GLN:HG2	2.00	0.43
1:A:476:ARG:HA	1:A:517:MET:SD	2.58	0.43
1:A:562:TYR:HE1	1:A:663:VAL:HG21	1.84	0.43
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.30	0.43
2:B:765:TYR:CD2	2:B:924:ILE:HG12	2.53	0.43
3:C:231:PRO:HB3	3:C:275:VAL:CG2	2.48	0.43
9:I:22:TYR:C	9:I:23:THR:CG2	2.91	0.43
15:O:271:LEU:HD23	15:O:272:ARG:H	1.84	0.43
15:O:538:ALA:O	15:O:541:ILE:HG22	2.19	0.43
16:P:183:TRP:O	16:P:187:SER:HB3	2.18	0.43
20:X:4:DT:H2'	20:X:5:DC:O5'	2.15	0.43
20:X:31:DG:H8	20:X:31:DG:O5'	2.01	0.43
21:Y:39:DC:H6	21:Y:39:DC:H2'	1.69	0.43
1:A:207:HIS:O	1:A:209:PRO:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HA	1:A:487:SER:HA	2.00	0.43
1:A:712:ILE:O	2:B:1001:LYS:NZ	2.49	0.43
1:A:730:LEU:O	1:A:733:ILE:HG22	2.18	0.43
2:B:112:LEU:HD23	2:B:113:THR:H	1.83	0.43
2:B:612:LEU:HA	2:B:675:ILE:HG23	2.01	0.43
2:B:696:SER:OG	2:B:697:PRO:HD3	2.19	0.43
2:B:763:SER:CB	2:B:765:TYR:H	2.31	0.43
13:M:121:ILE:HG21	13:M:179:LEU:HD21	2.01	0.43
13:M:126:ASP:HB2	13:M:129:ALA:HB2	1.99	0.43
16:P:175:ILE:HG22	16:P:179:LEU:CD1	2.49	0.43
18:R:171:THR:HG23	18:R:172:GLU:N	2.32	0.43
18:R:192:ALA:O	18:R:195:LYS:NZ	2.48	0.43
20:X:30:DT:H2''	20:X:31:DG:N7	2.33	0.43
1:A:541:LEU:HD11	1:A:694:MET:CE	2.49	0.43
1:A:753:GLN:HE22	1:A:765:LYS:HE2	1.83	0.43
2:B:324:ILE:HG23	2:B:325:GLU:N	2.33	0.43
2:B:496:MET:HG2	2:B:610:ARG:HD2	2.00	0.43
2:B:667:VAL:C	2:B:669:SER:H	2.27	0.43
3:C:152:ASP:HB3	3:C:155:GLU:OE1	2.18	0.43
3:C:244:ALA:O	3:C:247:PHE:HB3	2.19	0.43
5:E:157:SER:HB2	5:E:160:GLU:HG3	1.99	0.43
7:G:12:ARG:NH2	7:G:65:SER:OG	2.51	0.43
12:L:31:CYS:CB	12:L:34:CYS:HB2	2.49	0.43
15:O:347:ASP:HA	15:O:350:GLU:HG2	1.99	0.43
15:O:358:GLY:HA2	15:O:361:PHE:CD2	2.53	0.43
15:O:367:ALA:HB2	15:O:453:ILE:HD13	2.01	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.88	0.43
16:P:149:MET:SD	16:P:155:PRO:HD2	2.59	0.43
18:R:195:LYS:O	18:R:198:VAL:HB	2.18	0.43
18:R:470:GLN:HG2	18:R:475:ALA:O	2.18	0.43
18:R:619:ALA:O	18:R:623:LYS:HB2	2.18	0.43
19:S:517:GLU:O	19:S:520:LYS:HB3	2.18	0.43
20:X:30:DT:H3	21:Y:40:DA:N6	2.16	0.43
21:Y:59:DT:C2	21:Y:60:DA:C8	3.06	0.43
1:A:21:LEU:HD11	2:B:1133:LEU:HD11	2.00	0.43
1:A:228:LEU:HD12	1:A:229:ASN:CA	2.48	0.43
1:A:848:VAL:HG23	1:A:860:GLU:OE1	2.19	0.43
2:B:734:PRO:HB3	2:B:1023:TYR:CD2	2.53	0.43
2:B:774:ASN:HB2	2:B:941:ASP:O	2.19	0.43
2:B:803:GLN:O	2:B:805:ILE:HG12	2.18	0.43
5:E:80:VAL:HA	5:E:109:ILE:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:HIS:HB3	5:E:196:VAL:HG21	2.00	0.43
8:H:95:TYR:CZ	8:H:97:MET:SD	3.12	0.43
9:I:29:CYS:HA	13:M:183:PHE:HE2	1.84	0.43
15:O:125:GLU:C	15:O:127:ILE:H	2.25	0.43
15:O:175:LEU:HD21	15:O:184:LYS:HD3	2.00	0.43
15:O:289:LYS:NZ	15:O:320:GLU:HA	2.34	0.43
16:P:98:GLU:HB2	16:P:150:LEU:HD11	2.01	0.43
16:P:145:ARG:HB3	16:P:147:ILE:HG23	2.01	0.43
18:R:601:ASN:HB3	18:R:604:ASP:OD2	2.18	0.43
1:A:228:LEU:C	1:A:228:LEU:CD1	2.85	0.43
1:A:496:ARG:O	1:A:497:THR:HB	2.18	0.43
1:A:594:PRO:HB3	8:H:79:TRP:CD1	2.54	0.43
1:A:645:MET:SD	8:H:124:ARG:HB2	2.59	0.43
1:A:911:ILE:HG22	5:E:174:GLN:O	2.18	0.43
1:A:1272:VAL:HG13	1:A:1273:LYS:N	2.32	0.43
1:A:1441:LEU:HD23	7:G:53:THR:H	1.84	0.43
2:B:694:ASN:OD1	2:B:916:HIS:NE2	2.51	0.43
2:B:786:GLU:HA	2:B:903:ASN:HA	2.00	0.43
5:E:9:ILE:HD13	5:E:43:LYS:HD3	2.00	0.43
8:H:56:THR:HB	8:H:145:ARG:HG3	2.01	0.43
13:M:117:HIS:CG	13:M:118:LEU:N	2.87	0.43
15:O:282:ILE:H	15:O:282:ILE:HD12	1.84	0.43
15:O:483:LEU:HA	15:O:486:VAL:HG22	2.01	0.43
18:R:627:TRP:O	18:R:631:ASN:ND2	2.36	0.43
19:S:479:PRO:HB3	19:S:483:GLU:HB2	2.00	0.43
20:X:16:DA:H2"	20:X:17:DG:N9	2.34	0.43
1:A:8:GLU:OE1	1:A:8:GLU:N	2.51	0.43
1:A:857:SER:O	1:A:860:GLU:HG2	2.19	0.43
1:A:1224:ILE:HG13	1:A:1229:ARG:H	1.83	0.43
2:B:338:GLU:CD	2:B:339:ALA:N	2.76	0.43
2:B:403:ILE:HD12	2:B:403:ILE:HA	1.77	0.43
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.53	0.43
15:O:69:VAL:HG22	15:O:122:TYR:CD1	2.54	0.43
15:O:470:GLU:O	15:O:479:PRO:HD3	2.17	0.43
18:R:267:ALA:O	18:R:271:SER:OG	2.33	0.43
21:Y:20:DT:C5	21:Y:21:DT:C5	3.07	0.43
21:Y:45:DA:C6	21:Y:46:DA:C6	3.06	0.43
1:A:295:THR:O	1:A:298:LEU:HB3	2.19	0.42
1:A:792:LEU:HD11	8:H:19:ARG:NH2	2.33	0.42
1:A:816:GLN:N	1:A:846:GLY:O	2.52	0.42
1:A:822:ARG:NE	1:A:845:LYS:HB2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:GLN:CD	2:B:60:GLN:N	2.77	0.42
2:B:77:ILE:HG13	2:B:78:LYS:N	2.34	0.42
2:B:86:ASP:O	16:P:117:HIS:CD2	2.72	0.42
2:B:1095:CYS:O	2:B:1099:GLY:HA2	2.19	0.42
3:C:19:ASP:HB2	3:C:29:ASN:ND2	2.34	0.42
3:C:77:SER:O	3:C:210:LEU:HD12	2.19	0.42
3:C:152:ASP:O	3:C:154:LYS:N	2.49	0.42
3:C:209:ILE:HD12	3:C:209:ILE:HA	1.92	0.42
4:D:24:GLU:OE2	4:D:30:ASP:N	2.25	0.42
6:F:136:ARG:O	6:F:143:PHE:C	2.62	0.42
8:H:100:THR:OG1	8:H:138:GLU:HA	2.19	0.42
13:M:72:GLU:OE1	14:N:364:ARG:NH2	2.51	0.42
13:M:115:LYS:O	13:M:175:ARG:NH2	2.52	0.42
18:R:434:GLU:HA	18:R:436:LYS:N	2.33	0.42
1:A:336:MET:HG3	1:A:337:LEU:O	2.20	0.42
1:A:432:TYR:HD1	1:A:443:ASN:HA	1.84	0.42
1:A:1122:GLY:C	1:A:1124:PRO:HD2	2.43	0.42
1:A:1164:THR:CB	1:A:1271:VAL:HA	2.48	0.42
2:B:234:ILE:HG13	2:B:240:ILE:HG22	1.99	0.42
2:B:254:ALA:O	2:B:258:LYS:HG2	2.19	0.42
4:D:129:ALA:HB3	4:D:157:ILE:HG21	2.01	0.42
5:E:81:GLU:O	5:E:110:PHE:HA	2.20	0.42
15:O:500:LEU:HD11	15:O:543:TYR:CD2	2.54	0.42
15:O:547:GLU:O	15:O:548:ILE:HG13	2.19	0.42
15:O:591:LYS:HD3	16:P:308:GLU:HG3	2.01	0.42
18:R:590:THR:O	18:R:594:LYS:HG3	2.19	0.42
1:A:302:GLY:O	1:A:304:ASP:N	2.52	0.42
1:A:381:ILE:CD1	1:A:517:MET:HE2	2.50	0.42
1:A:496:ARG:HB2	2:B:1035:MET:SD	2.59	0.42
1:A:811:ALA:O	1:A:851:SER:OG	2.37	0.42
1:A:1024:LYS:HG3	1:A:1025:SER:N	2.35	0.42
2:B:228:LYS:HD3	2:B:244:HIS:HE2	1.85	0.42
2:B:553:TYR:HB3	2:B:598:ALA:N	2.34	0.42
3:C:229:LEU:HB3	3:C:293:ARG:NH1	2.34	0.42
6:F:81:THR:HG22	6:F:82:THR:N	2.34	0.42
7:G:203:ASP:HB3	7:G:211:TRP:NE1	2.33	0.42
7:G:207:LEU:HB3	7:G:210:TRP:CD2	2.54	0.42
8:H:95:TYR:OH	8:H:97:MET:SD	2.69	0.42
14:N:282:LEU:HA	14:N:285:ALA:HB3	2.01	0.42
14:N:310:PRO:HG2	14:N:420:PRO:HD3	2.00	0.42
15:O:133:SER:HB2	17:Q:58:TYR:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:271:LEU:HD23	15:O:272:ARG:N	2.34	0.42
15:O:496:ILE:HA	15:O:499:THR:HB	2.01	0.42
18:R:218:ARG:C	18:R:514:GLU:CG	2.92	0.42
18:R:511:TYR:HB2	18:R:519:LEU:HD12	2.01	0.42
20:X:3:DT:H2''	20:X:4:DT:OP2	2.19	0.42
1:A:366:GLY:O	2:B:1061:ARG:NH1	2.45	0.42
1:A:388:SER:OG	1:A:389:ILE:N	2.52	0.42
1:A:1189:ASP:OD2	1:A:1192:THR:N	2.53	0.42
2:B:87:VAL:O	2:B:88:ASP:C	2.62	0.42
2:B:555:VAL:CG1	2:B:563:GLY:H	2.31	0.42
2:B:710:ILE:O	2:B:751:ALA:HB1	2.20	0.42
2:B:776:SER:HB2	2:B:928:GLN:HB2	2.02	0.42
2:B:932:PRO:HB2	2:B:1004:LEU:HB3	2.01	0.42
4:D:11:LEU:HD23	4:D:12:SER:O	2.20	0.42
10:J:48:ARG:HG3	10:J:49:MET:HG3	2.01	0.42
12:L:48:CYS:SG	12:L:51:CYS:C	3.01	0.42
13:M:106:PHE:O	13:M:123:ILE:HG12	2.19	0.42
13:M:123:ILE:N	13:M:145:VAL:HG22	2.34	0.42
13:M:159:TYR:HB3	13:M:170:LEU:HG	2.02	0.42
15:O:54:LYS:HA	15:O:62:ALA:HB2	2.01	0.42
15:O:553:ARG:HB3	15:O:561:ARG:O	2.19	0.42
17:Q:1074:UNK:O	17:Q:1076:UNK:N	2.52	0.42
19:S:407:ASN:O	19:S:410:SER:N	2.49	0.42
1:A:91:PHE:CE2	1:A:96:PHE:HD1	2.35	0.42
1:A:114:LEU:CD1	1:A:148:CYS:HB2	2.49	0.42
1:A:413:ARG:O	1:A:416:LEU:N	2.52	0.42
2:B:234:ILE:CB	2:B:240:ILE:HG22	2.50	0.42
2:B:727:LEU:HD11	2:B:786:GLU:OE1	2.20	0.42
2:B:809:MET:HG2	2:B:811:VAL:HG23	2.01	0.42
3:C:309:THR:OG1	3:C:311:GLU:HG2	2.20	0.42
5:E:148:GLU:OE1	5:E:149:LEU:N	2.53	0.42
8:H:43:ASN:ND2	8:H:46:LEU:HD13	2.35	0.42
15:O:128:HIS:CE1	15:O:291:ARG:HH22	2.38	0.42
15:O:134:GLY:O	15:O:137:ILE:HB	2.19	0.42
16:P:69:GLU:HG3	16:P:70:LEU:N	2.29	0.42
16:P:209:ALA:O	16:P:212:VAL:HG12	2.19	0.42
16:P:256:VAL:HG22	16:P:257:THR:HG23	2.01	0.42
18:R:214:MET:C	18:R:258:ARG:HH22	2.27	0.42
18:R:402:LEU:HD22	18:R:476:ALA:HB1	2.00	0.42
20:X:8:DC:N4	20:X:9:DA:H62	2.17	0.42
20:X:19:DA:H4'	20:X:20:DA:OP1	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASP:O	1:A:48:PRO:HD3	2.19	0.42
1:A:172:GLY:HA2	1:A:175:ALA:HB3	2.00	0.42
1:A:566:HIS:CD2	1:A:568:ASP:HB3	2.54	0.42
1:A:1065:LYS:HA	1:A:1068:ARG:HB2	2.00	0.42
2:B:191:GLU:OE1	2:B:458:LEU:HB3	2.20	0.42
2:B:326:ALA:C	13:M:231:LEU:HD11	2.45	0.42
2:B:809:MET:HG2	2:B:811:VAL:CG2	2.50	0.42
2:B:909:GLY:O	2:B:1031:VAL:HB	2.19	0.42
2:B:931:MET:HB2	2:B:932:PRO:HD2	2.01	0.42
3:C:216:HIS:CD2	12:L:70:ARG:HB2	2.54	0.42
5:E:41:ASP:O	5:E:45:LYS:N	2.52	0.42
7:G:83:GLU:C	7:G:149:ARG:HA	2.45	0.42
7:G:207:LEU:HD23	7:G:209:SER:H	1.85	0.42
20:X:8:DC:H6	20:X:8:DC:H2'	1.69	0.42
21:Y:48:DT:C2	21:Y:49:DA:N7	2.87	0.42
21:Y:60:DA:H2'	21:Y:61:DT:H71	2.02	0.42
1:A:123:PHE:O	1:A:127:LEU:CD1	2.67	0.42
1:A:136:ARG:O	1:A:140:ILE:HG12	2.20	0.42
1:A:155:LEU:HD11	1:A:156:HIS:HD2	1.84	0.42
1:A:167:ALA:HB1	15:O:557:ARG:NE	2.35	0.42
1:A:636:PRO:HG2	1:A:643:ASN:HA	2.01	0.42
2:B:316:LYS:NZ	13:M:226:ARG:CZ	2.83	0.42
2:B:398:ASP:HB3	2:B:425:HIS:CE1	2.55	0.42
2:B:529:ILE:HD12	2:B:529:ILE:HA	1.95	0.42
2:B:932:PRO:HA	2:B:1005:TYR:O	2.19	0.42
2:B:943:ILE:HD12	2:B:944:MET:H	1.84	0.42
3:C:31:TRP:CG	3:C:32:ASN:H	2.38	0.42
4:D:126:GLN:O	4:D:127:LEU:O	2.37	0.42
5:E:22:MET:CE	5:E:26:ARG:HH21	2.33	0.42
6:F:80:ALA:C	6:F:81:THR:HG1	2.19	0.42
7:G:39:ILE:HG23	7:G:42:VAL:HG13	2.01	0.42
9:I:24:LEU:HG	9:I:33:PHE:HB2	2.02	0.42
15:O:183:MET:HB2	15:O:186:THR:HB	2.00	0.42
18:R:394:GLN:HB2	18:R:487:VAL:HG12	2.01	0.42
19:S:442:ILE:HA	19:S:445:LEU:HD12	2.01	0.42
1:A:284:ASP:O	1:A:286:THR:N	2.53	0.42
1:A:379:THR:HG22	1:A:380:VAL:N	2.34	0.42
1:A:786:ASP:OD2	3:C:9:TYR:HE2	2.02	0.42
1:A:968:GLY:O	1:A:972:GLU:HG2	2.19	0.42
1:A:1380:ARG:HH11	1:A:1385:GLN:NE2	2.07	0.42
2:B:260:CYS:O	2:B:346:ALA:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:MET:HE2	2:B:754:ASN:ND2	2.35	0.42
2:B:762:TYR:CG	2:B:763:SER:N	2.87	0.42
2:B:833:GLY:N	2:B:881:ILE:O	2.28	0.42
3:C:239:ILE:O	3:C:244:ALA:HB2	2.20	0.42
14:N:286:ASP:O	14:N:290:ILE:HG22	2.20	0.42
18:R:484:GLN:HA	18:R:544:LYS:HE2	2.02	0.42
18:R:540:LEU:HD13	18:R:549:ILE:HG23	2.02	0.42
1:A:118:THR:O	1:A:122:GLN:N	2.49	0.42
1:A:262:PRO:HB2	2:B:1134:SER:O	2.19	0.42
1:A:373:VAL:CG1	1:A:374:ASP:N	2.82	0.42
1:A:383:PRO:HG3	1:A:512:PHE:CZ	2.55	0.42
1:A:408:VAL:O	1:A:409:THR:CG2	2.68	0.42
2:B:96:VAL:HG13	2:B:97:ASP:N	2.35	0.42
2:B:489:LEU:HG	2:B:493:GLN:OE1	2.20	0.42
2:B:732:GLN:HE22	10:J:49:MET:HG2	1.85	0.42
2:B:834:MET:HE2	12:L:63:ARG:HD2	2.01	0.42
2:B:1039:ALA:HB3	18:R:20:ASN:OD1	2.19	0.42
3:C:326:GLU:HB2	11:K:125:MET:SD	2.60	0.42
9:I:22:TYR:C	9:I:23:THR:O	2.59	0.42
13:M:85:LEU:HD12	13:M:171:VAL:HG11	2.02	0.42
13:M:88:PHE:CZ	13:M:119:TRP:HE3	2.36	0.42
13:M:251:THR:HG23	13:M:254:GLN:CG	2.50	0.42
15:O:190:LEU:HG	15:O:193:GLN:HB3	2.01	0.42
15:O:199:TYR:C	15:O:200:LEU:HD12	2.45	0.42
15:O:478:VAL:HG12	15:O:479:PRO:O	2.20	0.42
16:P:209:ALA:C	16:P:211:ASN:N	2.78	0.42
16:P:221:ILE:HG21	16:P:240:ILE:HG21	2.01	0.42
19:S:299:UNK:CB	19:S:400:ASN:HD21	2.33	0.42
19:S:479:PRO:HB2	19:S:483:GLU:OE1	2.19	0.42
21:Y:14:DG:C2	21:Y:15:DT:C2	3.08	0.42
1:A:78:HIS:ND1	2:B:1090:PHE:HZ	2.18	0.42
1:A:91:PHE:HE2	1:A:96:PHE:CD1	2.37	0.42
1:A:283:ASP:O	1:A:284:ASP:C	2.63	0.42
1:A:381:ILE:HG22	1:A:382:SER:N	2.35	0.42
1:A:733:ILE:HG13	1:A:737:LYS:HE2	2.01	0.42
2:B:135:TYR:HE1	2:B:419:LEU:HB3	1.74	0.42
2:B:143:MET:HG2	2:B:144:HIS:H	1.85	0.42
2:B:180:ASP:OD2	2:B:460:ARG:NH2	2.38	0.42
2:B:364:LYS:O	2:B:366:ILE:HG23	2.18	0.42
2:B:591:TYR:HB3	2:B:653:GLU:HA	2.01	0.42
2:B:762:TYR:C	2:B:763:SER:HG	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:TYR:HA	3:C:191:ILE:O	2.18	0.42
3:C:195:LYS:HD2	10:J:57:ILE:CG2	2.49	0.42
3:C:229:LEU:HD23	3:C:293:ARG:NH1	2.35	0.42
5:E:63:ASN:HA	5:E:77:SER:HA	2.01	0.42
7:G:141:ASP:OD1	7:G:142:VAL:HG22	2.20	0.42
9:I:33:PHE:CE2	9:I:35:ILE:HA	2.55	0.42
13:M:117:HIS:CG	13:M:118:LEU:H	2.38	0.42
14:N:402:ASP:O	14:N:405:SER:HB3	2.20	0.42
15:O:125:GLU:HB2	15:O:128:HIS:HB2	1.97	0.42
16:P:106:TRP:NE1	16:P:145:ARG:HA	2.35	0.42
16:P:253:LEU:HB2	16:P:262:ARG:O	2.20	0.42
19:S:367:ASN:HB3	19:S:370:GLY:O	2.20	0.42
21:Y:41:DG:C6	21:Y:42:DA:C6	3.08	0.42
1:A:14:LYS:HE3	2:B:1142:ARG:CZ	2.50	0.41
1:A:721:ASP:H	1:A:724:LYS:NZ	2.17	0.41
1:A:912:VAL:HG11	1:A:1361:VAL:HG12	2.02	0.41
2:B:535:VAL:HG13	14:N:310:PRO:HB3	2.02	0.41
2:B:636:ASP:OD1	2:B:637:PHE:N	2.53	0.41
2:B:957:LYS:O	2:B:960:GLU:N	2.52	0.41
5:E:152:LYS:HE2	5:E:154:ILE:HD11	2.02	0.41
6:F:140:ASP:OD1	6:F:142:SER:N	2.52	0.41
7:G:147:ARG:NH2	7:G:211:TRP:HB2	2.35	0.41
15:O:190:LEU:HD11	15:O:199:TYR:HE1	1.85	0.41
16:P:206:VAL:HB	16:P:210:PRO:HA	2.02	0.41
18:R:128:SER:O	18:R:132:VAL:HG22	2.20	0.41
18:R:401:THR:HG23	18:R:446:LYS:HG2	2.01	0.41
18:R:485:ASN:ND2	18:R:542:GLY:H	2.17	0.41
1:A:134:ASN:O	1:A:137:ARG:HB2	2.20	0.41
1:A:318:TYR:CD1	1:A:336:MET:HE2	2.55	0.41
1:A:1323:PHE:HD1	1:A:1328:ILE:H	1.68	0.41
1:A:1454:GLU:HA	1:A:1457:LEU:HD12	2.01	0.41
2:B:65:PHE:O	2:B:68:PHE:HB3	2.19	0.41
2:B:234:ILE:CG1	2:B:240:ILE:HG22	2.50	0.41
2:B:556:TYR:CD1	2:B:561:LEU:HA	2.55	0.41
2:B:576:ARG:O	2:B:580:ARG:HG2	2.21	0.41
2:B:933:PHE:O	2:B:934:ASN:CG	2.63	0.41
3:C:93:GLN:HB2	3:C:96:VAL:HB	2.02	0.41
7:G:2:PHE:HE2	7:G:79:PRO:HB3	1.86	0.41
9:I:12:LEU:HD22	9:I:24:LEU:HD11	2.02	0.41
13:M:154:GLU:HB3	13:M:175:ARG:HA	2.02	0.41
14:N:290:ILE:HG21	14:N:384:LYS:NZ	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:506:ARG:O	15:O:510:CYS:N	2.46	0.41
15:O:634:GLU:O	15:O:637:VAL:N	2.52	0.41
18:R:83:ALA:O	18:R:87:LEU:HB2	2.19	0.41
19:S:416:TYR:OH	21:Y:64:DT:H5"	2.20	0.41
19:S:423:GLU:HA	19:S:426:ILE:HG12	2.02	0.41
19:S:427:LYS:HA	19:S:430:LYS:HD2	2.03	0.41
21:Y:10:DT:C2	21:Y:11:DG:C5	3.07	0.41
1:A:678:PHE:CD2	1:A:694:MET:HG2	2.55	0.41
1:A:1299:GLY:C	1:A:1301:ARG:N	2.79	0.41
2:B:855:PRO:HD2	18:R:106:GLN:NE2	2.34	0.41
3:C:270:ALA:O	3:C:271:ARG:HG2	2.20	0.41
4:D:127:LEU:HD23	7:G:147:ARG:CD	2.51	0.41
4:D:134:LEU:HD22	4:D:153:MET:SD	2.61	0.41
5:E:66:GLU:O	5:E:69:ILE:HG22	2.20	0.41
5:E:118:PRO:O	5:E:122:LYS:N	2.53	0.41
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.21	0.41
15:O:226:ILE:O	15:O:228:ARG:N	2.46	0.41
15:O:369:HIS:CG	15:O:370:LEU:N	2.89	0.41
16:P:25:LYS:HG3	16:P:26:GLY:N	2.35	0.41
18:R:515:LEU:HD23	18:R:515:LEU:HA	1.82	0.41
21:Y:28:DT:H2"	21:Y:29:DG:C8	2.55	0.41
1:A:332:VAL:HG13	1:A:333:ASN:N	2.30	0.41
1:A:958:ALA:O	1:A:961:GLU:HB2	2.20	0.41
2:B:249:GLU:H	2:B:308:LYS:HE2	1.85	0.41
2:B:553:TYR:HB3	2:B:598:ALA:CA	2.50	0.41
2:B:885:MET:HE2	2:B:897:LYS:HB3	2.02	0.41
5:E:96:PHE:O	5:E:100:ILE:HG12	2.19	0.41
6:F:131:PRO:C	6:F:132:LEU:HD12	2.46	0.41
7:G:96:GLY:CA	7:G:112:GLN:HG3	2.49	0.41
8:H:110:ASP:O	8:H:128:ASN:HA	2.20	0.41
15:O:369:HIS:ND1	15:O:370:LEU:N	2.68	0.41
18:R:131:TYR:HA	18:R:134:CYS:SG	2.59	0.41
19:S:506:GLN:O	19:S:510:LYS:CB	2.67	0.41
1:A:404:TYR:CE1	1:A:528:ARG:HD2	2.55	0.41
1:A:668:VAL:HG23	1:A:669:LEU:N	2.35	0.41
1:A:717:VAL:O	1:A:810:VAL:HG22	2.20	0.41
1:A:1130:ILE:HA	1:A:1362:MET:HE1	2.01	0.41
2:B:193:VAL:HG23	2:B:458:LEU:HB2	2.03	0.41
2:B:611:PRO:HG3	2:B:648:TYR:CE1	2.56	0.41
3:C:319:ARG:HB2	11:K:132:GLU:OE2	2.21	0.41
14:N:292:ARG:O	14:N:296:LYS:HG2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:256:VAL:O	16:P:260:CYS:HB3	2.19	0.41
18:R:484:GLN:NE2	20:X:16:DA:N3	2.68	0.41
18:R:537:LYS:O	18:R:538:ILE:HD13	2.21	0.41
1:A:91:PHE:CD1	1:A:224:PRO:HB3	2.52	0.41
1:A:610:PHE:CE1	1:A:697:MET:HE1	2.56	0.41
1:A:953:GLY:HA3	1:A:1061:ARG:CG	2.50	0.41
1:A:1281:ALA:HB1	1:A:1295:VAL:HG22	2.03	0.41
2:B:68:PHE:HD1	2:B:385:SER:HG	1.55	0.41
2:B:234:ILE:HD11	2:B:238:GLY:H	1.86	0.41
2:B:354:ARG:NH1	2:B:549:LEU:HD13	2.35	0.41
2:B:1147:PHE:HZ	7:G:60:LYS:HB3	1.85	0.41
3:C:91:VAL:HG23	3:C:200:GLN:HE22	1.85	0.41
5:E:180:ARG:HH12	5:E:191:LYS:HA	1.86	0.41
16:P:59:ASN:OD1	16:P:80:ALA:HB1	2.20	0.41
16:P:209:ALA:O	16:P:211:ASN:N	2.42	0.41
1:A:308:SER:O	1:A:312:MET:N	2.53	0.41
1:A:487:SER:OG	1:A:536:GLY:HA2	2.21	0.41
1:A:687:PRO:O	1:A:690:ALA:N	2.54	0.41
2:B:65:PHE:O	2:B:68:PHE:N	2.53	0.41
2:B:615:VAL:HA	2:B:620:SER:HA	2.02	0.41
2:B:723:THR:O	2:B:789:ARG:HA	2.21	0.41
2:B:947:HIS:O	2:B:950:PRO:HD2	2.21	0.41
3:C:44:ILE:HA	3:C:54:PHE:HB2	2.03	0.41
3:C:239:ILE:O	3:C:239:ILE:HD12	2.21	0.41
3:C:278:GLU:O	3:C:281:ARG:HG2	2.20	0.41
7:G:84:ILE:HG23	7:G:147:ARG:HB3	2.02	0.41
8:H:9:ILE:O	8:H:31:THR:HG22	2.20	0.41
14:N:286:ASP:OD2	14:N:384:LYS:HE3	2.20	0.41
15:O:155:LEU:O	15:O:159:ILE:HG12	2.21	0.41
15:O:328:ASP:OD1	15:O:329:PRO:HD3	2.20	0.41
15:O:571:THR:O	15:O:575:ASN:HB2	2.19	0.41
16:P:206:VAL:HB	16:P:210:PRO:HB3	2.01	0.41
20:X:15:DT:H2"	20:X:16:DA:C8	2.56	0.41
20:X:51:DA:C6	20:X:52:DA:C6	3.08	0.41
1:A:57:LYS:HA	1:A:68:ALA:HB3	2.03	0.41
1:A:132:VAL:HG13	1:A:136:ARG:HB2	2.01	0.41
1:A:220:ASP:HB3	15:O:549:GLN:HE22	1.86	0.41
1:A:389:ILE:O	1:A:390:ASP:OD1	2.37	0.41
1:A:822:ARG:CZ	1:A:845:LYS:HB2	2.51	0.41
1:A:1267:LEU:C	1:A:1269:ASP:H	2.29	0.41
2:B:217:GLN:HB3	2:B:356:VAL:CG1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:ASP:OD2	2:B:513:ASN:ND2	2.54	0.41
2:B:519:HIS:ND1	2:B:586:GLU:OE2	2.54	0.41
3:C:71:MET:HE1	3:C:314:PHE:HD1	1.86	0.41
3:C:123:ASP:OD1	3:C:124:GLU:N	2.53	0.41
4:D:14:TYR:CD1	4:D:15:GLU:CB	3.03	0.41
8:H:7:ASP:HB3	8:H:58:THR:HG23	2.03	0.41
11:K:55:SER:O	11:K:56:GLU:HG3	2.20	0.41
13:M:133:LYS:O	13:M:137:GLU:N	2.47	0.41
15:O:32:MET:C	15:O:34:ILE:H	2.29	0.41
16:P:309:VAL:HG21	16:P:311:TYR:CZ	2.56	0.41
17:Q:69:PRO:HG2	17:Q:70:PHE:CE2	2.55	0.41
18:R:195:LYS:HE2	18:R:195:LYS:HB2	1.86	0.41
18:R:196:ILE:O	18:R:199:VAL:HB	2.20	0.41
19:S:416:TYR:OH	19:S:419:PRO:HD3	2.21	0.41
21:Y:20:DT:C2'	21:Y:21:DT:H5'	2.51	0.41
21:Y:64:DT:H4'	21:Y:65:DG:H5'	2.02	0.41
1:A:11:LYS:HD3	2:B:1145:ASP:CA	2.49	0.41
1:A:163:VAL:HG13	1:A:184:ARG:HH12	1.86	0.41
1:A:258:TRP:CZ3	2:B:1136:ASN:HB2	2.56	0.41
1:A:330:ASP:CG	1:A:331:SER:N	2.77	0.41
1:A:484:SER:O	1:A:508:TYR:HE1	2.04	0.41
1:A:577:THR:HG21	11:K:81:MET:HE1	2.03	0.41
1:A:832:LEU:HD21	1:A:862:LEU:HD23	2.02	0.41
1:A:921:LEU:HG	1:A:1081:ALA:O	2.20	0.41
1:A:1383:VAL:HG22	1:A:1406:ASP:CG	2.46	0.41
2:B:72:ASP:O	2:B:76:ILE:HG12	2.20	0.41
2:B:258:LYS:HE2	2:B:265:ASP:HA	2.03	0.41
2:B:454:VAL:HG13	2:B:455:THR:HG23	2.02	0.41
2:B:726:TYR:O	2:B:727:LEU:HB3	2.21	0.41
2:B:757:VAL:HA	2:B:942:ILE:O	2.21	0.41
2:B:905:ARG:O	2:B:907:GLU:N	2.53	0.41
2:B:932:PRO:CB	2:B:1004:LEU:HB3	2.51	0.41
2:B:1106:TRP:CD1	7:G:163:PRO:HD3	2.55	0.41
3:C:45:SER:HB2	3:C:53:ASN:O	2.21	0.41
3:C:67:PHE:O	3:C:71:MET:HB2	2.21	0.41
3:C:260:GLU:N	3:C:263:ASP:HB2	2.36	0.41
4:D:3:VAL:HG13	7:G:7:ILE:HG22	2.03	0.41
4:D:130:ASN:O	4:D:133:HIS:HB2	2.20	0.41
7:G:126:SER:HB2	7:G:139:TYR:CB	2.45	0.41
9:I:3:SER:CB	9:I:12:LEU:HD12	2.51	0.41
12:L:60:ARG:NH1	12:L:61:THR:HG22	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:237:ALA:O	13:M:241:ALA:HB2	2.20	0.41
14:N:366:HIS:CG	14:N:367:LYS:H	2.38	0.41
14:N:394:VAL:HB	14:N:412:VAL:HB	2.01	0.41
15:O:41:THR:C	15:O:43:ASN:N	2.79	0.41
15:O:115:LYS:HB3	15:O:116:LYS:H	1.54	0.41
15:O:203:ILE:O	15:O:203:ILE:HG13	2.21	0.41
15:O:365:ASP:C	15:O:366:LEU:HD12	2.45	0.41
15:O:480:TYR:O	15:O:483:LEU:N	2.54	0.41
15:O:584:ASN:OD1	16:P:310:VAL:HG22	2.21	0.41
18:R:142:MET:HB2	18:R:181:PHE:HE1	1.86	0.41
18:R:227:CYS:HA	18:R:230:LEU:HD12	2.02	0.41
18:R:413:LEU:O	18:R:615:LEU:HD11	2.21	0.41
18:R:442:PHE:HD2	18:R:446:LYS:HB2	1.86	0.41
18:R:484:GLN:CD	20:X:16:DA:H1'	2.46	0.41
18:R:492:VAL:HB	18:R:494:PHE:CE2	2.56	0.41
20:X:59:DC:H2''	20:X:60:DA:OP2	2.20	0.41
21:Y:40:DA:C6	21:Y:41:DG:C6	3.09	0.41
21:Y:42:DA:C6	21:Y:43:DA:C6	3.09	0.41
1:A:5:VAL:HG23	7:G:38:ILE:C	2.46	0.41
1:A:34:VAL:HG23	1:A:52:GLY:C	2.46	0.41
1:A:296:SER:O	1:A:299:ILE:N	2.54	0.41
1:A:618:HIS:CD2	8:H:77:ARG:HH11	2.39	0.41
1:A:859:PRO:HD3	2:B:661:LEU:HD11	2.03	0.41
1:A:1124:PRO:O	1:A:1127:LYS:HB2	2.20	0.41
1:A:1202:ILE:HG23	1:A:1203:GLU:N	2.36	0.41
2:B:916:HIS:CG	2:B:957:LYS:HB2	2.56	0.41
3:C:59:ILE:HD13	3:C:63:ILE:CD1	2.50	0.41
15:O:60:ARG:HG3	15:O:61:ALA:N	2.36	0.41
15:O:337:GLN:HB3	15:O:342:ALA:HB2	2.02	0.41
15:O:644:LEU:HD12	17:Q:43:ILE:HD12	2.03	0.41
16:P:98:GLU:HB3	16:P:150:LEU:HD21	2.03	0.41
18:R:13:GLU:OE2	18:R:26:LYS:HE2	2.20	0.41
18:R:229:LEU:HD13	18:R:244:ILE:HD11	2.03	0.41
18:R:492:VAL:HG11	18:R:560:LEU:HD13	2.03	0.41
18:R:510:SER:HB3	18:R:520:ILE:HD11	2.03	0.41
20:X:22:DA:C2	20:X:23:DC:C2	3.08	0.41
1:A:32:VAL:HG11	1:A:57:LYS:CD	2.49	0.40
1:A:89:PRO:CG	1:A:228:LEU:CD2	2.96	0.40
1:A:179:ILE:HD13	15:O:557:ARG:HH21	1.78	0.40
1:A:261:LEU:HA	1:A:262:PRO:HD3	1.84	0.40
1:A:666:LYS:O	1:A:667:SER:OG	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ASP:OD1	1:A:789:ASN:HB2	2.21	0.40
1:A:1184:ILE:HD11	1:A:1260:MET:SD	2.61	0.40
1:A:1396:LEU:HD23	1:A:1396:LEU:HA	1.79	0.40
2:B:527:GLU:HB3	2:B:528:PRO:HD3	2.02	0.40
2:B:673:LEU:O	2:B:673:LEU:HD12	2.21	0.40
2:B:915:ARG:HD2	2:B:1023:TYR:CD2	2.50	0.40
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.54	0.40
3:C:255:VAL:HG22	3:C:256:ILE:N	2.36	0.40
5:E:136:ASN:ND2	5:E:138:ALA:HB3	2.37	0.40
6:F:93:ILE:HD11	6:F:134:ILE:HG12	2.03	0.40
8:H:12:VAL:HG22	8:H:26:ILE:HD11	2.01	0.40
9:I:11:MET:HG3	9:I:12:LEU:N	2.35	0.40
13:M:108:SER:HG	13:M:247:TRP:CD1	2.38	0.40
15:O:73:ARG:NE	15:O:121:TYR:OH	2.53	0.40
15:O:579:GLN:O	15:O:583:TRP:N	2.54	0.40
16:P:20:SER:HA	16:P:23:MET:HG2	2.02	0.40
18:R:14:ARG:HA	18:R:22:ASP:O	2.21	0.40
18:R:133:ALA:O	18:R:136:LYS:N	2.53	0.40
18:R:598:ASP:HB3	18:R:601:ASN:OD1	2.21	0.40
21:Y:56:DA:N6	21:Y:57:DT:O4	2.54	0.40
1:A:82:GLY:O	1:A:263:ALA:N	2.41	0.40
1:A:103:LEU:HD11	1:A:222:LEU:CD2	2.50	0.40
1:A:183:PHE:CG	1:A:184:ARG:N	2.89	0.40
1:A:292:ILE:HA	1:A:295:THR:HG22	2.03	0.40
1:A:559:THR:HG23	1:A:560:GLY:N	2.36	0.40
1:A:1373:ARG:HD3	1:A:1390:GLU:CD	2.46	0.40
2:B:58:VAL:HG11	2:B:470:MET:CE	2.51	0.40
2:B:386:LEU:HD23	2:B:386:LEU:HA	1.90	0.40
2:B:1054:ARG:C	2:B:1055:SER:HG	2.23	0.40
6:F:136:ARG:O	6:F:144:GLU:CB	2.69	0.40
14:N:389:THR:HG23	14:N:390:PHE:N	2.35	0.40
15:O:128:HIS:CE1	15:O:132:TYR:HE1	2.39	0.40
15:O:253:ILE:O	15:O:256:PRO:HD2	2.22	0.40
20:X:16:DA:H61	21:Y:55:DA:N6	2.14	0.40
21:Y:8:DC:C2	21:Y:9:DA:C5	3.10	0.40
1:A:403:THR:HG21	1:A:431:ASN:HD21	1.85	0.40
1:A:714:ILE:CD1	2:B:958:MET:HG2	2.51	0.40
1:A:891:LYS:HG3	1:A:1389:PHE:HD1	1.85	0.40
1:A:1027:GLY:C	1:A:1028:MET:HE2	2.47	0.40
2:B:305:ILE:HG22	2:B:325:GLU:HG2	2.03	0.40
2:B:637:PHE:CG	2:B:638:ASP:N	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:LEU:HA	2:B:1060:LEU:HD23	1.82	0.40
3:C:5:VAL:HG22	3:C:293:ARG:O	2.21	0.40
4:D:98:MET:HA	4:D:160:TYR:CZ	2.57	0.40
13:M:72:GLU:C	14:N:364:ARG:HD3	2.46	0.40
15:O:196:GLU:HG3	15:O:197:MET:N	2.28	0.40
16:P:48:LEU:O	16:P:52:VAL:HG23	2.22	0.40
18:R:213:TRP:HH2	18:R:497:ARG:HB3	1.84	0.40
18:R:218:ARG:HD3	21:Y:60:DA:P	2.62	0.40
20:X:3:DT:C2	20:X:4:DT:C4	3.10	0.40
1:A:478:PRO:HG3	21:Y:23:DT:O2	2.21	0.40
1:A:506:THR:HG21	1:A:554:THR:HG21	2.04	0.40
1:A:706:GLY:HA2	2:B:761:SER:O	2.21	0.40
1:A:976:ARG:HG2	1:A:1002:ARG:NH2	2.36	0.40
1:A:1447:LEU:HB3	1:A:1450:SER:HB3	2.04	0.40
2:B:86:ASP:O	2:B:87:VAL:HB	2.21	0.40
2:B:303:GLU:OE1	2:B:322:GLU:HA	2.21	0.40
2:B:945:ASN:OD1	2:B:946:PRO:HD2	2.21	0.40
3:C:96:VAL:O	3:C:97:LEU:C	2.64	0.40
5:E:153:HIS:ND1	5:E:184:VAL:HG11	2.37	0.40
13:M:230:SER:O	13:M:234:HIS:ND1	2.50	0.40
15:O:457:LEU:HD21	15:O:476:TYR:OH	2.22	0.40
1:A:216:LYS:HG3	1:A:217:ARG:N	2.37	0.40
1:A:329:SER:HB3	1:A:351:ARG:HB3	2.03	0.40
1:A:562:TYR:CE2	1:A:793:ILE:HG23	2.57	0.40
1:A:656:GLY:H	1:A:944:ASN:ND2	2.19	0.40
1:A:827:PHE:HE2	1:A:833:PRO:HD3	1.87	0.40
1:A:834:HIS:HA	2:B:659:ILE:O	2.21	0.40
1:A:923:PRO:HA	1:A:926:MET:HE2	2.04	0.40
1:A:935:PHE:HE1	1:A:1008:LEU:HD13	1.86	0.40
1:A:1260:MET:HB2	1:A:1260:MET:HE2	1.93	0.40
1:A:1332:ARG:NH2	5:E:200:ARG:HE	2.20	0.40
2:B:230:LYS:HB2	2:B:333:ALA:CB	2.51	0.40
2:B:377:LEU:HD12	2:B:377:LEU:C	2.47	0.40
2:B:650:ASP:OD1	2:B:651:VAL:N	2.55	0.40
2:B:924:ILE:HD13	2:B:924:ILE:HA	1.93	0.40
2:B:1101:MET:HE1	2:B:1130:GLN:HG3	2.04	0.40
3:C:274:THR:HG22	3:C:274:THR:O	2.22	0.40
4:D:126:GLN:HG2	7:G:84:ILE:O	2.20	0.40
7:G:126:SER:CB	7:G:139:TYR:HB3	2.49	0.40
7:G:141:ASP:O	7:G:144:GLU:HB2	2.22	0.40
14:N:364:ARG:O	14:N:371:LEU:HD12	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:53:VAL:HG23	15:O:57:LEU:HD12	2.04	0.40
15:O:205:LYS:HG3	15:O:206:LEU:N	2.36	0.40
15:O:528:MET:HE3	15:O:529:LYS:HG2	2.03	0.40
15:O:583:TRP:HH2	16:P:314:GLU:CG	2.19	0.40
17:Q:39:ILE:O	17:Q:39:ILE:HG23	2.22	0.40
18:R:195:LYS:O	18:R:199:VAL:HG23	2.21	0.40
18:R:488:GLY:N	18:R:540:LEU:O	2.46	0.40
19:S:364:LEU:HB2	19:S:373:ALA:O	2.21	0.40
20:X:60:DA:H2''	20:X:61:DT:OP2	2.21	0.40
20:X:64:DC:H2''	20:X:65:DC:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1422/1460 (97%)	1142 (80%)	260 (18%)	20 (1%)	9	39
2	B	1112/1149 (97%)	907 (82%)	185 (17%)	20 (2%)	6	35
3	C	333/335 (99%)	272 (82%)	58 (17%)	3 (1%)	14	49
4	D	113/161 (70%)	85 (75%)	26 (23%)	2 (2%)	6	35
5	E	213/215 (99%)	177 (83%)	35 (16%)	1 (0%)	24	61
6	F	81/155 (52%)	71 (88%)	9 (11%)	1 (1%)	10	42
7	G	178/212 (84%)	146 (82%)	27 (15%)	5 (3%)	4	27
8	H	136/146 (93%)	114 (84%)	21 (15%)	1 (1%)	18	55
9	I	40/110 (36%)	29 (72%)	8 (20%)	3 (8%)	1	12
10	J	65/70 (93%)	51 (78%)	14 (22%)	0	100	100
11	K	99/142 (70%)	79 (80%)	20 (20%)	0	100	100
12	L	44/70 (63%)	36 (82%)	8 (18%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	160/282 (57%)	128 (80%)	27 (17%)	5 (3%)	3	25
14	N	106/422 (25%)	80 (76%)	26 (24%)	0	100	100
15	O	533/654 (82%)	405 (76%)	116 (22%)	12 (2%)	5	31
16	P	271/317 (86%)	223 (82%)	45 (17%)	3 (1%)	11	44
17	Q	33/251 (13%)	27 (82%)	6 (18%)	0	100	100
18	R	514/736 (70%)	436 (85%)	75 (15%)	3 (1%)	21	58
19	S	172/594 (29%)	157 (91%)	15 (9%)	0	100	100
All	All	5625/7481 (75%)	4565 (81%)	981 (17%)	79 (1%)	11	39

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	236	SER
1	A	587	ILE
1	A	599	LYS
1	A	601	TYR
1	A	1371	ILE
2	B	416	TYR
2	B	417	ASP
2	B	427	ASN
2	B	587	PHE
2	B	823	SER
9	I	21	VAL
13	M	107	ILE
15	O	124	GLU
15	O	494	TYR
15	O	496	ILE
18	R	514	GLU
18	R	516	PHE
1	A	284	ASP
1	A	285	LEU
1	A	307	ILE
1	A	975	VAL
2	B	87	VAL
2	B	318	THR
4	D	129	ALA
9	I	23	THR
13	M	87	VAL
13	M	242	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	40	ARG
15	O	125	GLU
1	A	275	GLN
1	A	410	ARG
1	A	995	VAL
1	A	998	TYR
3	C	87	ASN
3	C	255	VAL
6	F	144	GLU
7	G	123	PRO
7	G	191	PRO
9	I	35	ILE
15	O	36	SER
16	P	203	LYS
1	A	39	LEU
1	A	233	GLN
1	A	277	SER
1	A	1300	LEU
1	A	1328	ILE
2	B	506	GLU
2	B	713	ILE
2	B	763	SER
3	C	88	ASN
5	E	147	HIS
15	O	146	VAL
15	O	516	LEU
2	B	767	ILE
4	D	127	LEU
7	G	160	PRO
8	H	77	ARG
13	M	84	SER
13	M	85	LEU
15	O	557	ARG
1	A	252	ARG
2	B	168	GLU
2	B	295	ILE
2	B	624	ASP
15	O	499	THR
2	B	1008	ILE
2	B	584	VAL
15	O	473	PRO
2	B	215	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	811	VAL
2	B	233	VAL
7	G	142	VAL
15	O	76	VAL
16	P	192	PRO
16	P	206	VAL
2	B	1137	ILE
7	G	158	VAL
18	R	154	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1232/1257 (98%)	1226 (100%)	6 (0%)	81	82
2	B	975/1006 (97%)	968 (99%)	7 (1%)	76	79
3	C	296/296 (100%)	293 (99%)	3 (1%)	68	76
4	D	110/145 (76%)	110 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	164/190 (86%)	161 (98%)	3 (2%)	51	67
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	38/98 (39%)	37 (97%)	1 (3%)	40	61
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	39 (98%)	1 (2%)	42	62
13	M	142/249 (57%)	141 (99%)	1 (1%)	76	79
14	N	92/360 (26%)	92 (100%)	0	100	100
15	O	495/593 (84%)	489 (99%)	6 (1%)	63	73
16	P	255/285 (90%)	255 (100%)	0	100	100
17	Q	31/195 (16%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	450/623 (72%)	448 (100%)	2 (0%)	84	83
19	S	157/494 (32%)	157 (100%)	0	100	100
All	All	5023/6505 (77%)	4993 (99%)	30 (1%)	76	80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	254	GLU
1	A	275	GLN
1	A	285	LEU
1	A	955	LEU
1	A	1145	LEU
2	B	59	LYS
2	B	316	LYS
2	B	427	ASN
2	B	587	PHE
2	B	741	ILE
2	B	772	VAL
2	B	1085	ILE
3	C	35	LYS
3	C	120	LEU
3	C	239	ILE
7	G	122	THR
7	G	124	GLU
7	G	125	GLU
9	I	24	LEU
12	L	61	THR
13	M	184	LYS
15	O	40	ARG
15	O	41	THR
15	O	187	ILE
15	O	496	ILE
15	O	516	LEU
15	O	557	ARG
18	R	514	GLU
18	R	515	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	156	HIS
1	A	233	GLN
1	A	275	GLN
1	A	315	HIS
1	A	320	GLN
1	A	386	ASN
1	A	437	ASN
1	A	509	ASN
1	A	518	ASN
1	A	520	HIS
1	A	523	GLN
1	A	533	ASN
1	A	555	GLN
1	A	566	HIS
1	A	589	HIS
1	A	618	HIS
1	A	619	ASN
1	A	625	ASN
1	A	688	GLN
1	A	808	GLN
1	A	828	GLN
1	A	838	ASN
1	A	913	GLN
1	A	1006	HIS
1	A	1058	GLN
1	A	1385	GLN
1	A	1395	HIS
2	B	116	HIS
2	B	140	ASN
2	B	197	GLN
2	B	203	ASN
2	B	217	GLN
2	B	244	HIS
2	B	275	ASN
2	B	286	ASN
2	B	299	GLN
2	B	334	HIS
2	B	374	ASN
2	B	397	ASN
2	B	411	ASN
2	B	425	HIS
2	B	441	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	519	HIS
2	B	600	HIS
2	B	626	HIS
2	B	693	HIS
2	B	717	GLN
2	B	754	ASN
2	B	803	GLN
2	B	902	GLN
2	B	918	GLN
2	B	928	GLN
2	B	1148	GLN
3	C	29	ASN
3	C	99	HIS
3	C	175	GLN
3	C	200	GLN
3	C	207	HIS
3	C	330	ASN
4	D	71	ASN
4	D	122	GLN
5	E	3	GLN
5	E	5	ASN
5	E	104	ASN
5	E	153	HIS
5	E	174	GLN
7	G	58	GLN
8	H	133	ASN
11	K	118	GLN
13	M	86	HIS
13	M	89	GLN
13	M	156	ASN
13	M	190	ASN
14	N	288	GLN
15	O	43	ASN
15	O	147	ASN
15	O	152	HIS
15	O	161	GLN
15	O	222	HIS
15	O	295	GLN
15	O	310	GLN
15	O	332	GLN
15	O	337	GLN
15	O	346	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	456	HIS
15	O	652	GLN
16	P	33	GLN
16	P	34	GLN
16	P	53	GLN
16	P	118	GLN
16	P	119	HIS
16	P	131	GLN
16	P	305	HIS
18	R	20	ASN
18	R	35	ASN
18	R	124	ASN
18	R	184	HIS
18	R	235	ASN
18	R	278	ASN
18	R	394	GLN
18	R	414	HIS
18	R	545	GLN
19	S	386	ASN
19	S	499	ASN
19	S	506	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	S	1
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	319:UNK	C	360:THR	N	37.31
1	Q	70:PHE	C	1070:UNK	N	13.25

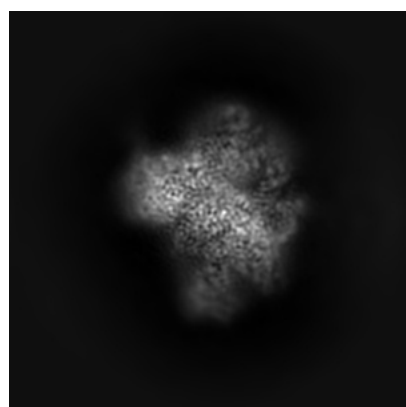
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7530. These allow visual inspection of the internal detail of the map and identification of artifacts.

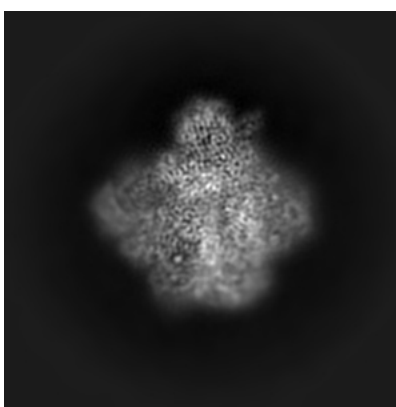
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

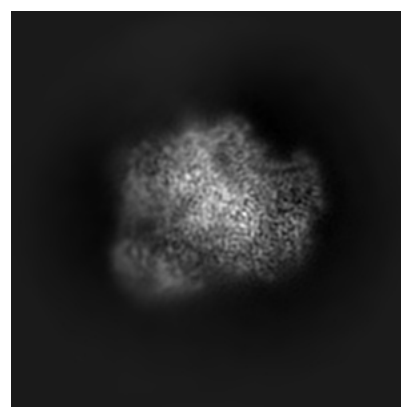
6.1.1 Primary map



X



Y

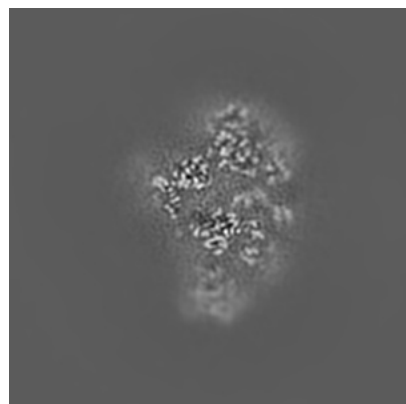


Z

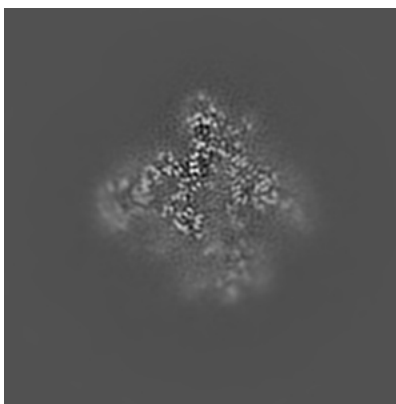
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

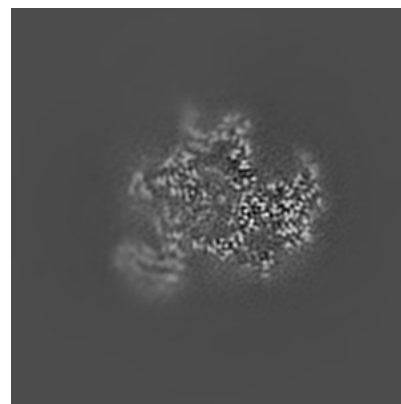
6.2.1 Primary map



X Index: 144



Y Index: 144

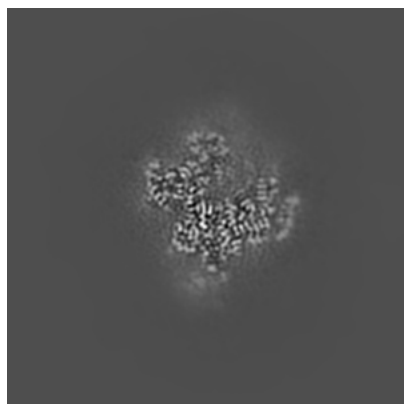


Z Index: 144

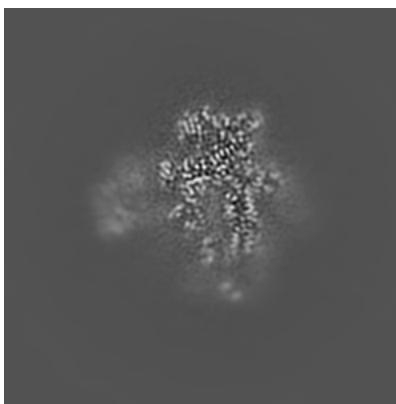
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

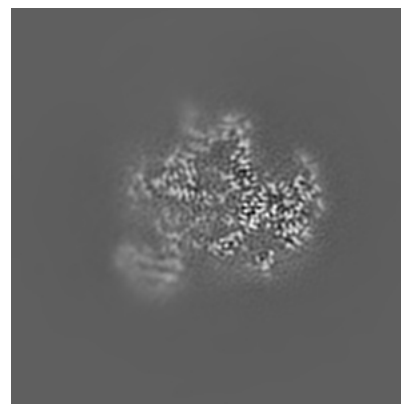
6.3.1 Primary map



X Index: 168



Y Index: 134

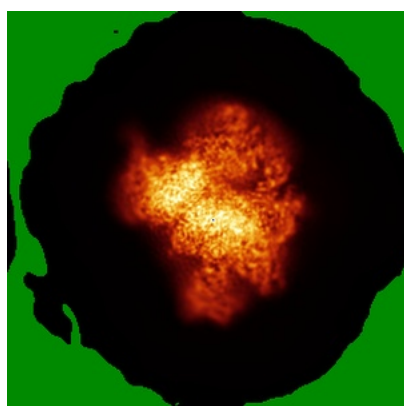


Z Index: 143

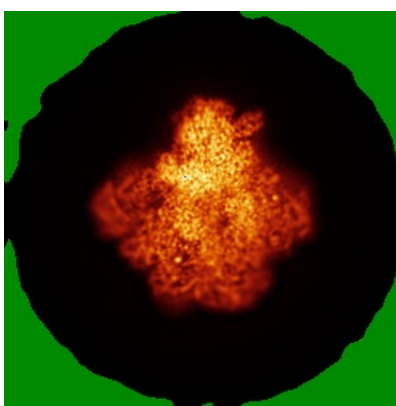
The images above show the largest variance slices of the map in three orthogonal directions.

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

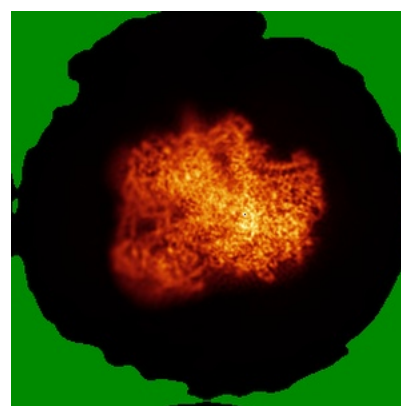
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

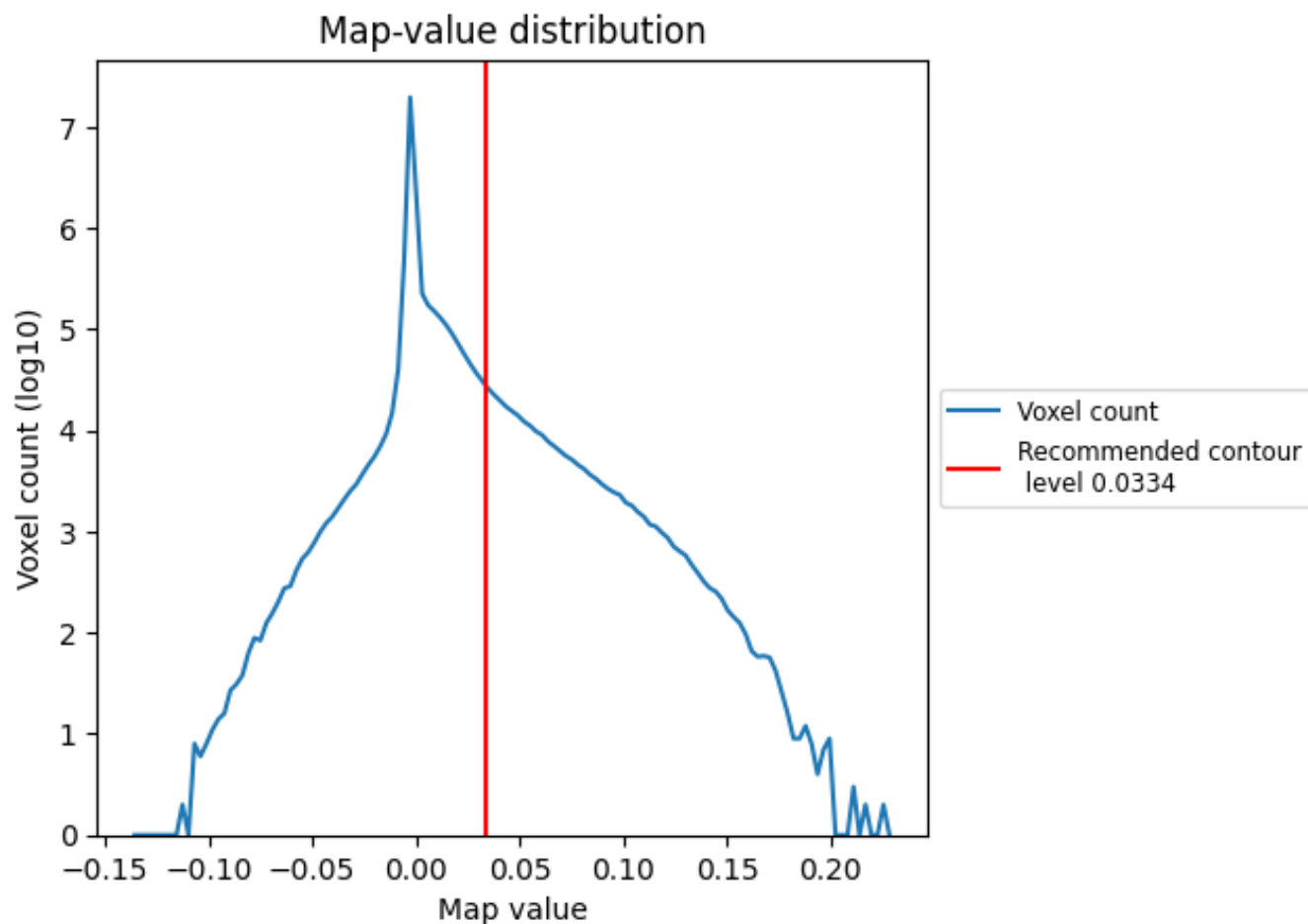
6.6 Mask visualisation

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

7 Map analysis [i](#)

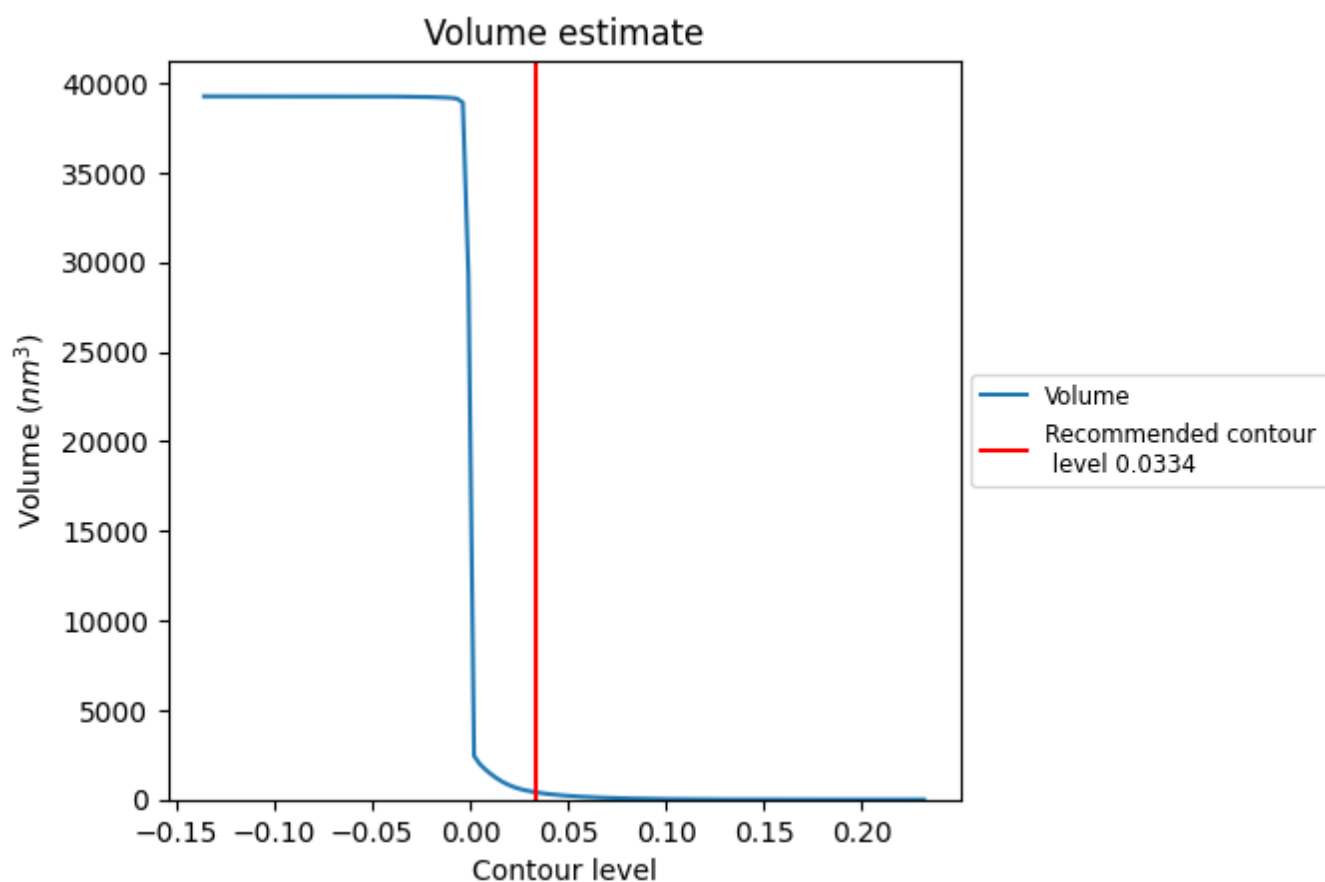
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

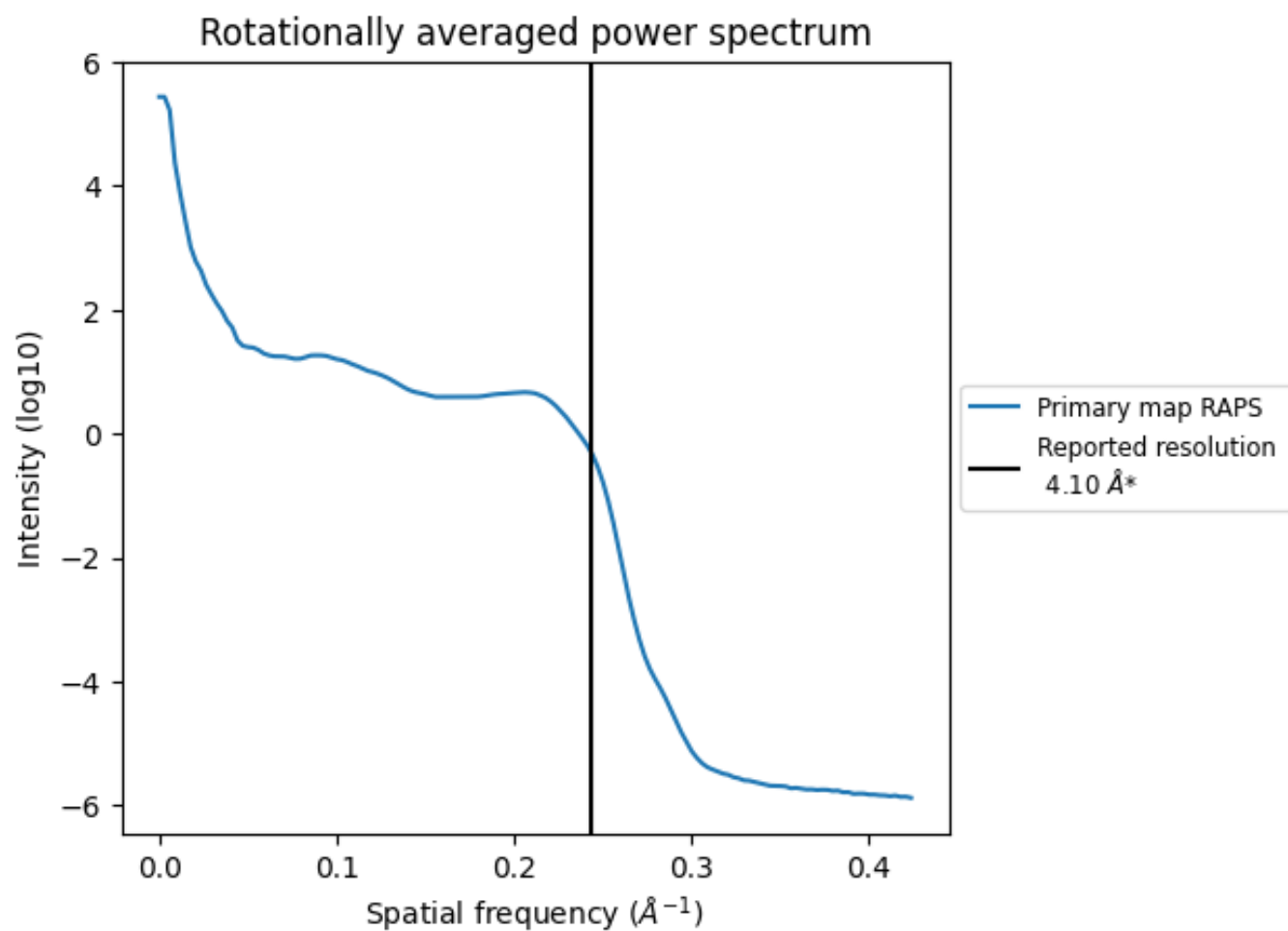
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 406 nm³; this corresponds to an approximate mass of 366 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

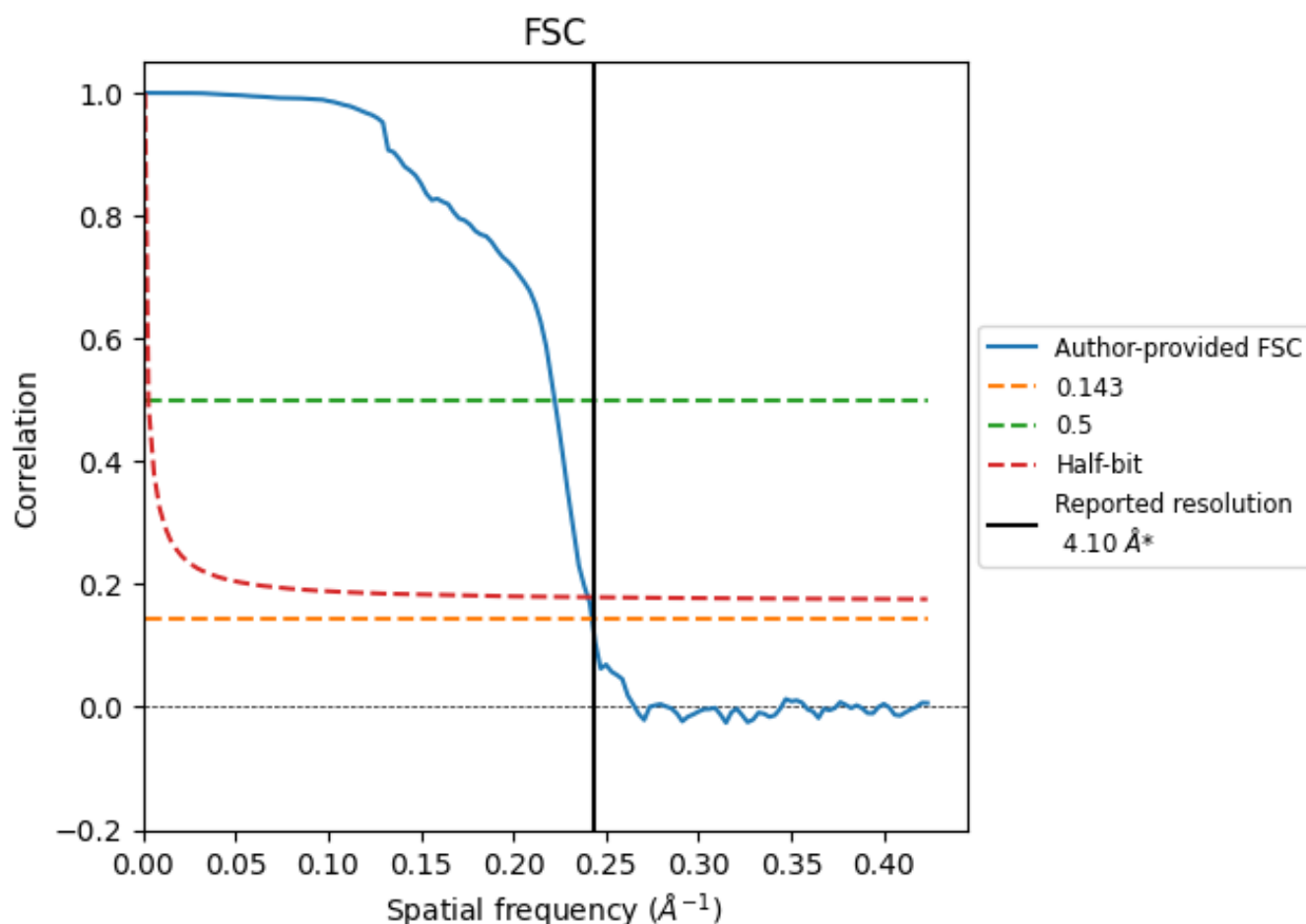


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.50	4.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

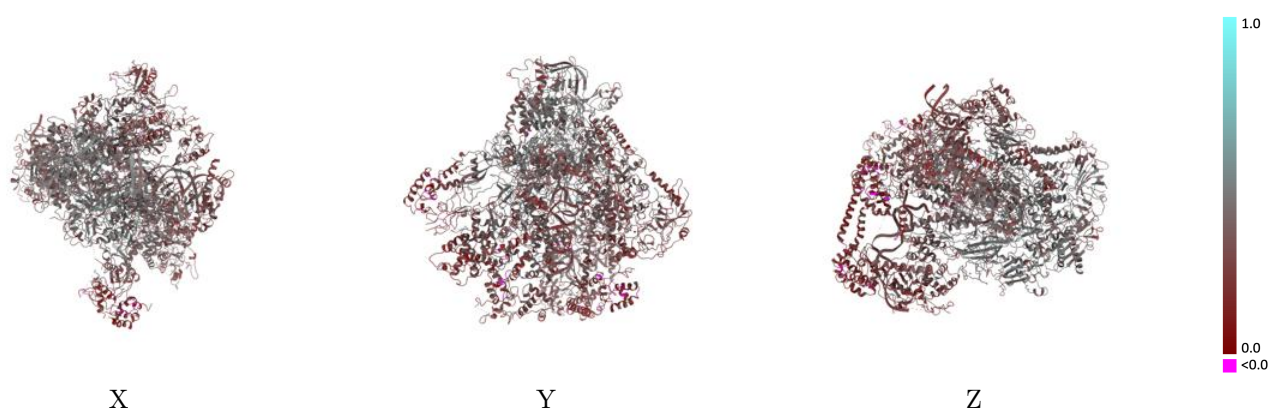
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7530 and PDB model 6CNB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

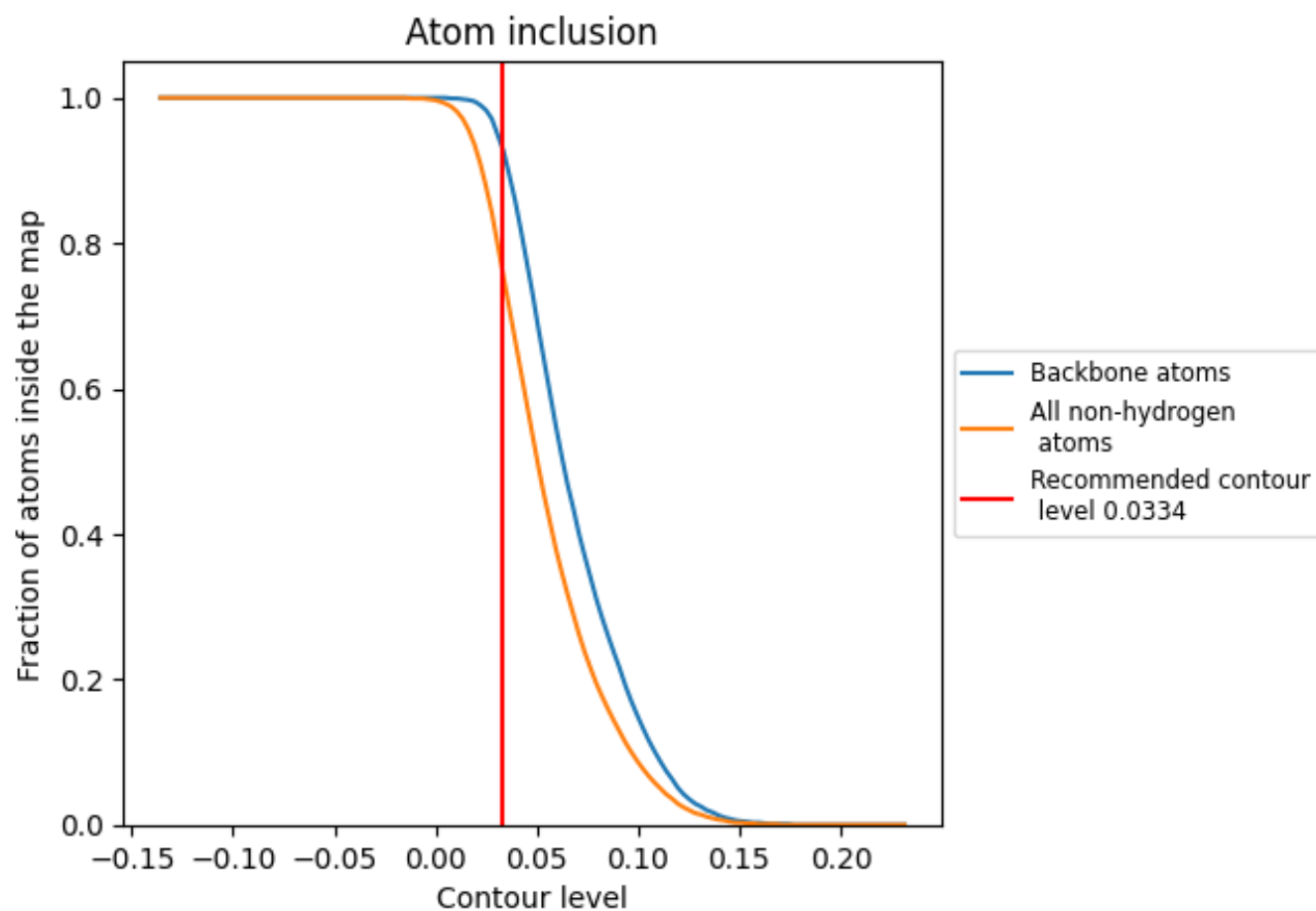


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.3550
A	 0.7800	 0.3950
B	 0.7980	 0.4100
C	 0.8810	 0.4270
D	 0.6120	 0.2080
E	 0.7900	 0.3510
F	 0.8790	 0.4450
G	 0.7440	 0.2830
H	 0.8350	 0.4160
I	 0.7350	 0.3120
J	 0.8950	 0.4390
K	 0.8610	 0.4380
L	 0.8210	 0.4270
M	 0.6700	 0.2820
N	 0.7000	 0.2880
O	 0.7070	 0.3040
P	 0.6070	 0.2680
Q	 0.8660	 0.3680
R	 0.6680	 0.2830
S	 0.5590	 0.2440
X	 0.8890	 0.3240
Y	 0.8460	 0.3270

