



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:33 PM UTC

PDB ID : 5N5Y / pdb_00005n5y
EMDB ID : EMD-3590
Title : Cryo-EM structure of RNA polymerase I in complex with Rrn3 and Core Factor (Orientation III)
Authors : Engel, C.; Gubbey, T.; Neyer, S.; Sainsbury, S.; Oberthuer, C.; Baejen, C.; Bernecky, C.; Cramer, P.
Deposited on : 2017-02-14
Resolution : 7.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

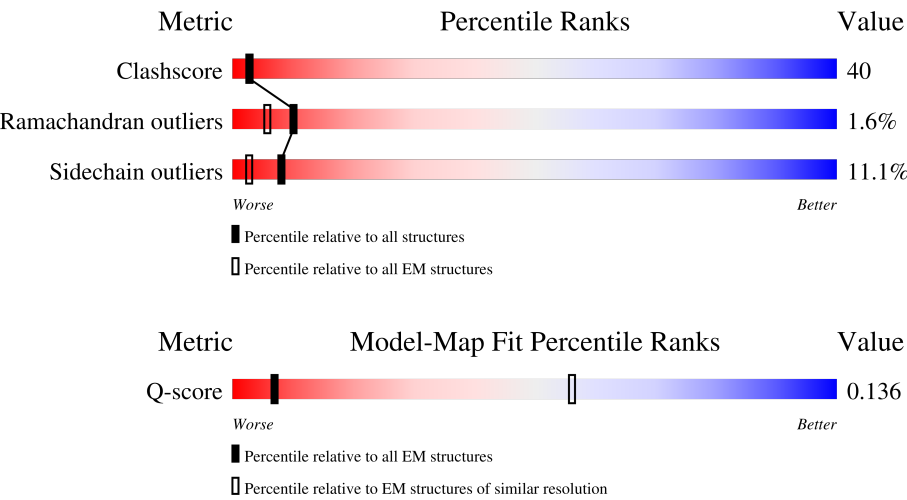
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 7.70 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.



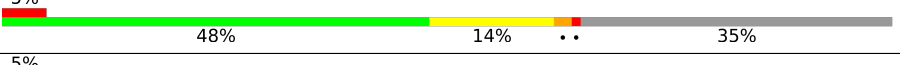
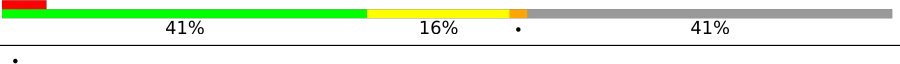
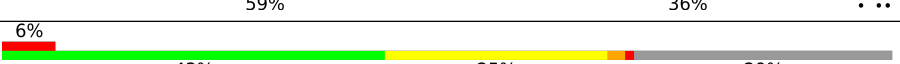
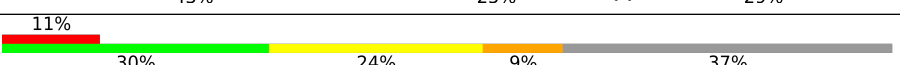
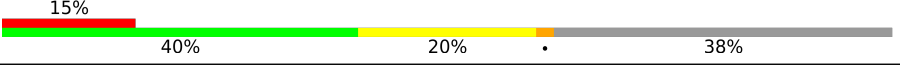
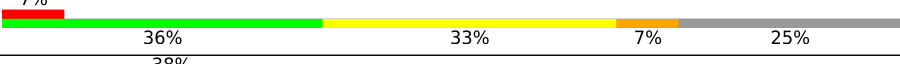
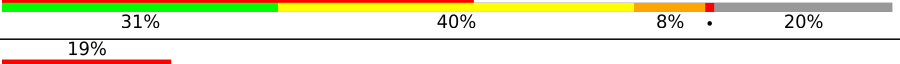
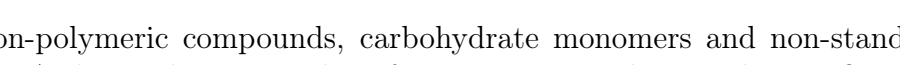
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	384 (7.20 - 8.20)

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	1664	
2	B	1203	
3	C	335	
4	D	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	
16	P	894	
17	Q	514	
18	R	507	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	SO4	R	601	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 48030 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1467	Total	C	N	O	S	0	0
			11598	7327	2017	2193	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0
			9312	5891	1633	1738	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1526	985	262	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	99	Total	C	N	O	S	0	0
			755	472	125	149	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	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
			793	496	130	162	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	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	108	Total	C	N	O		0	0
			856	543	142	171			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	473	Total	C	N	O	S	0	0
			3907	2533	642	711	21		

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	583	Total	C	N	O	S	0	0
			4729	3010	803	905	11		

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	410	Total	C	N	O	S	0	0
			3421	2219	579	603	20		

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	303	Total	C	N	O	S	0	0
			2535	1634	456	434	11		

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

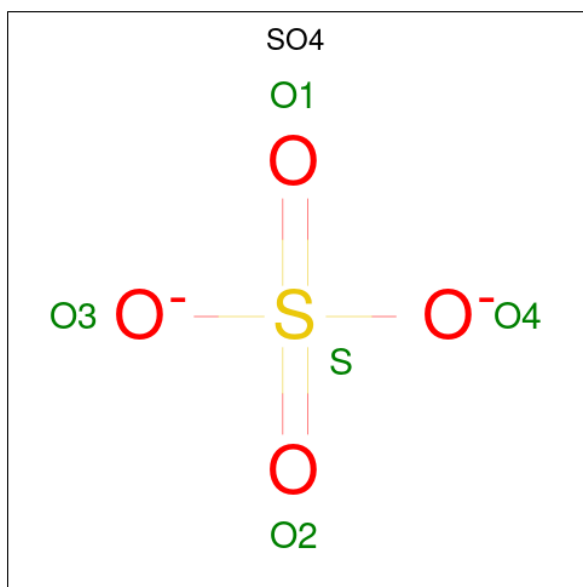
Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	
19	J	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
19	L	1	Total	Zn	0
			1	1	
19	Q	1	Total	Zn	0
			1	1	

- Molecule 20 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
20	P	1	Total	O	S	0
			5	4	1	
20	P	1	Total	O	S	0
			5	4	1	
20	P	1	Total	O	S	0
			5	4	1	
20	Q	1	Total	O	S	0
			5	4	1	
20	R	1	Total	O	S	0
			5	4	1	

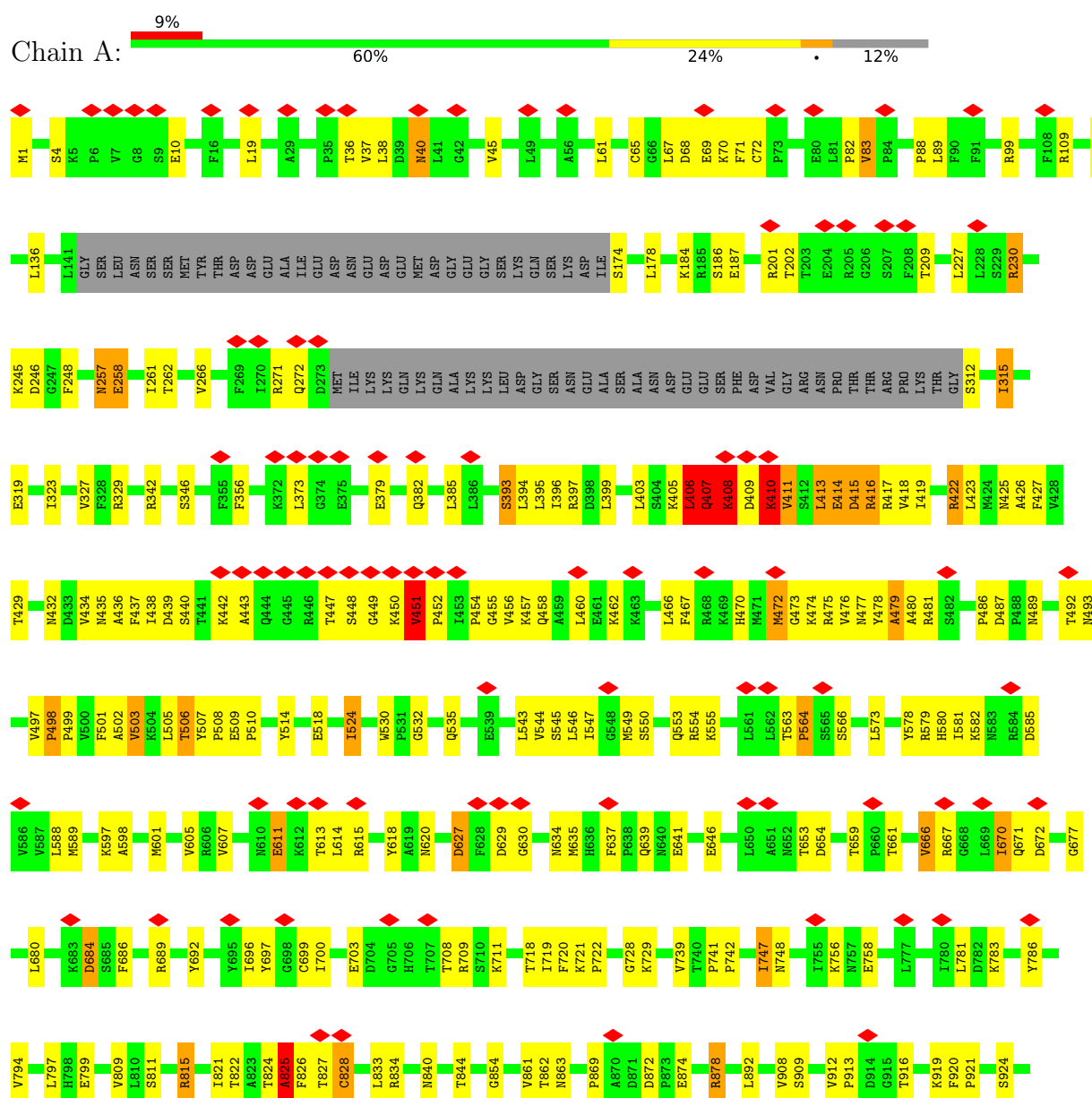
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

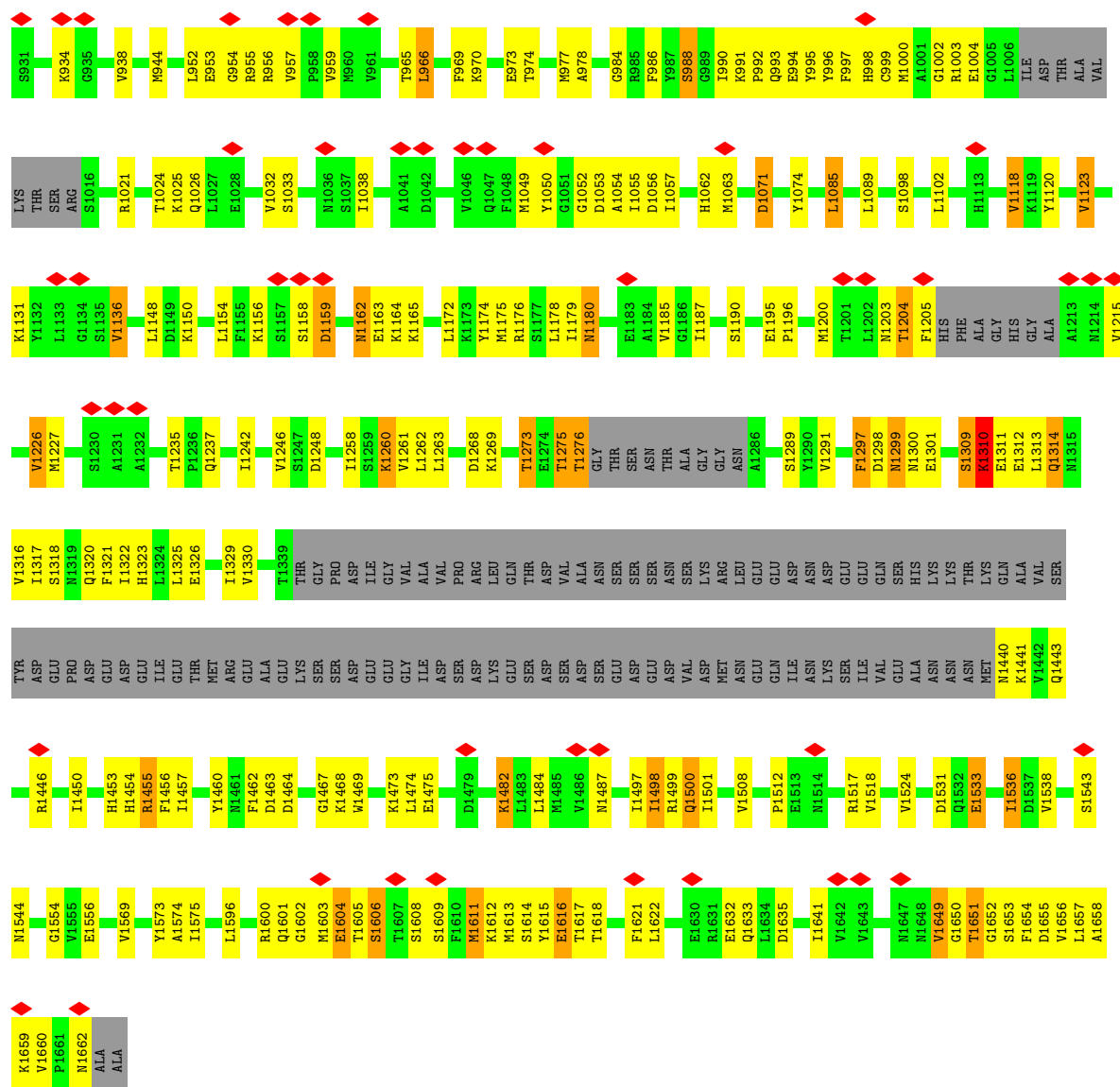
Mol	Chain	Residues	Atoms		AltConf
21	R	1	Total	Mg	0
			1	1	

3 Residue-property plots

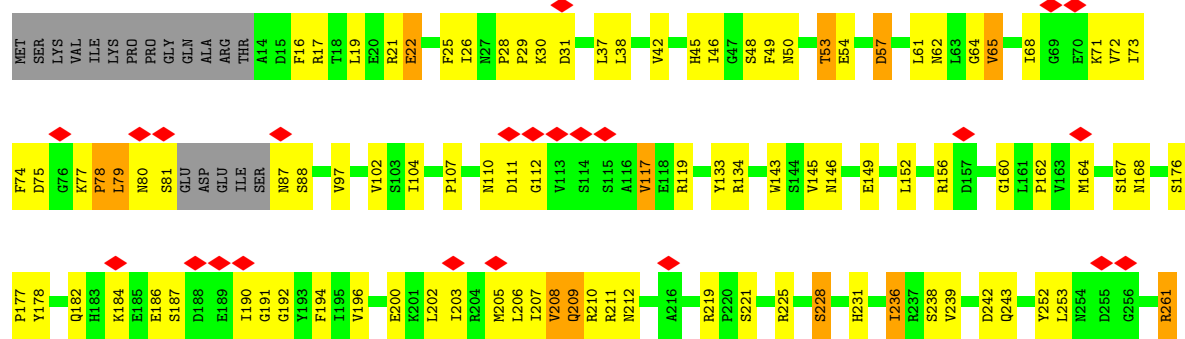
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

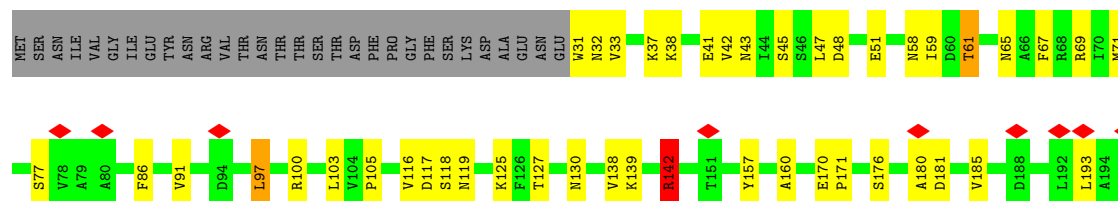
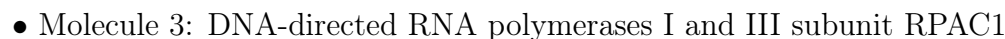
- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

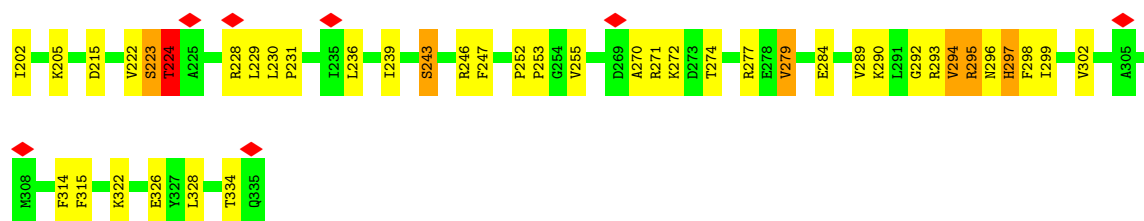




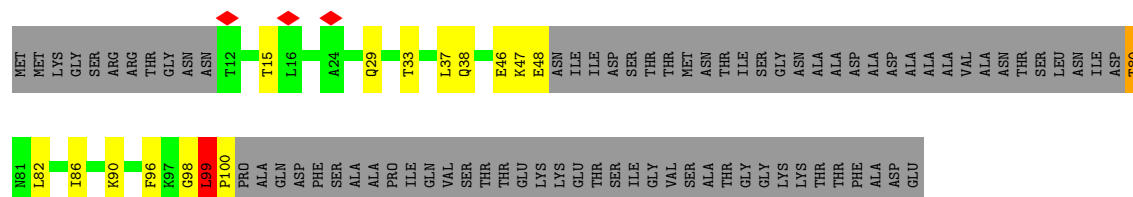
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135



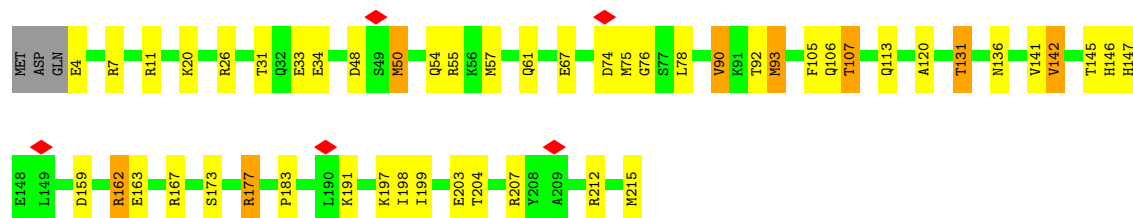
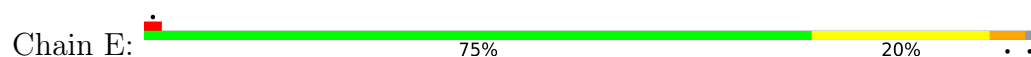




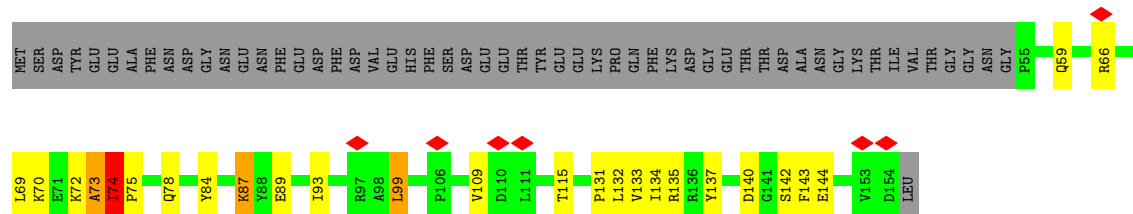
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



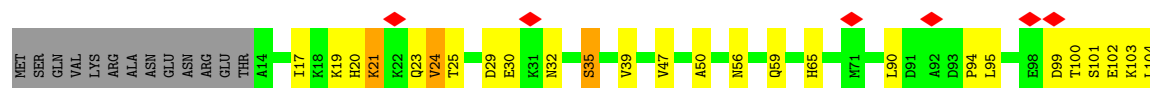
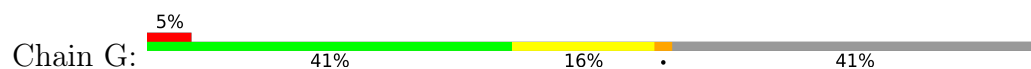
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

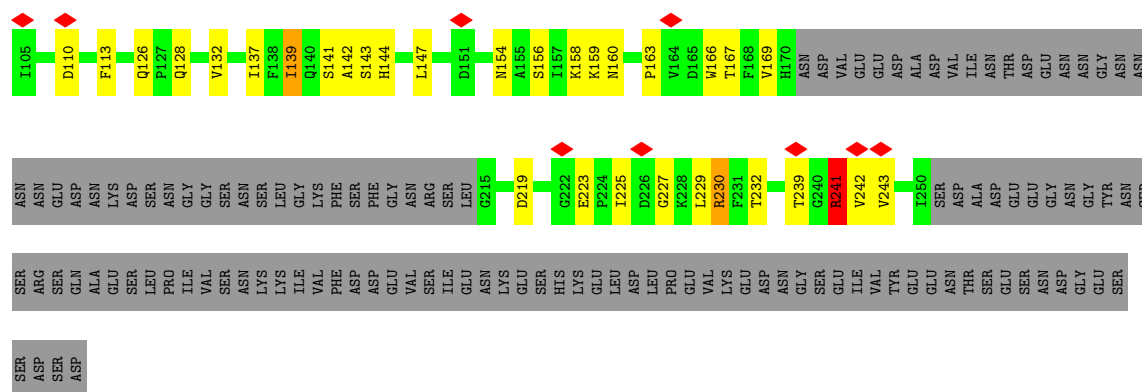


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

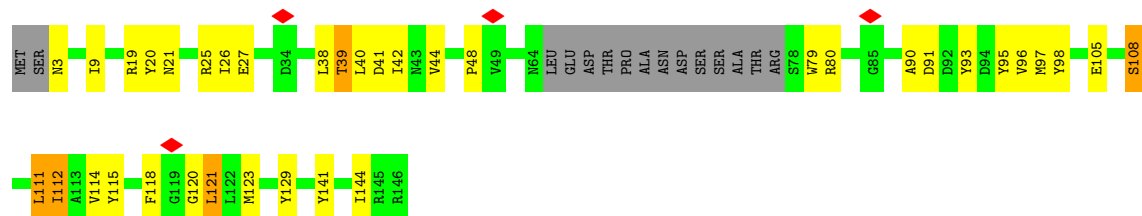


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

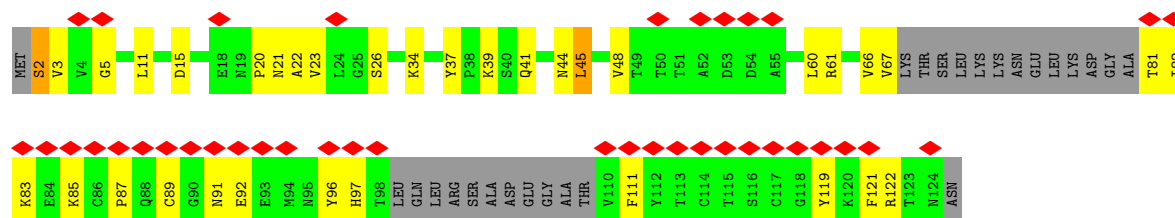




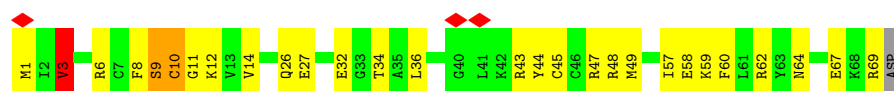
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



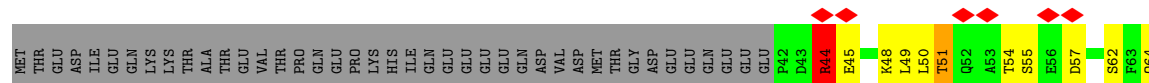
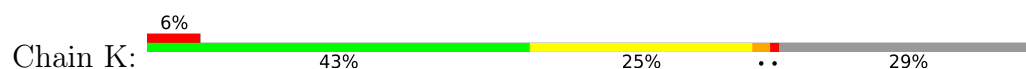
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

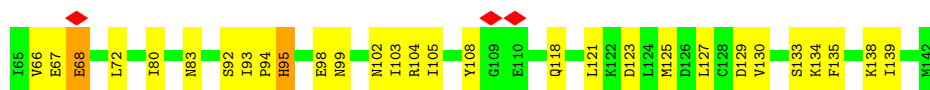


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

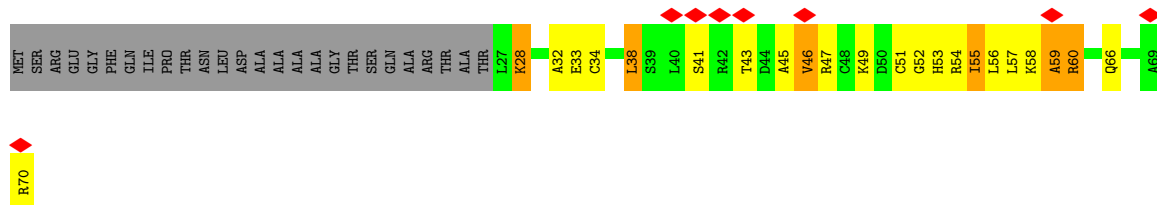
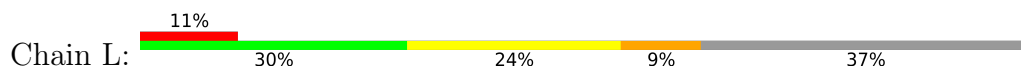


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

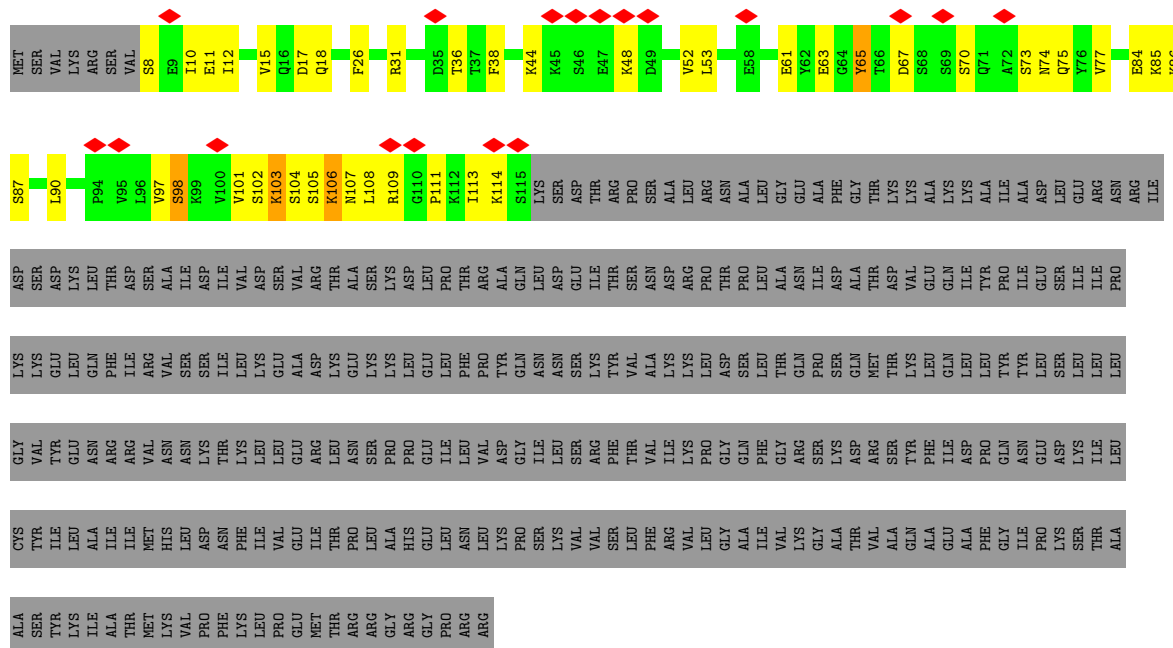




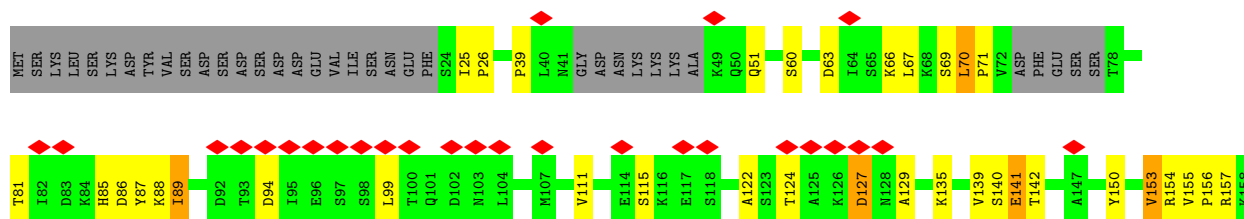
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



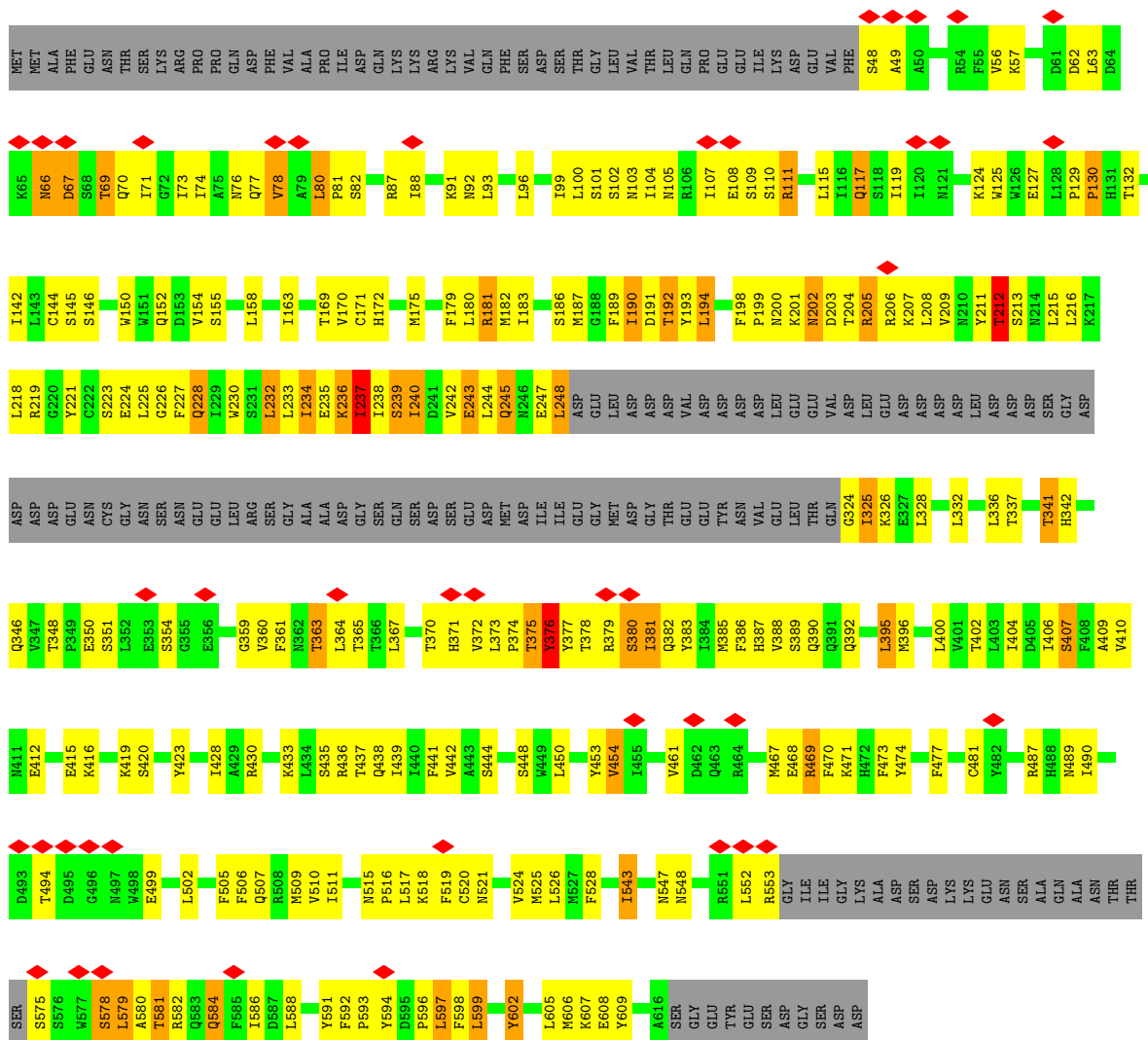
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



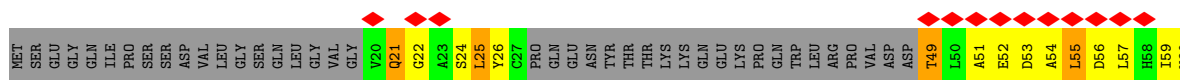
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

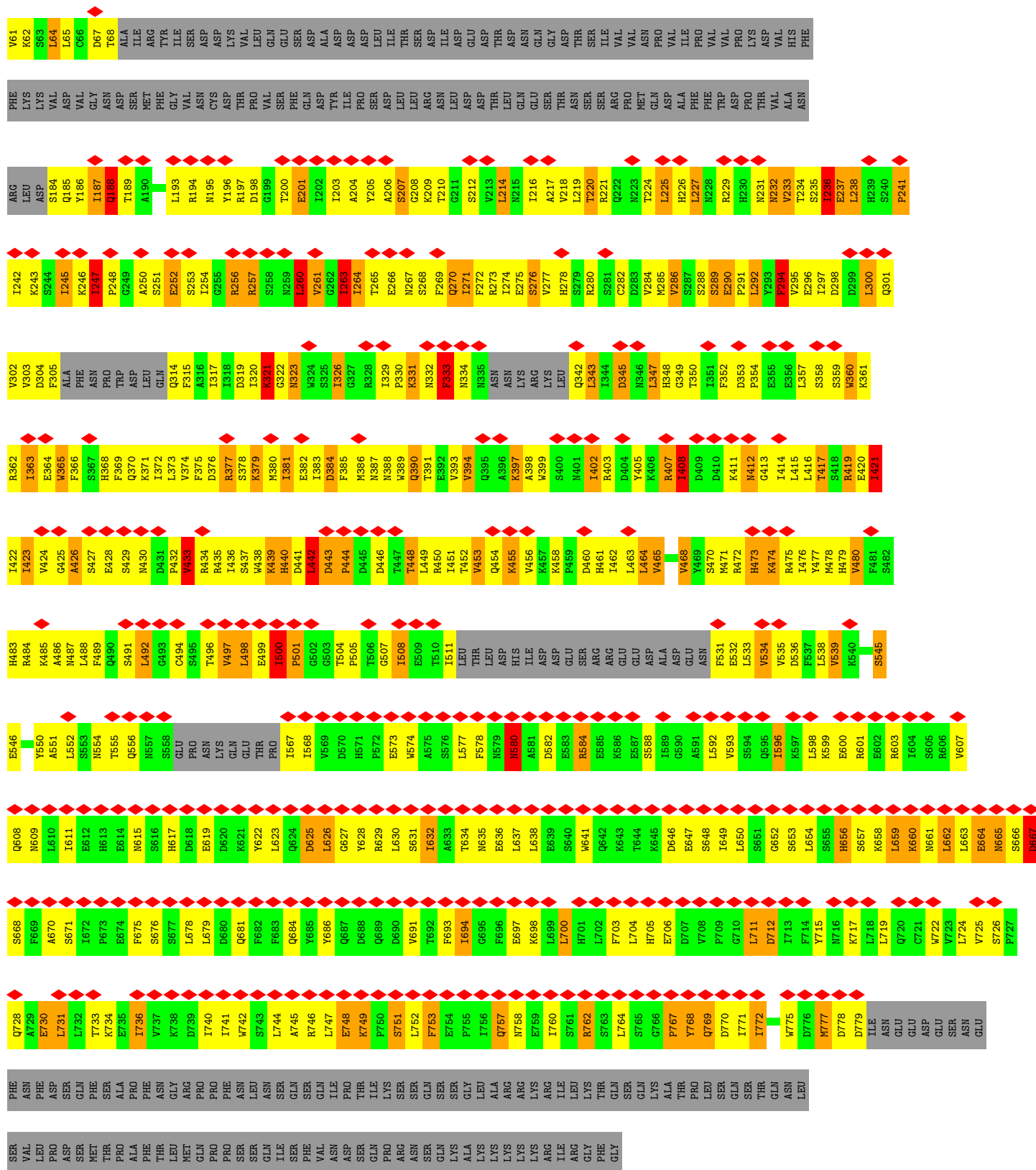


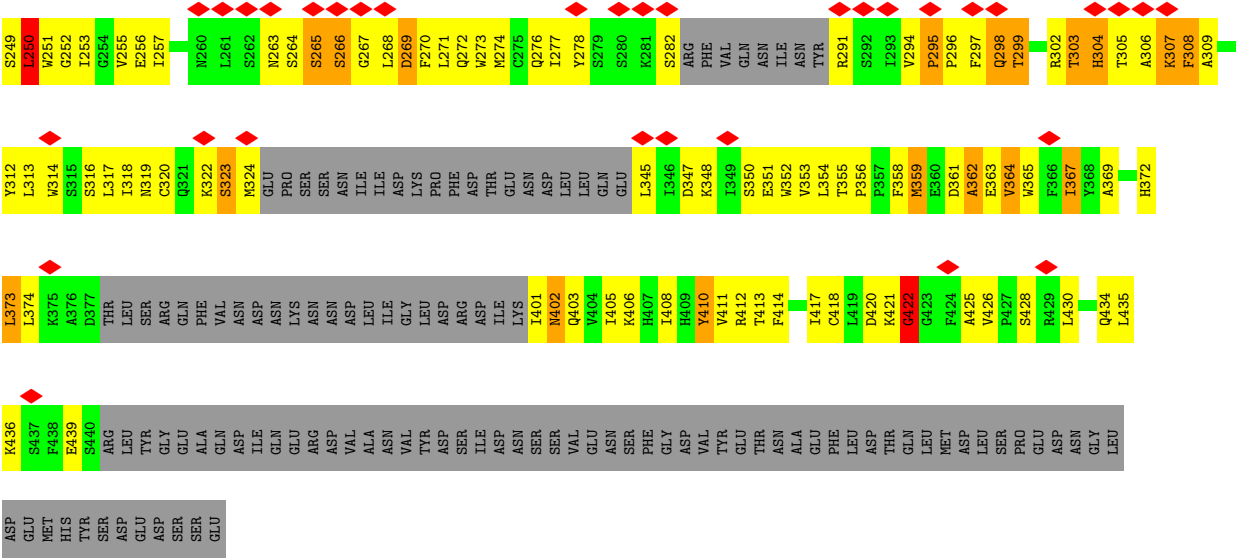
- Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3



- Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	0.068	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0205	Depositor
Map size ($\text{\AA}$)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	1/11809 (0.0%)	0.96	36/15943 (0.2%)
2	B	0.62	0/9518	0.98	36/12863 (0.3%)
3	C	0.53	0/2475	0.94	8/3354 (0.2%)
4	D	0.52	0/465	0.81	0/630
5	E	0.49	0/1771	0.88	3/2383 (0.1%)
6	F	0.58	0/838	0.85	0/1129
7	G	0.50	0/1563	0.84	3/2124 (0.1%)
8	H	0.52	0/1070	0.88	0/1449
9	I	0.53	0/765	0.87	0/1030
10	J	0.59	0/578	0.98	6/775 (0.8%)
11	K	0.54	0/804	0.93	6/1083 (0.6%)
12	L	0.50	0/354	0.91	2/468 (0.4%)
13	M	0.49	0/872	0.87	0/1170
14	N	0.48	0/1172	0.88	1/1580 (0.1%)
15	O	0.45	1/3996 (0.0%)	0.82	2/5401 (0.0%)
16	P	0.38	0/4822	0.74	6/6525 (0.1%)
17	Q	0.36	1/3502 (0.0%)	0.67	2/4727 (0.0%)
18	R	0.34	1/2592 (0.0%)	0.76	3/3486 (0.1%)
All	All	0.54	4/48966 (0.0%)	0.89	114/66120 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
2	B	0	4
3	C	0	1
6	F	0	1
12	L	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	3
14	N	0	1
15	O	0	4
16	P	0	26
17	Q	0	8
18	R	0	10
All	All	0	75

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	PHE	C-N	8.50	1.44	1.33
17	Q	15	CYS	CA-C	7.48	1.62	1.52
15	O	212	THR	CA-CB	5.50	1.62	1.53
18	R	206	ARG	CA-C	5.33	1.58	1.53

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	205	VAL	N-CA-C	18.74	128.15	110.53
18	R	206	ARG	N-CA-C	13.29	126.46	110.91
2	B	405	GLY	N-CA-C	-12.25	97.20	113.24
1	A	1071	ASP	N-CA-C	-9.88	97.50	110.53
3	C	223	SER	N-CA-C	-9.71	101.59	112.57
15	O	376	TYR	N-CA-C	-9.46	100.41	113.56
17	Q	7	GLY	C-N-CD	-9.27	87.00	125.00
1	A	956	ARG	CA-C-O	8.52	122.88	117.94
1	A	666	VAL	CB-CA-C	-8.46	102.36	110.65
2	B	537	SER	CA-C-N	-7.83	111.92	121.00
2	B	537	SER	C-N-CA	-7.83	111.92	121.00
16	P	442	LEU	CA-C-N	-7.77	113.31	123.34
16	P	442	LEU	C-N-CA	-7.77	113.31	123.34
2	B	1074	MET	N-CA-C	-7.70	102.86	111.71
3	C	279	VAL	CB-CA-C	-7.42	102.39	111.88
2	B	893	ASN	N-CA-C	7.38	120.25	111.02
1	A	201	ARG	N-CA-C	6.96	120.86	112.38
1	A	356	PHE	O-C-N	-6.79	113.22	122.94
2	B	894	LYS	CB-CA-C	-6.60	108.26	117.23
2	B	1103	VAL	CB-CA-C	-6.57	100.70	110.82
2	B	219	ARG	CA-C-N	6.55	128.03	119.84
2	B	219	ARG	C-N-CA	6.55	128.03	119.84
1	A	1123	VAL	CB-CA-C	-6.53	103.48	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	GLU	N-CA-C	6.47	119.73	109.50
2	B	1023	ARG	NE-CZ-NH2	-6.43	113.42	119.20
3	C	295	ARG	N-CA-C	6.41	118.06	111.14
1	A	397	ARG	CD-NE-CZ	6.39	133.34	124.40
2	B	261	ARG	CD-NE-CZ	6.32	133.25	124.40
2	B	622	ILE	CB-CA-C	-6.29	102.87	112.05
10	J	64	ASN	CA-C-N	6.28	125.98	119.82
10	J	64	ASN	C-N-CA	6.28	125.98	119.82
5	E	203	GLU	N-CA-C	-6.24	104.58	111.82
2	B	452	ARG	NE-CZ-NH2	-6.12	113.69	119.20
2	B	72	VAL	N-CA-C	6.06	117.20	108.48
2	B	448	ARG	NE-CZ-NH2	-6.03	113.77	119.20
2	B	452	ARG	CD-NE-CZ	6.01	132.81	124.40
1	A	329	ARG	NE-CZ-NH2	-5.97	113.82	119.20
16	P	394	VAL	N-CA-C	5.96	119.39	111.17
2	B	658	LEU	N-CA-C	-5.92	100.90	109.31
1	A	258	GLU	N-CA-C	5.92	118.21	111.11
2	B	832	TRP	CA-C-N	5.89	127.20	119.84
2	B	832	TRP	C-N-CA	5.89	127.20	119.84
1	A	416	ARG	NE-CZ-NH2	-5.84	113.94	119.20
2	B	429	ARG	NE-CZ-NH2	-5.84	113.95	119.20
1	A	329	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	956	ARG	CB-CA-C	-5.76	108.77	117.07
16	P	188	GLN	N-CA-C	5.76	123.06	110.80
2	B	448	ARG	CD-NE-CZ	5.74	132.43	124.40
16	P	443	ASP	N-CA-C	5.73	119.39	108.97
5	E	167	ARG	NE-CZ-NH2	-5.69	114.08	119.20
2	B	634	ARG	CD-NE-CZ	5.67	132.34	124.40
11	K	95	HIS	CA-C-N	5.66	126.92	119.84
11	K	95	HIS	C-N-CA	5.66	126.92	119.84
11	K	44	ARG	CD-NE-CZ	5.66	132.32	124.40
17	Q	15	CYS	CA-C-O	-5.66	112.41	120.16
1	A	1261	VAL	N-CA-C	5.65	116.25	108.12
1	A	1203	ASN	N-CA-C	5.64	117.65	109.07
1	A	422	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	659	THR	CA-C-N	-5.62	113.97	119.64
1	A	659	THR	C-N-CA	-5.62	113.97	119.64
1	A	356	PHE	CA-C-N	5.61	130.68	122.77
1	A	356	PHE	C-N-CA	5.61	130.68	122.77
1	A	416	ARG	CD-NE-CZ	5.59	132.23	124.40
2	B	429	ARG	CD-NE-CZ	5.59	132.23	124.40
11	K	44	ARG	NE-CZ-NH2	-5.58	114.18	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	250	LEU	CA-CB-CG	5.57	135.78	116.30
1	A	1498	ILE	N-CA-C	5.56	115.75	110.42
16	P	333	PHE	N-CA-C	5.55	117.44	108.34
1	A	549	MET	N-CA-C	5.52	119.10	110.32
1	A	498	PRO	CA-C-N	5.52	125.35	119.28
1	A	498	PRO	C-N-CA	5.52	125.35	119.28
12	L	28	LYS	N-CA-C	5.52	118.05	111.71
1	A	825	ALA	CB-CA-C	-5.49	110.27	116.63
2	B	634	ARG	NE-CZ-NH2	-5.49	114.26	119.20
2	B	1082	HIS	N-CA-C	5.48	117.34	111.36
2	B	261	ARG	NE-CZ-NH2	-5.48	114.27	119.20
10	J	3	VAL	CA-C-N	-5.45	114.34	119.85
10	J	3	VAL	C-N-CA	-5.45	114.34	119.85
3	C	142	ARG	CD-NE-CZ	5.45	132.02	124.40
7	G	241	ARG	CD-NE-CZ	5.39	131.95	124.40
14	N	127	ASP	N-CA-C	-5.39	106.19	114.16
5	E	167	ARG	CD-NE-CZ	5.38	131.93	124.40
12	L	52	GLY	N-CA-C	-5.38	107.84	115.43
1	A	397	ARG	NE-CZ-NH1	5.36	126.86	121.50
2	B	1072	GLY	CA-C-N	5.35	127.89	120.29
2	B	1072	GLY	C-N-CA	5.35	127.89	120.29
7	G	241	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	A	825	ALA	N-CA-C	5.34	117.11	108.08
15	O	580	ALA	N-CA-C	-5.34	105.36	111.07
1	A	245	LYS	N-CA-C	5.34	117.98	109.65
1	A	1543	SER	CA-C-N	5.29	127.80	120.29
1	A	1543	SER	C-N-CA	5.29	127.80	120.29
1	A	1482	LYS	N-CA-C	5.28	117.89	110.23
1	A	397	ARG	NE-CZ-NH2	-5.28	114.45	119.20
3	C	185	VAL	CA-C-N	-5.26	114.50	119.76
3	C	185	VAL	C-N-CA	-5.26	114.50	119.76
2	B	1048	SER	N-CA-C	5.25	116.81	111.14
7	G	219	ASP	N-CA-C	5.24	116.75	109.31
1	A	329	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	422	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	342	ARG	CD-NE-CZ	5.17	131.63	124.40
10	J	9	SER	CA-C-N	5.16	127.45	120.44
10	J	9	SER	C-N-CA	5.16	127.45	120.44
2	B	1054	SER	N-CA-C	5.13	117.53	111.33
3	C	142	ARG	NE-CZ-NH2	-5.10	114.61	119.20
11	K	83	ASN	CA-C-N	5.10	124.76	119.56
11	K	83	ASN	C-N-CA	5.10	124.76	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1524	VAL	N-CA-C	5.09	115.45	108.12
2	B	314	LYS	N-CA-C	-5.09	103.76	110.43
2	B	88	SER	N-CA-C	5.08	118.08	109.76
2	B	1110	ILE	CB-CA-C	-5.08	105.46	111.65
2	B	511	GLN	N-CA-C	-5.06	107.15	113.38
2	B	261	ARG	NE-CZ-NH1	5.06	126.56	121.50
2	B	448	ARG	NE-CZ-NH1	5.03	126.53	121.50

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1180	ASN	Peptide
1	A	1260	LYS	Peptide
1	A	1297	PHE	Peptide
1	A	1309	SER	Peptide
1	A	1310	LYS	Peptide
1	A	1649	VAL	Peptide
1	A	405	LYS	Peptide
1	A	406	LEU	Peptide
1	A	407	GLN	Peptide
1	A	410	LYS	Peptide
1	A	411	VAL	Peptide
1	A	506	THR	Peptide
1	A	781	LEU	Peptide
1	A	825	ALA	Peptide
1	A	828	CYS	Peptide
2	B	1049	THR	Peptide
2	B	1068	GLY	Peptide
2	B	404	LEU	Peptide
2	B	550	ARG	Peptide
3	C	294	VAL	Peptide
6	F	73	ALA	Peptide
12	L	59	ALA	Peptide
12	L	60	ARG	Peptide
13	M	103	LYS	Peptide
13	M	106	LYS	Peptide
13	M	107	ASN	Peptide
14	N	141	GLU	Peptide
15	O	236	LYS	Peptide
15	O	243	GLU	Peptide
15	O	375	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
15	O	380	SER	Peptide
16	P	216	ILE	Peptide
16	P	236	ILE	Peptide
16	P	238	LEU	Peptide
16	P	247	ILE	Peptide
16	P	256	ARG	Peptide
16	P	260	LEU	Peptide
16	P	263	ILE	Peptide
16	P	270	GLN	Peptide
16	P	289	SER	Peptide
16	P	294	PHE	Peptide
16	P	295	VAL	Peptide
16	P	333	PHE	Peptide
16	P	365	TRP	Peptide
16	P	393	VAL	Peptide
16	P	408	ILE	Peptide
16	P	433	VAL	Peptide
16	P	442	LEU	Peptide
16	P	485	LYS	Peptide
16	P	500	ILE	Peptide
16	P	51	ALA	Peptide
16	P	52	GLU	Peptide
16	P	580	ASN	Peptide
16	P	661	ASN	Peptide
16	P	667	ASP	Peptide
16	P	767	PRO	Peptide
16	P	769	GLN	Peptide
17	Q	148	PRO	Peptide
17	Q	15	CYS	Peptide
17	Q	17	SER	Peptide
17	Q	221	PRO	Peptide
17	Q	25	GLY	Peptide
17	Q	29	CYS	Peptide
17	Q	290	THR	Peptide
17	Q	4	PHE	Peptide
18	R	154	LYS	Peptide
18	R	206	ARG	Peptide
18	R	247	ILE	Peptide
18	R	263	ASN	Peptide
18	R	265	SER	Peptide
18	R	303	THR	Peptide
18	R	304	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	R	422	GLY	Peptide
18	R	425	ALA	Peptide
18	R	9	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11598	0	11666	1191	0
2	B	9312	0	9200	1004	0
3	C	2423	0	2412	143	0
4	D	459	0	462	8	0
5	E	1735	0	1764	33	0
6	F	823	0	839	96	0
7	G	1526	0	1534	155	0
8	H	1052	0	1021	57	0
9	I	755	0	728	108	0
10	J	569	0	584	56	0
11	K	793	0	790	58	0
12	L	352	0	371	59	0
13	M	856	0	852	60	0
14	N	1151	0	1168	167	0
15	O	3907	0	3902	416	0
16	P	4729	0	4670	585	0
17	Q	3421	0	3463	452	0
18	R	2535	0	2606	609	0
19	A	2	0	0	1	0
19	B	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	Q	1	0	0	0	0
20	P	15	0	0	2	0
20	Q	5	0	0	1	0
20	R	5	0	0	4	0
21	R	1	0	0	0	0
All	All	48030	0	48032	3867	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 40.

All (3867) 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)
3:C:272:LYS:HA	14:N:175:TYR:CE1	1.16	1.69
1:A:990:ILE:CB	1:A:994:GLU:HB2	1.19	1.66
1:A:995:TYR:CD2	2:B:708:ASP:HA	1.29	1.65
16:P:473:HIS:CD2	18:R:1:MET:HB2	1.16	1.63
17:Q:20:TRP:CZ3	17:Q:22:ILE:CG2	1.76	1.62
15:O:248:LEU:HD12	15:O:598:PHE:CD2	1.32	1.61
17:Q:12:THR:HG21	17:Q:33:HIS:CE1	1.12	1.60
17:Q:20:TRP:HZ3	17:Q:22:ILE:CG2	1.10	1.60
6:F:72:LYS:HB3	6:F:142:SER:CA	1.30	1.59
1:A:545:SER:HB2	17:Q:34:VAL:CG2	1.14	1.59
13:M:102:SER:HB3	13:M:105:SER:CB	1.28	1.58
17:Q:12:THR:CG2	17:Q:33:HIS:HE1	1.10	1.58
15:O:200:ASN:HB2	17:Q:14:ASN:CB	1.34	1.57
18:R:5:PRO:HG2	18:R:217:THR:CG2	1.16	1.57
1:A:1322:ILE:HG22	1:A:1454:HIS:CD2	1.37	1.57
1:A:1484:LEU:HD13	2:B:305:ARG:CZ	1.24	1.56
7:G:143:SER:HB2	15:O:104:ILE:CG2	1.36	1.55
2:B:152:LEU:CB	2:B:443:LYS:HE3	1.37	1.55
15:O:200:ASN:CG	17:Q:14:ASN:HB2	1.30	1.54
1:A:1575:ILE:CG1	9:I:122:ARG:NH1	1.68	1.54
7:G:143:SER:CB	15:O:104:ILE:HG22	1.33	1.53
2:B:152:LEU:HB3	2:B:443:LYS:CE	1.34	1.53
15:O:200:ASN:CB	17:Q:14:ASN:HB2	1.07	1.53
15:O:248:LEU:CD1	15:O:598:PHE:CD2	1.92	1.52
1:A:990:ILE:HB	1:A:994:GLU:CB	1.06	1.52
15:O:248:LEU:CD1	15:O:598:PHE:CE2	1.93	1.51
1:A:1049:MET:HG2	1:A:1052:GLY:C	1.30	1.51
2:B:679:GLN:CG	14:N:157:ARG:N	1.75	1.50
16:P:473:HIS:HD2	18:R:1:MET:CB	1.19	1.50
15:O:248:LEU:HD12	15:O:598:PHE:CE2	0.97	1.49
1:A:545:SER:CB	17:Q:34:VAL:HG21	1.01	1.49
2:B:527:PHE:CD1	2:B:666:PRO:HG3	1.47	1.49
3:C:272:LYS:CA	14:N:175:TYR:CE1	1.92	1.48
3:C:253:PRO:CD	14:N:180:PHE:HB3	1.09	1.48
1:A:547:ILE:CD1	17:Q:26:ARG:NH1	1.68	1.48
6:F:72:LYS:CD	6:F:142:SER:HB3	1.43	1.48
2:B:143:TRP:HB2	2:B:446:MET:CE	1.43	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:PHE:CZ	2:B:666:PRO:HA	1.49	1.47
2:B:207:ILE:HG13	2:B:503:VAL:CG2	1.41	1.47
16:P:436:ILE:HG22	18:R:142:ARG:C	1.07	1.46
18:R:5:PRO:CG	18:R:217:THR:CB	1.92	1.46
18:R:251:TRP:CE3	18:R:307:LYS:HE3	1.50	1.46
1:A:547:ILE:HD11	17:Q:26:ARG:NH1	1.18	1.45
2:B:848:ILE:CB	12:L:60:ARG:HD2	1.46	1.45
17:Q:358:PRO:CA	18:R:206:ARG:HH12	1.29	1.45
3:C:58:ASN:HA	3:C:296:ASN:ND2	1.18	1.44
7:G:141:SER:HB3	15:O:142:ILE:CD1	1.46	1.44
2:B:68:ILE:HG21	2:B:71:LYS:NZ	1.32	1.43
2:B:1089:GLN:CG	2:B:1093:LEU:HD22	1.46	1.43
18:R:5:PRO:CG	18:R:217:THR:HB	1.44	1.43
14:N:87:TYR:CA	14:N:141:GLU:HA	1.48	1.43
1:A:597:LYS:HB2	2:B:1082:HIS:NE2	1.23	1.42
1:A:878:ARG:HB3	9:I:67:VAL:CG1	1.47	1.42
18:R:251:TRP:CE3	18:R:307:LYS:CE	2.01	1.42
1:A:1297:PHE:CE2	1:A:1301:GLU:OE1	1.70	1.41
1:A:629:ASP:C	2:B:926:VAL:HG21	1.42	1.41
1:A:429:THR:HG21	18:R:406:LYS:CE	1.50	1.41
3:C:272:LYS:HA	14:N:175:TYR:CZ	1.51	1.41
16:P:397:LYS:HZ1	18:R:85:ARG:NH1	1.18	1.41
1:A:756:LYS:CD	9:I:85:LYS:NZ	1.79	1.41
7:G:159:LYS:H	15:O:105:ASN:ND2	0.91	1.41
6:F:72:LYS:CB	6:F:142:SER:HA	1.50	1.40
15:O:240:ILE:HG22	15:O:380:SER:CB	1.48	1.40
1:A:1326:GLU:CD	1:A:1455:ARG:N	1.76	1.40
2:B:679:GLN:CG	14:N:156:PRO:C	1.92	1.40
2:B:143:TRP:CE3	2:B:446:MET:HG3	1.57	1.40
1:A:597:LYS:HB2	2:B:1082:HIS:CD2	1.58	1.38
3:C:253:PRO:HD2	14:N:180:PHE:CB	1.31	1.38
2:B:207:ILE:CG1	2:B:503:VAL:HG21	1.49	1.38
13:M:102:SER:CB	13:M:105:SER:HB3	1.13	1.38
16:P:397:LYS:HE2	18:R:85:ARG:NE	1.38	1.38
1:A:1322:ILE:HD12	1:A:1457:ILE:CD1	1.53	1.37
7:G:141:SER:CB	15:O:142:ILE:HD12	1.54	1.37
16:P:397:LYS:HZ1	18:R:85:ARG:CZ	1.36	1.37
16:P:436:ILE:CG2	18:R:142:ARG:O	1.72	1.37
6:F:74:ILE:O	7:G:95:LEU:CD1	1.69	1.36
7:G:159:LYS:N	15:O:105:ASN:ND2	1.70	1.36
1:A:1322:ILE:CG2	1:A:1454:HIS:CG	2.08	1.35

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:5:PRO:CG	18:R:217:THR:CG2	2.01	1.35
15:O:200:ASN:CB	17:Q:14:ASN:CB	1.95	1.35
17:Q:351:ASN:HB3	17:Q:369:TRP:CH2	1.61	1.35
1:A:999:CYS:HA	2:B:712:SER:CB	1.54	1.34
16:P:397:LYS:CE	18:R:85:ARG:NE	1.90	1.34
1:A:547:ILE:HD12	17:Q:26:ARG:CZ	1.53	1.34
2:B:743:ARG:NH2	10:J:60:PHE:CZ	1.96	1.34
2:B:143:TRP:CG	2:B:446:MET:SD	2.21	1.34
2:B:848:ILE:HB	12:L:60:ARG:CD	1.56	1.34
15:O:234:ILE:CG2	15:O:237:ILE:HG12	1.41	1.34
2:B:1002:LYS:HD3	14:N:166:LEU:O	1.16	1.34
7:G:141:SER:CB	15:O:142:ILE:CD1	2.06	1.34
17:Q:356:VAL:HG11	18:R:208:TYR:CD1	1.62	1.34
2:B:796:ARG:NE	10:J:8:PHE:O	1.58	1.33
1:A:1276:THR:OG1	9:I:45:LEU:HD12	1.22	1.33
1:A:1482:LYS:CE	2:B:304:ASP:OD1	1.74	1.33
18:R:199:LYS:HE3	20:R:601:SO4:O2	1.27	1.33
1:A:1326:GLU:OE2	1:A:1454:HIS:HB3	1.26	1.32
16:P:397:LYS:NZ	18:R:85:ARG:NH1	1.74	1.32
1:A:503:VAL:HA	1:A:580:HIS:CD2	1.61	1.32
1:A:1297:PHE:CD2	1:A:1301:GLU:OE1	1.81	1.32
1:A:545:SER:CB	17:Q:34:VAL:CG2	1.77	1.32
2:B:68:ILE:CG2	2:B:71:LYS:NZ	1.91	1.32
7:G:159:LYS:CB	15:O:105:ASN:HD22	1.43	1.32
2:B:549:CYS:SG	2:B:649:MET:HG2	1.70	1.31
1:A:1326:GLU:OE2	1:A:1455:ARG:N	1.60	1.31
2:B:143:TRP:CD2	2:B:446:MET:HG3	1.65	1.31
2:B:322:ASN:ND2	13:M:108:LEU:O	1.57	1.31
2:B:890:ASP:O	12:L:54:ARG:HD3	1.24	1.31
2:B:1072:GLY:C	2:B:1075:GLU:HG2	1.55	1.31
1:A:547:ILE:CD1	17:Q:26:ARG:CZ	2.08	1.31
1:A:1322:ILE:HG22	1:A:1454:HIS:CG	1.62	1.31
17:Q:26:ARG:HB3	17:Q:34:VAL:CG1	1.61	1.31
1:A:1299:ASN:OD1	1:A:1467:GLY:CA	1.71	1.30
3:C:272:LYS:HA	14:N:175:TYR:CD1	1.63	1.30
7:G:24:VAL:O	7:G:128:GLN:HB2	1.17	1.30
1:A:990:ILE:HA	1:A:994:GLU:OE1	1.30	1.30
2:B:19:LEU:CD1	10:J:26:GLN:OE1	1.78	1.30
1:A:1276:THR:OG1	9:I:45:LEU:CD1	1.79	1.30
1:A:535:GLN:NE2	17:Q:26:ARG:HD3	1.43	1.30
2:B:527:PHE:CZ	2:B:666:PRO:CA	2.13	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:15:GLN:OE1	18:R:184:ASN:ND2	1.63	1.30
2:B:682:GLN:C	14:N:154:ARG:HH21	1.37	1.29
16:P:390:GLN:CB	18:R:150:GLN:O	1.78	1.29
14:N:86:ASP:C	14:N:141:GLU:HG3	1.58	1.29
1:A:547:ILE:HD12	17:Q:26:ARG:NH2	1.46	1.29
2:B:1003:ALA:O	14:N:170:HIS:N	1.66	1.29
15:O:200:ASN:CG	17:Q:14:ASN:CB	2.05	1.29
16:P:436:ILE:HG22	18:R:142:ARG:O	1.23	1.29
1:A:756:LYS:HD3	9:I:85:LYS:NZ	0.97	1.28
16:P:198:ASP:CB	16:P:205:TYR:O	1.79	1.28
16:P:397:LYS:NZ	18:R:85:ARG:CZ	1.94	1.28
16:P:436:ILE:CG2	18:R:142:ARG:C	2.02	1.28
18:R:177:LEU:O	18:R:185:LYS:HE2	1.13	1.28
18:R:199:LYS:HE2	18:R:204:GLU:CA	1.61	1.28
13:M:102:SER:O	13:M:106:LYS:N	1.66	1.28
1:A:995:TYR:OH	2:B:707:SER:CB	1.79	1.27
2:B:75:ASP:HB3	2:B:440:PHE:CE2	1.67	1.27
2:B:527:PHE:CE1	2:B:666:PRO:HG3	1.69	1.27
2:B:679:GLN:HG2	14:N:157:ARG:N	0.96	1.27
17:Q:12:THR:CG2	17:Q:33:HIS:CE1	1.95	1.27
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG23	1.48	1.27
2:B:682:GLN:C	14:N:154:ARG:NH2	1.91	1.27
16:P:198:ASP:HB2	16:P:205:TYR:O	1.27	1.27
1:A:435:ASN:HB3	1:A:442:LYS:CB	1.64	1.27
3:C:253:PRO:HD2	14:N:180:PHE:CG	1.68	1.27
1:A:1326:GLU:CD	1:A:1454:HIS:HB3	1.57	1.26
2:B:682:GLN:CA	14:N:154:ARG:HH21	1.46	1.26
16:P:433:VAL:HA	18:R:145:SER:OG	1.24	1.26
1:A:990:ILE:HG13	1:A:995:TYR:N	1.47	1.26
2:B:1072:GLY:O	2:B:1075:GLU:HG2	1.26	1.26
7:G:159:LYS:HD2	15:O:103:ASN:OD1	1.09	1.26
18:R:199:LYS:CE	18:R:204:GLU:HB3	1.65	1.26
2:B:683:ASN:N	14:N:154:ARG:NH2	1.84	1.26
2:B:679:GLN:HG3	14:N:156:PRO:C	1.55	1.25
17:Q:358:PRO:HA	18:R:206:ARG:NH1	1.51	1.25
18:R:199:LYS:HE2	18:R:204:GLU:CB	1.64	1.25
2:B:143:TRP:CB	2:B:446:MET:CE	2.13	1.25
16:P:397:LYS:CE	18:R:85:ARG:CZ	2.14	1.25
1:A:878:ARG:CG	9:I:66:VAL:HG23	1.65	1.25
1:A:1330:VAL:HG21	1:A:1455:ARG:CZ	1.66	1.25
17:Q:351:ASN:CB	17:Q:369:TRP:CH2	2.20	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1603:MET:HE2	1:A:1615:TYR:CD2	1.73	1.24
2:B:1089:GLN:HG3	2:B:1093:LEU:CG	1.65	1.24
1:A:1322:ILE:CG2	1:A:1454:HIS:CD2	2.19	1.24
2:B:207:ILE:CG1	2:B:503:VAL:CG2	2.07	1.24
16:P:397:LYS:NZ	18:R:85:ARG:CD	2.00	1.23
1:A:1180:ASN:OD1	6:F:87:LYS:HD3	1.33	1.23
14:N:87:TYR:HA	14:N:141:GLU:CA	1.69	1.23
15:O:376:TYR:CE2	15:O:377:TYR:CE2	2.24	1.23
1:A:1322:ILE:HG21	1:A:1454:HIS:ND1	1.54	1.22
1:A:1650:GLY:O	1:A:1652:GLY:N	1.73	1.22
14:N:86:ASP:O	14:N:141:GLU:HG3	1.37	1.22
15:O:374:PRO:C	15:O:376:TYR:HB3	1.64	1.22
1:A:403:LEU:HD11	1:A:419:ILE:CG2	1.68	1.22
1:A:545:SER:CA	17:Q:34:VAL:HG21	1.70	1.22
16:P:443:ASP:O	18:R:3:GLU:HB2	1.31	1.22
1:A:458:GLN:O	1:A:462:LYS:HB2	1.36	1.22
1:A:1484:LEU:CD1	2:B:305:ARG:CZ	2.17	1.21
1:A:1575:ILE:HG13	9:I:122:ARG:CZ	1.70	1.21
14:N:86:ASP:O	14:N:141:GLU:CG	1.88	1.21
18:R:6:ILE:HD11	18:R:213:ILE:CG2	1.70	1.21
2:B:68:ILE:CG2	2:B:71:LYS:HZ3	1.51	1.21
1:A:474:LYS:NZ	2:B:1096:SER:OG	1.74	1.21
2:B:182:GLN:NE2	10:J:69:ARG:HB3	1.55	1.21
1:A:991:LYS:N	1:A:994:GLU:HG3	1.54	1.21
13:M:61:GLU:OE2	13:M:106:LYS:CD	1.87	1.21
17:Q:417:PHE:CE2	18:R:270:PHE:CD1	2.28	1.21
7:G:144:HIS:CG	15:O:146:SER:OG	1.92	1.21
1:A:1329:ILE:HG21	1:A:1456:PHE:CE2	1.75	1.20
3:C:253:PRO:O	14:N:179:ASP:O	1.58	1.20
6:F:72:LYS:HD2	6:F:142:SER:CB	1.69	1.20
1:A:991:LYS:CB	1:A:993:GLN:HB2	1.71	1.20
1:A:824:THR:HB	2:B:1023:ARG:HB2	1.22	1.20
1:A:1003:ARG:NH2	2:B:530:PRO:O	1.74	1.20
1:A:1326:GLU:OE2	1:A:1454:HIS:CB	1.90	1.20
2:B:207:ILE:CD1	2:B:503:VAL:HG21	1.72	1.20
1:A:478:TYR:HA	2:B:1048:SER:O	1.38	1.20
3:C:274:THR:CA	14:N:172:ALA:HB2	1.71	1.20
3:C:296:ASN:O	3:C:298:PHE:CD1	1.94	1.19
1:A:566:SER:CB	15:O:235:GLU:CD	2.15	1.19
1:A:995:TYR:CD2	2:B:708:ASP:CA	2.23	1.19
16:P:436:ILE:CG2	18:R:141:TRP:O	1.91	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:248:LYS:CG	18:R:298:GLN:HE22	1.54	1.19
1:A:1314:GLN:NE2	1:A:1446:ARG:NH1	1.89	1.19
2:B:1072:GLY:N	2:B:1075:GLU:CG	2.04	1.19
2:B:943:ILE:HD12	10:J:44:TYR:CZ	1.78	1.19
1:A:474:LYS:NZ	2:B:1092:LEU:HD23	1.55	1.19
1:A:878:ARG:CG	9:I:67:VAL:HG13	1.73	1.19
1:A:878:ARG:CD	9:I:66:VAL:CG2	2.21	1.19
2:B:1120:ILE:HD12	15:O:117:GLN:NE2	1.58	1.18
15:O:200:ASN:HB2	17:Q:14:ASN:CA	1.73	1.18
3:C:58:ASN:CA	3:C:296:ASN:ND2	2.06	1.18
15:O:247:GLU:OE1	15:O:325:ILE:CG1	1.85	1.18
16:P:475:ARG:CB	18:R:1:MET:CE	2.15	1.18
1:A:1313:LEU:HG	1:A:1462:PHE:CE1	1.79	1.18
16:P:399:TRP:CH2	18:R:291:ARG:O	1.95	1.18
1:A:547:ILE:CD1	17:Q:26:ARG:NH2	2.07	1.18
2:B:683:ASN:N	14:N:154:ARG:HH22	1.37	1.18
7:G:24:VAL:O	7:G:128:GLN:CB	1.91	1.18
1:A:474:LYS:CE	2:B:1092:LEU:HD23	1.73	1.17
1:A:1326:GLU:OE1	1:A:1454:HIS:HA	1.45	1.17
7:G:241:ARG:HH11	15:O:189:PHE:CB	1.55	1.17
17:Q:417:PHE:CE2	18:R:270:PHE:HD1	1.60	1.17
18:R:5:PRO:CG	18:R:217:THR:HG21	1.66	1.17
1:A:1050:TYR:CZ	1:A:1179:ILE:HG12	1.79	1.17
16:P:382:GLU:OE1	18:R:146:SER:CB	1.93	1.17
2:B:143:TRP:CD2	2:B:446:MET:CG	2.26	1.17
2:B:679:GLN:HG3	14:N:156:PRO:CA	1.75	1.17
6:F:72:LYS:CA	6:F:142:SER:HB2	1.75	1.17
18:R:6:ILE:HD11	18:R:213:ILE:CB	1.74	1.17
1:A:1322:ILE:HB	1:A:1454:HIS:CE1	1.79	1.17
2:B:152:LEU:HD22	2:B:443:LYS:HD2	1.24	1.17
2:B:894:LYS:HD3	12:L:47:ARG:CZ	1.74	1.17
18:R:199:LYS:HE3	18:R:203:SER:O	1.41	1.17
1:A:477:ASN:O	2:B:1047:ARG:HD3	1.44	1.17
1:A:436:ALA:O	1:A:440:SER:N	1.77	1.16
16:P:475:ARG:CB	18:R:1:MET:HE1	1.63	1.16
18:R:4:VAL:HG21	18:R:214:VAL:HG22	1.23	1.16
18:R:251:TRP:CZ3	18:R:307:LYS:HE2	1.80	1.16
16:P:438:TRP:CD1	18:R:141:TRP:CZ2	2.33	1.16
1:A:438:ILE:O	1:A:457:LYS:CD	1.94	1.16
1:A:953:GLU:HA	1:A:1205:PHE:CD2	1.81	1.16
2:B:1072:GLY:N	2:B:1075:GLU:HG3	1.59	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:TYR:HD2	2:B:708:ASP:CA	1.59	1.15
1:A:1657:LEU:O	6:F:133:VAL:N	1.76	1.15
1:A:1657:LEU:HD22	7:G:104:LEU:CD1	1.74	1.15
2:B:19:LEU:HD13	10:J:26:GLN:OE1	1.30	1.15
7:G:141:SER:HB2	15:O:142:ILE:HD12	1.20	1.15
2:B:266:LYS:HG3	2:B:473:GLN:O	1.46	1.15
16:P:185:GLN:HA	18:R:196:GLU:O	1.42	1.15
16:P:436:ILE:HG23	18:R:141:TRP:O	0.97	1.15
1:A:435:ASN:O	1:A:439:ASP:O	1.61	1.15
16:P:390:GLN:HB2	18:R:150:GLN:O	1.37	1.15
1:A:1049:MET:CG	1:A:1052:GLY:C	2.18	1.15
2:B:149:GLU:OE1	2:B:441:LYS:NZ	1.80	1.15
2:B:894:LYS:CG	12:L:54:ARG:HH22	1.53	1.15
1:A:990:ILE:HD11	1:A:995:TYR:HA	1.24	1.15
3:C:274:THR:HA	14:N:172:ALA:CB	1.75	1.15
1:A:1482:LYS:HE2	2:B:304:ASP:OD1	0.96	1.14
2:B:266:LYS:HE3	2:B:473:GLN:O	1.46	1.14
1:A:952:LEU:HD22	1:A:1004:GLU:HG3	1.15	1.14
2:B:566:TYR:HD2	13:M:73:SER:OG	1.23	1.14
2:B:894:LYS:HD3	12:L:47:ARG:NE	1.63	1.14
17:Q:22:ILE:CD1	17:Q:24:ASP:OD2	1.96	1.14
1:A:1329:ILE:CG2	1:A:1456:PHE:CE2	2.31	1.14
1:A:1657:LEU:HD22	7:G:104:LEU:HD13	1.14	1.14
2:B:985:ILE:O	14:N:160:VAL:HG23	1.46	1.14
14:N:87:TYR:CZ	14:N:141:GLU:OE1	2.01	1.14
1:A:991:LYS:H	1:A:994:GLU:CG	1.60	1.14
3:C:253:PRO:CD	14:N:180:PHE:CB	1.85	1.14
17:Q:417:PHE:CZ	18:R:270:PHE:HD1	1.65	1.14
1:A:438:ILE:O	1:A:457:LYS:HD2	1.42	1.14
1:A:436:ALA:HB2	1:A:443:ALA:HB2	1.15	1.13
2:B:1089:GLN:CG	2:B:1093:LEU:CD2	2.24	1.13
15:O:240:ILE:CG2	15:O:380:SER:HB3	1.77	1.13
17:Q:134:LYS:O	17:Q:138:LEU:HB2	1.47	1.13
18:R:203:SER:HA	20:R:601:SO4:O3	1.38	1.13
1:A:403:LEU:CD1	1:A:419:ILE:HG21	1.78	1.13
2:B:1072:GLY:H	2:B:1075:GLU:HG3	1.08	1.13
2:B:1093:LEU:HG	2:B:1094:ASN:OD1	1.45	1.13
7:G:159:LYS:HD2	15:O:103:ASN:CG	1.72	1.13
15:O:248:LEU:HD11	15:O:598:PHE:HD2	1.05	1.13
17:Q:9:ILE:HG13	17:Q:10:CYS:H	1.06	1.13
18:R:5:PRO:CD	18:R:217:THR:OG1	1.95	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:NZ	2:B:1092:LEU:CD2	2.11	1.12
1:A:1276:THR:N	9:I:45:LEU:O	1.80	1.12
2:B:1072:GLY:H	2:B:1075:GLU:CG	1.59	1.12
1:A:756:LYS:CD	9:I:85:LYS:HZ1	1.49	1.12
1:A:1556:GLU:OE2	5:E:212:ARG:NH1	1.82	1.12
18:R:248:LYS:HG2	18:R:298:GLN:NE2	1.62	1.12
1:A:435:ASN:O	1:A:439:ASP:HB3	1.50	1.12
1:A:506:THR:HG22	1:A:579:ARG:C	1.74	1.12
2:B:894:LYS:CG	12:L:54:ARG:NH2	1.92	1.12
1:A:990:ILE:CA	1:A:994:GLU:HB2	1.78	1.12
7:G:241:ARG:HH11	15:O:189:PHE:HB2	1.10	1.12
16:P:348:HIS:CD2	18:R:154:LYS:HD3	1.82	1.12
1:A:566:SER:CB	15:O:235:GLU:OE2	1.96	1.12
3:C:334:THR:HG21	11:K:44:ARG:HB3	1.29	1.12
7:G:143:SER:O	15:O:105:ASN:ND2	1.82	1.12
1:A:472:MET:HB3	2:B:1073:GLU:CB	1.80	1.11
3:C:230:LEU:HD12	3:C:231:PRO:HD2	1.22	1.11
18:R:248:LYS:CG	18:R:298:GLN:NE2	2.12	1.11
1:A:1326:GLU:OE2	1:A:1454:HIS:C	1.93	1.11
2:B:1002:LYS:CD	14:N:166:LEU:O	1.99	1.11
1:A:429:THR:CG2	18:R:406:LYS:HE3	1.81	1.11
1:A:878:ARG:CB	9:I:67:VAL:CG1	2.27	1.11
15:O:376:TYR:CZ	15:O:377:TYR:CE2	2.37	1.11
2:B:145:VAL:HG11	2:B:441:LYS:HG2	1.24	1.11
1:A:475:ARG:CZ	2:B:1061:LYS:HB2	1.81	1.11
2:B:1003:ALA:HA	14:N:169:GLU:H	1.04	1.11
2:B:849:GLY:C	12:L:60:ARG:HH22	1.58	1.10
17:Q:358:PRO:CA	18:R:206:ARG:NH1	2.11	1.10
1:A:503:VAL:HG23	1:A:530:TRP:HB2	1.29	1.10
1:A:1482:LYS:O	2:B:308:LEU:HD21	1.50	1.10
1:A:474:LYS:HE3	2:B:1092:LEU:CD2	1.80	1.10
1:A:474:LYS:O	2:B:1070:ARG:CB	2.00	1.10
1:A:545:SER:H	17:Q:34:VAL:HG23	1.08	1.10
1:A:1299:ASN:OD1	1:A:1467:GLY:HA3	1.39	1.10
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.13	1.10
15:O:373:LEU:O	15:O:376:TYR:HB2	1.51	1.10
2:B:551:ILE:HG21	2:B:647:SER:HA	1.29	1.09
2:B:985:ILE:HB	14:N:160:VAL:CG2	1.82	1.09
13:M:61:GLU:OE2	13:M:106:LYS:HD3	1.44	1.09
17:Q:188:ALA:HB3	17:Q:384:GLN:CG	1.82	1.09
17:Q:356:VAL:HG11	18:R:208:TYR:CE1	1.85	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:MET:HE2	1:A:472:MET:HA	1.31	1.09
15:O:579:LEU:HA	15:O:582:ARG:HB3	1.24	1.09
18:R:4:VAL:CG2	18:R:214:VAL:HG22	1.83	1.09
1:A:1600:ARG:NH2	1:A:1617:THR:OG1	1.83	1.09
2:B:143:TRP:HB2	2:B:446:MET:HE1	1.31	1.09
2:B:143:TRP:HB2	2:B:446:MET:HE3	1.18	1.09
16:P:397:LYS:NZ	18:R:85:ARG:HD3	1.62	1.09
17:Q:26:ARG:HB3	17:Q:34:VAL:HG13	1.12	1.09
1:A:1314:GLN:HE21	1:A:1446:ARG:NH1	1.46	1.09
6:F:72:LYS:HA	6:F:142:SER:HB2	1.21	1.09
6:F:74:ILE:CG1	6:F:75:PRO:HD2	1.83	1.09
15:O:234:ILE:HG22	15:O:237:ILE:HG12	1.25	1.09
15:O:374:PRO:O	15:O:376:TYR:HB3	1.53	1.09
17:Q:417:PHE:HE2	18:R:270:PHE:CD1	1.69	1.09
1:A:566:SER:HB2	15:O:235:GLU:CD	1.77	1.08
1:A:990:ILE:HB	1:A:994:GLU:HB3	1.17	1.08
1:A:1322:ILE:CD1	1:A:1457:ILE:HD11	1.83	1.08
1:A:1575:ILE:N	9:I:122:ARG:NH1	2.00	1.08
3:C:272:LYS:HG2	14:N:175:TYR:CD1	1.88	1.08
18:R:5:PRO:CD	18:R:217:THR:CB	2.31	1.08
1:A:1049:MET:HG2	1:A:1053:ASP:N	1.66	1.08
2:B:527:PHE:CE1	2:B:666:PRO:CG	2.35	1.08
2:B:849:GLY:CA	12:L:60:ARG:HH22	1.57	1.08
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG22	1.58	1.08
1:A:1003:ARG:HH21	2:B:530:PRO:C	1.61	1.08
1:A:476:VAL:HG22	2:B:1070:ARG:H	1.15	1.08
1:A:1326:GLU:CD	1:A:1454:HIS:CB	2.26	1.08
15:O:376:TYR:CE2	15:O:377:TYR:HE2	1.66	1.08
16:P:184:SER:HB3	18:R:198:LEU:CB	1.75	1.08
1:A:878:ARG:HB3	9:I:67:VAL:HG11	1.16	1.08
16:P:622:TYR:O	16:P:626:LEU:HB2	1.54	1.08
1:A:486:PRO:O	2:B:781:TYR:CD2	2.06	1.07
1:A:597:LYS:CB	2:B:1082:HIS:NE2	2.17	1.07
1:A:999:CYS:HA	2:B:712:SER:HB2	1.32	1.07
3:C:253:PRO:N	14:N:180:PHE:CD1	2.19	1.07
15:O:200:ASN:ND2	17:Q:14:ASN:O	1.86	1.07
1:A:474:LYS:HZ2	2:B:1092:LEU:HA	1.11	1.07
1:A:1322:ILE:HB	1:A:1454:HIS:NE2	1.68	1.07
2:B:943:ILE:HD12	10:J:44:TYR:CE1	1.88	1.07
6:F:72:LYS:CD	6:F:142:SER:CB	2.28	1.07
7:G:141:SER:HB3	15:O:142:ILE:HD13	1.35	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ALA:C	1:A:439:ASP:C	2.22	1.07
1:A:954:GLY:HA3	1:A:1205:PHE:HB3	1.27	1.07
1:A:1314:GLN:NE2	1:A:1446:ARG:HD2	1.67	1.07
1:A:474:LYS:CE	2:B:1092:LEU:CD2	2.32	1.07
1:A:834:ARG:NH2	2:B:994:ASP:OD1	1.87	1.07
1:A:506:THR:HG22	1:A:579:ARG:O	1.53	1.07
1:A:1049:MET:HB3	1:A:1052:GLY:CA	1.84	1.07
7:G:159:LYS:CD	15:O:103:ASN:OD1	2.02	1.07
1:A:564:PRO:HG2	15:O:370:THR:O	1.53	1.06
2:B:1089:GLN:HG3	2:B:1093:LEU:CB	1.82	1.06
18:R:251:TRP:CE3	18:R:307:LYS:HE2	1.86	1.06
1:A:878:ARG:HG2	9:I:67:VAL:HG13	1.09	1.06
1:A:1322:ILE:HG21	1:A:1454:HIS:CG	1.81	1.06
16:P:436:ILE:HB	18:R:143:THR:HG23	1.30	1.06
1:A:88:PRO:CG	1:A:438:ILE:HD12	1.83	1.06
3:C:58:ASN:CA	3:C:296:ASN:HD21	1.65	1.06
6:F:74:ILE:O	7:G:95:LEU:HD11	1.43	1.06
17:Q:351:ASN:HB3	17:Q:369:TRP:CZ3	1.89	1.06
1:A:1003:ARG:NH2	2:B:530:PRO:C	2.14	1.06
1:A:1317:ILE:CG2	1:A:1460:TYR:HE1	1.69	1.06
1:A:1575:ILE:HG13	9:I:122:ARG:NH1	0.74	1.06
2:B:49:PHE:HB2	2:B:164:MET:CE	1.84	1.06
1:A:597:LYS:CB	2:B:1082:HIS:CD2	2.38	1.06
1:A:566:SER:HB3	15:O:235:GLU:CD	1.77	1.05
1:A:1326:GLU:OE1	1:A:1454:HIS:CA	2.03	1.05
2:B:1092:LEU:HA	2:B:1096:SER:HB2	1.35	1.05
1:A:1050:TYR:CE1	1:A:1179:ILE:HG12	1.90	1.05
1:A:1313:LEU:HG	1:A:1462:PHE:CZ	1.90	1.05
1:A:1660:VAL:O	7:G:102:GLU:HG2	1.54	1.05
2:B:143:TRP:CD2	2:B:446:MET:SD	2.49	1.05
16:P:197:ARG:NE	16:P:261:VAL:H	1.54	1.05
2:B:207:ILE:CD1	2:B:503:VAL:CG2	2.34	1.05
17:Q:17:SER:O	17:Q:29:CYS:HB2	1.55	1.05
1:A:422:ARG:NH1	18:R:412:ARG:NH1	2.04	1.05
1:A:566:SER:HB3	15:O:235:GLU:OE2	1.56	1.05
1:A:1600:ARG:CD	1:A:1616:GLU:OE1	2.05	1.05
2:B:527:PHE:CE2	2:B:666:PRO:HA	1.89	1.05
15:O:240:ILE:HG22	15:O:380:SER:HB3	1.06	1.05
16:P:389:TRP:HH2	18:R:148:ASN:N	1.54	1.05
18:R:6:ILE:CD1	18:R:213:ILE:HB	1.87	1.05
1:A:545:SER:N	17:Q:34:VAL:CG2	2.18	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:434:ARG:HG2	18:R:143:THR:CG2	1.87	1.05
1:A:503:VAL:CA	1:A:580:HIS:CD2	2.23	1.04
1:A:1298:ASP:OD1	1:A:1468:LYS:NZ	1.90	1.04
16:P:434:ARG:HG2	18:R:143:THR:HG21	1.38	1.04
17:Q:356:VAL:HG13	18:R:212:HIS:CE1	1.91	1.04
16:P:22:GLY:CA	18:R:139:GLU:OE2	2.04	1.04
1:A:1297:PHE:CE2	1:A:1301:GLU:CD	2.34	1.04
1:A:1322:ILE:CB	1:A:1454:HIS:CE1	2.40	1.04
2:B:889:GLY:HA3	12:L:54:ARG:O	1.56	1.04
16:P:475:ARG:HB3	18:R:1:MET:CE	1.85	1.04
17:Q:15:CYS:HB3	17:Q:17:SER:N	1.70	1.04
18:R:4:VAL:HG21	18:R:214:VAL:CG2	1.88	1.04
1:A:425:ASN:CG	18:R:406:LYS:HZ2	1.64	1.04
1:A:615:ARG:NH1	2:B:929:ARG:HE	1.54	1.04
1:A:878:ARG:CD	9:I:66:VAL:HG23	1.68	1.04
1:A:1049:MET:CB	1:A:1052:GLY:HA2	1.88	1.04
1:A:477:ASN:O	2:B:1047:ARG:CD	2.06	1.04
1:A:629:ASP:C	2:B:926:VAL:CG2	2.31	1.04
2:B:551:ILE:HG23	2:B:648:ARG:N	1.73	1.04
15:O:234:ILE:HG23	15:O:237:ILE:HG12	1.37	1.04
16:P:436:ILE:HG22	18:R:143:THR:N	1.72	1.04
16:P:472:ARG:CZ	18:R:200:THR:HG23	1.87	1.04
18:R:5:PRO:HD3	18:R:217:THR:OG1	1.55	1.04
1:A:1657:LEU:CD2	7:G:104:LEU:HD13	1.88	1.03
15:O:243:GLU:OE1	15:O:328:LEU:HD23	1.58	1.03
17:Q:413:LEU:HG	18:R:273:TRP:HZ2	1.16	1.03
1:A:1049:MET:CG	1:A:1053:ASP:N	2.21	1.03
1:A:1322:ILE:CG2	1:A:1454:HIS:CE1	2.41	1.03
2:B:1089:GLN:HG2	2:B:1093:LEU:HD22	1.07	1.03
6:F:72:LYS:HB3	6:F:142:SER:CB	1.87	1.03
7:G:143:SER:HB3	15:O:104:ILE:H	0.90	1.03
17:Q:417:PHE:CZ	18:R:270:PHE:CD1	2.45	1.03
18:R:314:TRP:NE1	18:R:363:GLU:OE2	1.92	1.03
1:A:476:VAL:O	2:B:1068:GLY:HA3	1.57	1.03
2:B:182:GLN:HE22	10:J:69:ARG:HB3	1.23	1.03
3:C:296:ASN:O	3:C:298:PHE:CE1	2.10	1.03
16:P:486:ALA:O	18:R:137:SER:N	1.92	1.03
17:Q:5:ILE:O	17:Q:19:LEU:O	1.74	1.03
1:A:938:VAL:HG22	9:I:82:ILE:CD1	1.88	1.03
2:B:527:PHE:CD1	2:B:666:PRO:CG	2.40	1.03
1:A:503:VAL:CG2	1:A:530:TRP:HB2	1.88	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ASP:CG	8:H:20:TYR:HB3	1.83	1.03
1:A:721:LYS:O	8:H:96:VAL:N	1.91	1.03
16:P:382:GLU:OE1	18:R:146:SER:HB3	1.56	1.03
1:A:545:SER:HB2	17:Q:34:VAL:HG22	1.41	1.02
1:A:991:LYS:HB2	1:A:993:GLN:HB2	1.35	1.02
2:B:681:ILE:HB	14:N:154:ARG:HG3	1.40	1.02
7:G:144:HIS:CD2	15:O:146:SER:CA	2.42	1.02
18:R:199:LYS:HE2	18:R:204:GLU:HB3	1.22	1.02
1:A:1310:LYS:HG2	1:A:1311:GLU:CD	1.77	1.02
1:A:1317:ILE:HG21	1:A:1460:TYR:HE1	1.22	1.02
7:G:144:HIS:CD2	15:O:146:SER:HA	1.93	1.02
15:O:379:ARG:HA	15:O:379:ARG:HH11	1.22	1.02
17:Q:188:ALA:CB	17:Q:384:GLN:CG	2.36	1.02
1:A:878:ARG:HG2	9:I:66:VAL:HG23	1.38	1.02
2:B:566:TYR:CD2	13:M:73:SER:OG	2.11	1.02
2:B:1089:GLN:HG3	2:B:1093:LEU:CD1	1.87	1.02
7:G:159:LYS:HB2	15:O:105:ASN:HD22	1.24	1.02
1:A:472:MET:CB	2:B:1073:GLU:HB2	1.89	1.02
1:A:878:ARG:CG	9:I:66:VAL:CG2	2.36	1.02
16:P:432:PRO:O	18:R:145:SER:OG	1.78	1.02
1:A:909:SER:HA	9:I:83:LYS:NZ	1.75	1.02
1:A:1314:GLN:CD	1:A:1446:ARG:HD2	1.84	1.02
3:C:253:PRO:CD	14:N:180:PHE:CD1	2.43	1.02
16:P:397:LYS:NZ	18:R:85:ARG:NE	2.00	1.02
6:F:72:LYS:CB	6:F:142:SER:CB	2.37	1.01
16:P:473:HIS:CD2	18:R:1:MET:SD	2.53	1.01
17:Q:413:LEU:HG	18:R:273:TRP:CZ2	1.95	1.01
2:B:143:TRP:CE2	2:B:446:MET:HB2	1.96	1.01
3:C:229:LEU:HD22	3:C:295:ARG:O	1.61	1.01
16:P:22:GLY:N	18:R:139:GLU:OE2	1.93	1.01
18:R:6:ILE:HD11	18:R:213:ILE:HB	1.37	1.01
1:A:995:TYR:OH	2:B:707:SER:HB2	0.83	1.01
3:C:228:ARG:NH1	14:N:173:THR:O	1.90	1.01
18:R:199:LYS:CE	18:R:204:GLU:CA	2.37	1.01
2:B:143:TRP:CB	2:B:446:MET:SD	2.48	1.01
18:R:5:PRO:HG2	18:R:217:THR:CB	1.75	1.01
18:R:15:GLN:CD	18:R:184:ASN:HD22	1.69	1.01
1:A:486:PRO:HD2	2:B:928:SER:OG	1.60	1.01
2:B:1071:VAL:HG21	2:B:1091:ARG:HG3	1.41	1.01
15:O:332:LEU:HD11	15:O:380:SER:OG	1.61	1.01
1:A:954:GLY:CA	1:A:1205:PHE:HB3	1.89	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:ILE:CG1	1:A:995:TYR:N	2.24	1.00
1:A:991:LYS:HB3	1:A:993:GLN:CD	1.84	1.00
2:B:894:LYS:HG3	12:L:54:ARG:NH2	1.41	1.00
3:C:293:ARG:H	3:C:295:ARG:CZ	1.74	1.00
17:Q:12:THR:CB	17:Q:33:HIS:CE1	2.44	1.00
1:A:88:PRO:HG2	1:A:438:ILE:CD1	1.91	1.00
16:P:274:ILE:O	16:P:289:SER:HB2	1.57	1.00
1:A:1314:GLN:NE2	1:A:1446:ARG:HH11	1.48	1.00
2:B:75:ASP:HB3	2:B:440:PHE:CZ	1.96	1.00
3:C:253:PRO:HD2	14:N:180:PHE:CD1	1.95	1.00
16:P:399:TRP:HH2	18:R:291:ARG:O	1.35	1.00
17:Q:9:ILE:HB	17:Q:16:PRO:HB2	1.43	1.00
17:Q:188:ALA:HB3	17:Q:384:GLN:HG2	1.43	1.00
18:R:177:LEU:O	18:R:185:LYS:CE	2.08	1.00
1:A:1322:ILE:HD12	1:A:1457:ILE:HD11	1.04	1.00
7:G:24:VAL:HA	7:G:25:THR:HA	1.44	1.00
15:O:240:ILE:O	15:O:380:SER:OG	1.80	1.00
2:B:19:LEU:HD11	10:J:26:GLN:OE1	1.61	1.00
7:G:159:LYS:CB	15:O:105:ASN:ND2	2.23	1.00
16:P:185:GLN:HG3	18:R:190:SER:HB3	1.42	1.00
1:A:995:TYR:CE2	2:B:708:ASP:HA	1.97	1.00
2:B:143:TRP:CZ3	2:B:446:MET:HG3	1.96	1.00
2:B:1072:GLY:O	2:B:1075:GLU:CG	2.09	1.00
18:R:5:PRO:HG2	18:R:217:THR:HG22	1.44	1.00
1:A:953:GLU:C	1:A:1205:PHE:CG	2.40	0.99
2:B:1092:LEU:O	2:B:1096:SER:HB3	1.59	0.99
7:G:143:SER:CB	15:O:104:ILE:H	1.74	0.99
13:M:102:SER:O	13:M:105:SER:N	1.95	0.99
17:Q:351:ASN:CA	17:Q:369:TRP:CH2	2.45	0.99
1:A:995:TYR:CZ	2:B:715:ASN:ND2	2.29	0.99
1:A:998:HIS:NE2	2:B:711:GLN:HG3	1.75	0.99
15:O:202:ASN:HB3	17:Q:31:TYR:OH	1.62	0.99
1:A:408:LYS:CB	1:A:411:VAL:HB	1.92	0.99
1:A:1050:TYR:CG	1:A:1179:ILE:HG21	1.96	0.99
6:F:74:ILE:HG12	6:F:75:PRO:CD	1.91	0.99
15:O:348:THR:HG22	15:O:351:SER:HB3	1.42	0.99
17:Q:22:ILE:CD1	17:Q:26:ARG:NE	2.25	0.99
16:P:389:TRP:CH2	18:R:148:ASN:N	2.29	0.99
1:A:435:ASN:HB3	1:A:442:LYS:HB3	1.43	0.99
15:O:376:TYR:CE1	15:O:588:LEU:CD2	2.45	0.99
16:P:184:SER:HB3	18:R:198:LEU:H	1.25	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:86:ASP:O	14:N:142:THR:N	1.94	0.99
16:P:397:LYS:CE	18:R:85:ARG:CD	2.40	0.99
1:A:435:ASN:HB3	1:A:442:LYS:HB2	1.40	0.99
1:A:1314:GLN:HE22	1:A:1446:ARG:HD2	1.28	0.99
18:R:6:ILE:HD11	18:R:213:ILE:HG22	1.42	0.99
1:A:478:TYR:CA	2:B:1048:SER:O	2.10	0.99
16:P:397:LYS:HZ1	18:R:85:ARG:NE	1.58	0.99
1:A:1330:VAL:CG2	1:A:1455:ARG:CZ	2.41	0.98
2:B:143:TRP:CE3	2:B:446:MET:CG	2.46	0.98
7:G:144:HIS:NE2	15:O:145:SER:HB3	1.78	0.98
18:R:199:LYS:CE	18:R:204:GLU:CB	2.32	0.98
2:B:824:HIS:ND1	2:B:897:GLU:OE1	1.90	0.98
7:G:143:SER:HB3	15:O:104:ILE:N	1.75	0.98
1:A:566:SER:HB2	15:O:235:GLU:OE1	1.61	0.98
2:B:1072:GLY:CA	2:B:1075:GLU:HG2	1.93	0.98
1:A:1276:THR:CB	9:I:45:LEU:HD12	1.93	0.98
1:A:1482:LYS:HE2	2:B:304:ASP:CG	1.87	0.98
2:B:697:LEU:HB2	2:B:702:ASN:ND2	1.77	0.98
3:C:41:GLU:OE2	11:K:138:LYS:HE3	1.64	0.98
3:C:272:LYS:CA	14:N:175:TYR:CZ	2.16	0.98
1:A:480:ALA:CB	2:B:1046:VAL:HG23	1.93	0.98
1:A:990:ILE:CB	1:A:994:GLU:CB	1.98	0.98
1:A:1317:ILE:CG2	1:A:1460:TYR:CE1	2.45	0.98
1:A:438:ILE:O	1:A:457:LYS:CB	2.12	0.98
1:A:721:LYS:NZ	8:H:90:ALA:O	1.97	0.98
1:A:1314:GLN:NE2	1:A:1446:ARG:CD	2.25	0.98
16:P:397:LYS:HZ3	18:R:85:ARG:HD3	1.13	0.98
1:A:422:ARG:HH12	18:R:412:ARG:CZ	1.77	0.98
1:A:995:TYR:CZ	2:B:707:SER:HB2	1.98	0.97
2:B:71:LYS:HD3	2:B:421:LEU:HD13	1.46	0.97
2:B:1003:ALA:HA	14:N:169:GLU:N	1.78	0.97
1:A:1276:THR:HG1	9:I:45:LEU:HD12	1.18	0.97
13:M:102:SER:O	13:M:105:SER:CA	2.11	0.97
1:A:472:MET:HB3	2:B:1073:GLU:HB2	0.99	0.97
1:A:991:LYS:H	1:A:994:GLU:HG3	0.82	0.97
1:A:953:GLU:CA	1:A:1205:PHE:CD2	2.46	0.97
2:B:943:ILE:CD1	10:J:44:TYR:CE1	2.46	0.97
16:P:184:SER:CA	18:R:198:LEU:HB3	1.94	0.97
1:A:909:SER:HA	9:I:83:LYS:CE	1.93	0.97
2:B:152:LEU:HD22	2:B:443:LYS:CD	1.94	0.97
2:B:207:ILE:HD11	2:B:503:VAL:HG21	1.43	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:475:ARG:HB3	18:R:1:MET:HE1	0.99	0.97
1:A:535:GLN:HE22	17:Q:26:ARG:CD	1.77	0.97
18:R:248:LYS:HG3	18:R:298:GLN:HE22	1.26	0.97
2:B:550:ARG:HB2	2:B:650:LEU:HB2	1.47	0.97
1:A:995:TYR:HH	2:B:707:SER:HB2	1.22	0.97
17:Q:15:CYS:SG	17:Q:17:SER:HB2	2.05	0.97
1:A:545:SER:H	17:Q:34:VAL:CG2	1.74	0.97
1:A:615:ARG:HH22	2:B:929:ARG:HG2	1.27	0.97
1:A:999:CYS:CA	2:B:712:SER:CB	2.43	0.97
1:A:1050:TYR:CD1	1:A:1179:ILE:HG21	1.99	0.97
2:B:207:ILE:HG13	2:B:503:VAL:HG22	1.47	0.97
2:B:75:ASP:CB	2:B:440:PHE:CE2	2.47	0.96
15:O:376:TYR:HE1	15:O:588:LEU:CD2	1.77	0.96
16:P:185:GLN:HB3	18:R:195:LEU:HB3	1.47	0.96
2:B:679:GLN:HG2	14:N:156:PRO:C	1.67	0.96
1:A:88:PRO:HG2	1:A:438:ILE:HD12	0.97	0.96
2:B:202:LEU:HD22	2:B:488:ALA:HB2	1.46	0.96
1:A:1049:MET:HB3	1:A:1052:GLY:N	1.79	0.96
1:A:1326:GLU:CD	1:A:1454:HIS:CA	2.38	0.96
13:M:102:SER:OG	13:M:105:SER:N	1.96	0.96
1:A:474:LYS:NZ	2:B:1092:LEU:HA	1.80	0.96
2:B:1089:GLN:HG3	2:B:1093:LEU:CD2	1.90	0.96
6:F:66:ARG:NH2	7:G:90:LEU:CD1	2.29	0.96
17:Q:193:PHE:CD2	18:R:208:TYR:CD2	2.53	0.96
2:B:68:ILE:HG23	2:B:71:LYS:HZ2	1.23	0.96
16:P:436:ILE:HB	18:R:143:THR:CG2	1.95	0.96
1:A:474:LYS:O	2:B:1070:ARG:CA	2.14	0.96
1:A:474:LYS:O	2:B:1070:ARG:HA	1.65	0.96
2:B:796:ARG:CZ	10:J:8:PHE:O	2.14	0.96
1:A:953:GLU:HG2	1:A:1205:PHE:CE2	1.99	0.96
15:O:243:GLU:HB3	15:O:332:LEU:HD13	1.48	0.96
1:A:990:ILE:CD1	1:A:995:TYR:HA	1.96	0.96
15:O:200:ASN:CG	17:Q:14:ASN:CG	2.34	0.96
17:Q:371:GLU:HG3	18:R:231:LEU:CD1	1.96	0.96
18:R:6:ILE:CD1	18:R:213:ILE:CG2	2.43	0.95
2:B:68:ILE:CG2	2:B:71:LYS:HZ2	1.65	0.95
16:P:349:GLY:HA2	18:R:153:ASN:O	1.64	0.95
17:Q:22:ILE:HD11	17:Q:26:ARG:NE	1.81	0.95
18:R:199:LYS:HE2	18:R:204:GLU:N	1.82	0.95
1:A:429:THR:CG2	18:R:406:LYS:CE	2.42	0.95
1:A:862:THR:CB	9:I:67:VAL:HG12	1.95	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1484:LEU:HD13	2:B:305:ARG:NH1	1.80	0.95
17:Q:410:ARG:NH2	18:R:278:TYR:OH	1.99	0.95
1:A:1322:ILE:CD1	1:A:1457:ILE:CD1	2.43	0.95
2:B:152:LEU:CA	2:B:443:LYS:HE3	1.96	0.95
2:B:209:GLN:HG2	2:B:210:ARG:H	1.32	0.95
15:O:376:TYR:OH	15:O:588:LEU:HD21	1.65	0.95
18:R:199:LYS:CE	18:R:203:SER:O	2.13	0.95
1:A:545:SER:CA	17:Q:34:VAL:CG2	2.36	0.95
1:A:547:ILE:CD1	17:Q:26:ARG:HH22	1.71	0.95
1:A:1484:LEU:HD13	2:B:305:ARG:NE	1.81	0.95
6:F:75:PRO:CG	6:F:78:GLN:HB2	1.96	0.95
1:A:1322:ILE:CB	1:A:1454:HIS:NE2	2.30	0.95
2:B:49:PHE:HB2	2:B:164:MET:HE3	1.47	0.95
1:A:474:LYS:O	2:B:1070:ARG:HB2	1.66	0.95
15:O:247:GLU:OE1	15:O:325:ILE:HG12	1.10	0.95
1:A:429:THR:HG23	18:R:406:LYS:HZ1	1.31	0.95
2:B:548:LYS:HE3	2:B:695:ASN:CG	1.92	0.95
2:B:1089:GLN:CG	2:B:1093:LEU:HD13	1.96	0.95
13:M:102:SER:CB	13:M:105:SER:CB	2.02	0.95
17:Q:341:ARG:NH1	17:Q:369:TRP:HE1	1.65	0.95
2:B:1093:LEU:O	2:B:1098:TYR:HB2	1.67	0.94
16:P:443:ASP:O	18:R:3:GLU:CB	2.15	0.94
2:B:207:ILE:HG13	2:B:503:VAL:HG23	1.48	0.94
6:F:74:ILE:HG12	6:F:75:PRO:HD2	0.95	0.94
1:A:545:SER:N	17:Q:34:VAL:HG23	1.77	0.94
17:Q:9:ILE:CG1	17:Q:10:CYS:H	1.79	0.94
1:A:588:LEU:HD21	2:B:1087:LEU:HD13	1.48	0.94
1:A:1049:MET:CB	1:A:1052:GLY:CA	2.44	0.94
16:P:433:VAL:CA	18:R:145:SER:OG	2.13	0.94
16:P:436:ILE:HG21	18:R:142:ARG:O	1.67	0.94
1:A:506:THR:HA	1:A:579:ARG:O	1.67	0.94
1:A:543:LEU:HB2	17:Q:34:VAL:O	1.67	0.94
1:A:672:ASP:OD2	2:B:777:SER:HB3	1.67	0.94
1:A:991:LYS:HB3	1:A:993:GLN:OE1	1.64	0.94
2:B:679:GLN:HG3	14:N:155:VAL:O	1.64	0.94
2:B:75:ASP:N	2:B:440:PHE:HE2	1.65	0.94
2:B:1003:ALA:CA	14:N:169:GLU:H	1.80	0.94
17:Q:358:PRO:HA	18:R:206:ARG:HH12	0.78	0.94
15:O:63:LEU:HD12	15:O:71:ILE:HG13	1.47	0.94
16:P:184:SER:HB3	18:R:198:LEU:N	1.81	0.94
16:P:390:GLN:HB3	18:R:150:GLN:O	1.68	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:351:ASN:CG	17:Q:369:TRP:CZ2	2.45	0.94
18:R:251:TRP:HE3	18:R:307:LYS:CE	1.69	0.94
1:A:1600:ARG:HD2	1:A:1616:GLU:OE1	1.67	0.94
2:B:1089:GLN:HG3	2:B:1093:LEU:HD13	1.49	0.94
15:O:376:TYR:CZ	15:O:588:LEU:HD21	2.03	0.94
1:A:506:THR:CB	1:A:579:ARG:O	2.16	0.94
17:Q:341:ARG:NH1	17:Q:369:TRP:NE1	2.16	0.94
2:B:682:GLN:CA	14:N:154:ARG:NH2	2.22	0.93
1:A:506:THR:CG2	1:A:579:ARG:O	2.15	0.93
1:A:938:VAL:HG22	9:I:82:ILE:HD13	1.49	0.93
2:B:145:VAL:HG21	2:B:441:LYS:HA	1.47	0.93
17:Q:22:ILE:HD12	17:Q:24:ASP:OD2	1.68	0.93
1:A:990:ILE:HD12	1:A:994:GLU:C	1.92	0.93
1:A:1484:LEU:HD13	2:B:305:ARG:NH2	1.82	0.93
2:B:182:GLN:NE2	10:J:69:ARG:CB	2.32	0.93
18:R:199:LYS:CE	20:R:601:SO4:O2	2.17	0.93
1:A:991:LYS:HB3	1:A:993:GLN:HB2	1.50	0.93
2:B:202:LEU:HD23	2:B:202:LEU:H	1.34	0.93
2:B:1002:LYS:HD3	14:N:166:LEU:C	1.93	0.93
15:O:376:TYR:CD1	15:O:419:LYS:HE2	2.02	0.93
1:A:613:THR:HG21	2:B:913:ILE:CG2	1.98	0.93
2:B:1072:GLY:N	2:B:1075:GLU:HG2	1.80	0.93
16:P:405:TYR:HE1	16:P:414:ILE:HG23	1.31	0.93
1:A:953:GLU:C	1:A:1205:PHE:CB	2.42	0.93
2:B:1089:GLN:HG3	2:B:1093:LEU:HB2	1.42	0.93
15:O:233:LEU:O	15:O:237:ILE:HD12	1.65	0.93
18:R:5:PRO:HG3	18:R:217:THR:CB	1.71	0.93
1:A:756:LYS:CD	9:I:85:LYS:HZ3	1.76	0.92
16:P:24:SER:HB2	18:R:318:ILE:HD11	1.50	0.92
1:A:1049:MET:HB3	1:A:1052:GLY:HA2	1.42	0.92
2:B:1002:LYS:HD2	14:N:166:LEU:HB2	1.51	0.92
16:P:399:TRP:CZ3	18:R:291:ARG:O	2.22	0.92
17:Q:188:ALA:HB3	17:Q:384:GLN:CB	1.98	0.92
2:B:849:GLY:CA	12:L:60:ARG:NH2	2.17	0.92
2:B:1089:GLN:HG2	2:B:1093:LEU:CD2	1.90	0.92
17:Q:26:ARG:CB	17:Q:34:VAL:HG13	1.99	0.92
1:A:436:ALA:HA	1:A:439:ASP:O	1.68	0.92
1:A:720:PHE:CE2	8:H:141:TYR:HE2	1.86	0.92
2:B:890:ASP:O	12:L:54:ARG:CD	2.15	0.92
16:P:184:SER:HA	18:R:198:LEU:HB3	1.49	0.92
2:B:549:CYS:SG	2:B:649:MET:CG	2.57	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:15:CYS:HB3	17:Q:16:PRO:CA	2.00	0.92
17:Q:417:PHE:HE2	18:R:270:PHE:CE1	1.86	0.92
3:C:272:LYS:HG2	14:N:175:TYR:HD1	1.28	0.92
3:C:294:VAL:O	3:C:297:HIS:HB3	1.70	0.92
1:A:630:GLY:N	2:B:926:VAL:HG21	1.84	0.92
2:B:266:LYS:CG	2:B:473:GLN:O	2.18	0.92
18:R:199:LYS:HZ1	18:R:204:GLU:HA	1.35	0.92
1:A:436:ALA:O	1:A:439:ASP:C	2.11	0.92
1:A:684:ASP:OD2	8:H:20:TYR:HB3	1.69	0.92
1:A:1604:GLU:O	1:A:1612:LYS:HE2	1.70	0.92
16:P:184:SER:CB	18:R:198:LEU:H	1.83	0.92
1:A:403:LEU:O	1:A:406:LEU:HG	1.70	0.91
1:A:1317:ILE:HG21	1:A:1460:TYR:CE1	2.01	0.91
2:B:548:LYS:HE3	2:B:695:ASN:OD1	1.70	0.91
1:A:435:ASN:CB	1:A:442:LYS:CB	2.49	0.91
1:A:1049:MET:HB3	1:A:1052:GLY:H	1.35	0.91
2:B:64:GLY:HA2	2:B:242:ASP:CB	2.00	0.91
6:F:66:ARG:NH2	7:G:90:LEU:HD12	1.85	0.91
7:G:159:LYS:HB3	15:O:105:ASN:HD22	1.34	0.91
16:P:354:PRO:HG3	18:R:31:PHE:CD2	2.05	0.91
1:A:1310:LYS:CG	1:A:1311:GLU:CD	2.26	0.91
2:B:152:LEU:HB3	2:B:443:LYS:HE2	1.50	0.91
20:Q:1002:SO4:O4	18:R:1:MET:N	2.03	0.91
15:O:248:LEU:CD1	15:O:598:PHE:HE2	1.54	0.91
1:A:990:ILE:HG13	1:A:995:TYR:H	1.35	0.91
2:B:1151:ILE:HG12	7:G:21:LYS:HZ2	1.35	0.91
16:P:436:ILE:CB	18:R:143:THR:HG23	1.99	0.91
1:A:436:ALA:CB	1:A:443:ALA:HB2	2.00	0.91
1:A:545:SER:HB3	17:Q:34:VAL:CG2	1.96	0.91
1:A:634:ASN:ND2	2:B:1069:ILE:HG21	1.85	0.91
1:A:862:THR:HB	9:I:67:VAL:HG12	1.50	0.91
1:A:878:ARG:CB	9:I:67:VAL:HG13	1.97	0.91
17:Q:15:CYS:CB	17:Q:16:PRO:HA	1.99	0.91
17:Q:356:VAL:CG1	18:R:208:TYR:CD1	2.52	0.91
1:A:425:ASN:ND2	18:R:405:ILE:HG21	1.84	0.91
1:A:995:TYR:OH	2:B:715:ASN:ND2	2.04	0.91
1:A:1650:GLY:C	1:A:1652:GLY:H	1.79	0.91
2:B:894:LYS:HG3	12:L:54:ARG:HH22	0.74	0.91
17:Q:9:ILE:HG13	17:Q:10:CYS:N	1.77	0.91
1:A:429:THR:CG2	18:R:406:LYS:HZ1	1.83	0.91
1:A:670:ILE:HG12	2:B:783:MET:CE	2.01	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ARG:CD	9:I:66:VAL:HG21	2.00	0.91
2:B:266:LYS:CE	2:B:473:GLN:O	2.19	0.91
1:A:1313:LEU:CG	1:A:1462:PHE:CZ	2.54	0.90
15:O:247:GLU:OE1	15:O:325:ILE:HA	1.71	0.90
1:A:407:GLN:HE21	1:A:407:GLN:H	0.94	0.90
3:C:272:LYS:CG	14:N:175:TYR:CE1	2.54	0.90
18:R:173:MET:HG3	18:R:188:PHE:HZ	1.36	0.90
18:R:201:SER:O	18:R:205:VAL:CG2	2.20	0.90
16:P:434:ARG:N	18:R:145:SER:HA	1.85	0.90
18:R:199:LYS:CD	18:R:204:GLU:HB3	2.00	0.90
1:A:486:PRO:O	2:B:781:TYR:CE2	2.25	0.90
1:A:507:TYR:CE1	1:A:508:PRO:O	2.24	0.90
18:R:202:THR:HA	18:R:205:VAL:HG21	1.52	0.90
18:R:203:SER:CA	20:R:601:SO4:O3	2.18	0.90
1:A:470:HIS:HD2	2:B:1058:GLN:OE1	1.54	0.90
1:A:579:ARG:HH12	1:A:581:ILE:HA	1.34	0.90
17:Q:3:THR:HG22	17:Q:20:TRP:HB2	1.53	0.90
1:A:438:ILE:O	1:A:457:LYS:HB2	1.72	0.90
15:O:247:GLU:OE1	15:O:325:ILE:CB	2.20	0.90
16:P:443:ASP:HB3	18:R:3:GLU:OE2	1.72	0.90
1:A:1326:GLU:OE1	1:A:1455:ARG:N	2.03	0.90
1:A:826:PHE:CD1	2:B:777:SER:HB2	2.07	0.90
1:A:878:ARG:HD2	9:I:66:VAL:HG21	1.54	0.90
16:P:390:GLN:O	18:R:150:GLN:N	2.04	0.90
1:A:408:LYS:CA	1:A:411:VAL:HB	2.02	0.89
3:C:274:THR:HA	14:N:172:ALA:HB2	0.90	0.89
17:Q:19:LEU:HD11	17:Q:27:ARG:HB3	1.54	0.89
2:B:551:ILE:CG2	2:B:647:SER:HA	2.02	0.89
1:A:436:ALA:HB2	1:A:443:ALA:CB	2.01	0.89
2:B:679:GLN:CG	14:N:156:PRO:CA	2.43	0.89
2:B:1092:LEU:CA	2:B:1096:SER:HB2	2.02	0.89
16:P:694:ILE:HB	16:P:746:ARG:HD3	1.54	0.89
17:Q:188:ALA:HB3	17:Q:384:GLN:HB3	1.55	0.89
17:Q:341:ARG:CZ	17:Q:369:TRP:HE1	1.85	0.89
1:A:474:LYS:HZ1	2:B:1092:LEU:CD2	1.82	0.89
16:P:248:PRO:HD2	16:P:267:ASN:HB3	1.54	0.89
18:R:202:THR:HA	18:R:205:VAL:CG2	2.02	0.89
16:P:197:ARG:HE	16:P:261:VAL:H	1.16	0.89
1:A:581:ILE:HG13	1:A:585:ASP:OD2	1.71	0.89
1:A:1314:GLN:OE1	1:A:1446:ARG:HD2	1.73	0.89
6:F:70:LYS:CD	7:G:95:LEU:HD23	2.01	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:OD1	18:R:355:THR:CG2	2.20	0.89
1:A:474:LYS:HZ1	2:B:1092:LEU:HD22	1.34	0.89
1:A:627:ASP:O	2:B:784:ASP:HB3	1.73	0.89
18:R:5:PRO:HG2	18:R:217:THR:HG21	0.89	0.89
1:A:403:LEU:CD1	1:A:419:ILE:CG2	2.45	0.89
1:A:435:ASN:O	1:A:439:ASP:CB	2.21	0.89
1:A:1326:GLU:CD	1:A:1454:HIS:C	2.39	0.89
7:G:144:HIS:NE2	15:O:145:SER:CB	2.34	0.89
1:A:1314:GLN:HE22	1:A:1446:ARG:CD	1.83	0.89
2:B:64:GLY:HA2	2:B:242:ASP:HB3	1.54	0.89
15:O:376:TYR:CE1	15:O:588:LEU:HD21	2.07	0.89
14:N:86:ASP:O	14:N:141:GLU:HG2	1.71	0.89
2:B:534:PRO:HA	2:B:720:GLN:OE1	1.73	0.88
17:Q:193:PHE:O	18:R:209:ARG:NH1	2.06	0.88
3:C:272:LYS:CG	14:N:175:TYR:CD1	2.56	0.88
1:A:413:LEU:O	1:A:416:ARG:HG2	1.73	0.88
1:A:1276:THR:C	9:I:44:ASN:HA	1.99	0.88
16:P:433:VAL:HA	18:R:145:SER:CB	2.03	0.88
2:B:75:ASP:N	2:B:440:PHE:CE2	2.41	0.88
7:G:241:ARG:NH1	15:O:189:PHE:CB	2.35	0.88
3:C:58:ASN:HA	3:C:296:ASN:HD22	1.38	0.88
6:F:70:LYS:HD3	7:G:95:LEU:HD23	1.53	0.88
15:O:373:LEU:O	15:O:376:TYR:CB	2.21	0.88
1:A:1482:LYS:CD	2:B:304:ASP:OD1	2.22	0.88
2:B:800:TYR:OH	2:B:908:ARG:NH2	2.07	0.88
3:C:229:LEU:O	3:C:293:ARG:NH1	2.07	0.88
1:A:579:ARG:NH1	1:A:581:ILE:HA	1.88	0.88
2:B:145:VAL:CG1	2:B:441:LYS:HG2	2.04	0.88
17:Q:15:CYS:HB3	17:Q:16:PRO:C	1.98	0.88
18:R:199:LYS:CE	18:R:204:GLU:HA	2.03	0.88
1:A:543:LEU:O	17:Q:34:VAL:O	1.92	0.88
15:O:234:ILE:CG2	15:O:237:ILE:CG1	2.31	0.88
18:R:4:VAL:CG2	18:R:214:VAL:HG13	2.04	0.88
18:R:6:ILE:CD1	18:R:213:ILE:CB	2.50	0.88
1:A:1263:LEU:HA	1:A:1498:ILE:HD11	1.53	0.88
2:B:1151:ILE:HG12	7:G:21:LYS:NZ	1.88	0.88
7:G:144:HIS:NE2	15:O:145:SER:C	2.31	0.88
16:P:397:LYS:NZ	18:R:85:ARG:HH11	1.50	0.88
1:A:1322:ILE:CG2	1:A:1454:HIS:NE2	2.37	0.88
2:B:26:ILE:O	10:J:62:ARG:NH1	2.05	0.88
16:P:390:GLN:O	18:R:149:LYS:C	2.17	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ILE:CG1	17:Q:26:ARG:HH22	1.87	0.87
16:P:197:ARG:HD2	16:P:261:VAL:N	1.89	0.87
1:A:634:ASN:HD21	2:B:1069:ILE:HG21	1.37	0.87
1:A:954:GLY:N	1:A:1205:PHE:CB	2.37	0.87
1:A:998:HIS:O	2:B:712:SER:OG	1.92	0.87
1:A:1484:LEU:CD1	2:B:305:ARG:NE	2.35	0.87
3:C:293:ARG:H	3:C:295:ARG:NH1	1.72	0.87
1:A:474:LYS:HZ2	2:B:1092:LEU:HD23	1.34	0.87
1:A:1317:ILE:HG22	1:A:1460:TYR:CE1	2.09	0.87
2:B:143:TRP:CB	2:B:446:MET:HE1	1.94	0.87
2:B:266:LYS:HE3	2:B:473:GLN:C	1.99	0.87
17:Q:29:CYS:SG	17:Q:33:HIS:HB2	2.15	0.87
1:A:1053:ASP:O	1:A:1055:ILE:HG12	1.73	0.87
15:O:517:LEU:HD23	15:O:525:MET:HE3	1.56	0.87
17:Q:12:THR:CB	17:Q:33:HIS:ND1	2.37	0.87
1:A:966:LEU:HD21	1:A:997:PHE:CE1	2.09	0.87
1:A:474:LYS:HZ3	2:B:1096:SER:CB	1.88	0.87
17:Q:20:TRP:CH2	17:Q:22:ILE:CG2	2.56	0.87
18:R:15:GLN:CD	18:R:184:ASN:ND2	2.29	0.87
15:O:376:TYR:CZ	15:O:377:TYR:CZ	2.63	0.87
15:O:376:TYR:HE1	15:O:588:LEU:HD22	1.38	0.87
1:A:1085:LEU:HD22	6:F:84:TYR:OH	1.74	0.87
17:Q:378:LEU:HD23	18:R:216:LEU:HD21	1.56	0.87
1:A:1484:LEU:HD23	2:B:304:ASP:HB3	1.56	0.87
7:G:159:LYS:H	15:O:105:ASN:CG	1.82	0.87
7:G:159:LYS:N	15:O:105:ASN:HD21	1.50	0.87
7:G:159:LYS:CA	15:O:105:ASN:ND2	2.38	0.87
2:B:149:GLU:OE1	2:B:441:LYS:CE	2.23	0.86
15:O:243:GLU:OE1	15:O:328:LEU:CD2	2.08	0.86
16:P:389:TRP:CH2	18:R:149:LYS:N	2.42	0.86
1:A:1314:GLN:NE2	1:A:1446:ARG:CZ	2.38	0.86
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.57	0.86
15:O:238:ILE:O	15:O:242:VAL:HG23	1.75	0.86
18:R:168:ILE:HG23	18:R:169:PRO:HD3	1.58	0.86
1:A:408:LYS:HA	1:A:411:VAL:HB	1.55	0.86
2:B:143:TRP:CE2	2:B:446:MET:CG	2.58	0.86
6:F:74:ILE:O	7:G:95:LEU:HD13	1.72	0.86
13:M:102:SER:O	13:M:105:SER:C	2.17	0.86
1:A:954:GLY:N	1:A:1205:PHE:HB2	1.90	0.86
1:A:1056:ASP:HA	1:A:1179:ILE:HD13	1.57	0.86
16:P:185:GLN:HA	18:R:196:GLU:C	1.99	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:389:TRP:HH2	18:R:148:ASN:H	1.19	0.86
17:Q:409:ALA:O	17:Q:413:LEU:HB2	1.74	0.86
3:C:37:LYS:O	11:K:134:LYS:NZ	2.09	0.86
1:A:478:TYR:CD1	2:B:1048:SER:O	2.29	0.86
1:A:613:THR:HG21	2:B:913:ILE:HG21	1.57	0.86
1:A:756:LYS:CG	9:I:85:LYS:NZ	2.38	0.86
2:B:527:PHE:HZ	2:B:666:PRO:HA	1.39	0.86
3:C:230:LEU:HD12	3:C:231:PRO:CD	2.04	0.86
1:A:436:ALA:CA	1:A:439:ASP:O	2.24	0.86
3:C:293:ARG:N	3:C:295:ARG:NH1	2.23	0.86
1:A:40:ASN:ND2	18:R:355:THR:HG22	1.89	0.86
1:A:1326:GLU:OE2	1:A:1454:HIS:CA	2.24	0.86
2:B:143:TRP:CE3	2:B:446:MET:HE3	2.11	0.86
17:Q:20:TRP:CZ3	17:Q:22:ILE:HG21	2.08	0.86
2:B:679:GLN:CD	14:N:157:ARG:CA	2.48	0.86
16:P:397:LYS:HZ2	18:R:85:ARG:NH1	1.71	0.86
16:P:438:TRP:CG	18:R:141:TRP:CZ2	2.62	0.86
1:A:1606:SER:CB	1:A:1611:MET:HE3	2.06	0.85
2:B:679:GLN:CD	14:N:157:ARG:HA	1.99	0.85
1:A:1330:VAL:HG21	1:A:1455:ARG:NE	1.91	0.85
2:B:1089:GLN:CG	2:B:1093:LEU:HB2	2.06	0.85
6:F:74:ILE:C	7:G:95:LEU:HD11	2.00	0.85
16:P:436:ILE:HB	18:R:143:THR:HA	1.58	0.85
18:R:201:SER:O	18:R:205:VAL:HG23	1.75	0.85
1:A:756:LYS:CG	9:I:85:LYS:HZ2	1.89	0.85
1:A:1322:ILE:HD12	1:A:1457:ILE:HD12	1.57	0.85
2:B:143:TRP:CE2	2:B:446:MET:CB	2.58	0.85
16:P:184:SER:HB3	18:R:198:LEU:CA	2.07	0.85
2:B:849:GLY:HA3	12:L:60:ARG:NH2	1.89	0.85
6:F:72:LYS:CB	6:F:142:SER:HB2	2.05	0.85
1:A:477:ASN:C	2:B:1047:ARG:HD3	2.01	0.85
1:A:477:ASN:ND2	2:B:1049:THR:OG1	2.09	0.85
1:A:1032:VAL:HG21	1:A:1050:TYR:CD1	2.11	0.85
1:A:1660:VAL:O	7:G:102:GLU:HA	1.74	0.85
2:B:143:TRP:CE2	2:B:446:MET:HG3	2.11	0.85
1:A:475:ARG:HB3	2:B:1059:PRO:HB2	1.57	0.85
1:A:1262:LEU:CD2	1:A:1497:ILE:HG12	2.06	0.85
1:A:1313:LEU:HD23	1:A:1462:PHE:HZ	1.38	0.85
7:G:144:HIS:ND1	15:O:146:SER:OG	2.10	0.85
16:P:397:LYS:CE	18:R:85:ARG:HD3	2.04	0.85
1:A:990:ILE:HD12	1:A:994:GLU:O	1.77	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:CD2	1:A:1462:PHE:HZ	1.88	0.85
2:B:399:HIS:O	2:B:400:GLN:HG2	1.77	0.85
17:Q:26:ARG:CB	17:Q:34:VAL:CG1	2.53	0.85
1:A:535:GLN:HE22	17:Q:26:ARG:HD3	1.06	0.84
3:C:322:LYS:HE3	11:K:129:ASP:OD1	1.77	0.84
18:R:251:TRP:CD2	18:R:307:LYS:HE3	2.11	0.84
15:O:181:ARG:HB2	15:O:181:ARG:HH11	1.41	0.84
1:A:475:ARG:NH2	2:B:1061:LYS:HB2	1.91	0.84
2:B:346:ASP:OD1	13:M:113:ILE:HG23	1.76	0.84
1:A:1032:VAL:HG21	1:A:1050:TYR:CE1	2.12	0.84
7:G:141:SER:HB3	15:O:142:ILE:HD11	1.59	0.84
7:G:241:ARG:NH1	15:O:189:PHE:HB3	1.92	0.84
15:O:240:ILE:CG2	15:O:380:SER:CB	2.42	0.84
15:O:247:GLU:OE1	15:O:325:ILE:CA	2.25	0.84
17:Q:413:LEU:CG	18:R:273:TRP:HZ2	1.90	0.84
2:B:346:ASP:H	13:M:113:ILE:HG12	1.40	0.84
2:B:1049:THR:HG23	2:B:1050:GLY:N	1.92	0.84
13:M:61:GLU:OE2	13:M:106:LYS:CE	2.13	0.84
2:B:894:LYS:CD	12:L:47:ARG:NE	2.40	0.84
1:A:399:LEU:HD21	1:A:423:LEU:HG	1.59	0.84
1:A:475:ARG:CZ	2:B:1061:LYS:CB	2.56	0.84
1:A:429:THR:CG2	18:R:406:LYS:NZ	2.40	0.84
7:G:241:ARG:HH11	15:O:189:PHE:HB3	1.40	0.84
1:A:564:PRO:CG	15:O:370:THR:O	2.25	0.84
2:B:697:LEU:HB2	2:B:702:ASN:CG	2.03	0.84
18:R:5:PRO:HG3	18:R:217:THR:HB	0.84	0.84
1:A:1322:ILE:HG21	1:A:1454:HIS:CE1	2.08	0.84
2:B:1069:ILE:O	2:B:1070:ARG:HB3	1.76	0.84
17:Q:193:PHE:CE2	18:R:208:TYR:CD2	2.66	0.84
18:R:362:ALA:HB2	18:R:421:LYS:HB3	1.59	0.84
1:A:458:GLN:O	1:A:462:LYS:CB	2.26	0.83
2:B:894:LYS:CG	12:L:54:ARG:CZ	2.56	0.83
2:B:985:ILE:HB	14:N:160:VAL:HG21	1.59	0.83
3:C:59:ILE:O	3:C:296:ASN:HB2	1.78	0.83
13:M:102:SER:CB	13:M:105:SER:H	1.90	0.83
13:M:102:SER:C	13:M:105:SER:H	1.86	0.83
15:O:200:ASN:HB2	17:Q:14:ASN:HA	1.58	0.83
16:P:185:GLN:HB3	18:R:195:LEU:CB	2.08	0.83
1:A:429:THR:HG21	18:R:406:LYS:HE3	0.86	0.83
1:A:718:THR:O	8:H:98:TYR:N	2.11	0.83
2:B:25:PHE:CE1	10:J:59:LYS:HD2	2.13	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1089:GLN:CB	2:B:1093:LEU:HD22	2.09	0.83
1:A:999:CYS:HA	2:B:712:SER:HB3	1.57	0.83
1:A:629:ASP:OD1	2:B:926:VAL:HG23	1.79	0.83
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	1.58	0.83
2:B:985:ILE:HB	14:N:160:VAL:HG22	1.59	0.83
1:A:532:GLY:C	1:A:580:HIS:HD1	1.86	0.83
2:B:743:ARG:NH2	10:J:60:PHE:HZ	1.71	0.83
2:B:864:ASP:HB3	17:Q:412:LYS:CE	2.07	0.83
15:O:584:GLN:OE1	15:O:584:GLN:N	2.11	0.83
16:P:389:TRP:HH2	18:R:148:ASN:CA	1.91	0.83
2:B:848:ILE:CA	12:L:60:ARG:HD2	2.08	0.83
2:B:1092:LEU:HA	2:B:1096:SER:CB	2.09	0.83
17:Q:101:LYS:HG2	17:Q:152:LEU:HD11	1.58	0.83
1:A:966:LEU:CD2	1:A:997:PHE:CE1	2.61	0.83
2:B:623:ASP:O	2:B:648:ARG:NH1	2.10	0.83
2:B:1002:LYS:HD2	14:N:166:LEU:CB	2.09	0.83
1:A:986:PHE:CD2	2:B:958:MET:HE2	2.13	0.83
15:O:245:GLN:NE2	15:O:379:ARG:HB2	1.93	0.83
1:A:672:ASP:OD1	2:B:777:SER:OG	1.96	0.83
1:A:938:VAL:CG2	9:I:82:ILE:HD13	2.07	0.83
2:B:119:ARG:CZ	12:L:53:HIS:CE1	2.61	0.83
2:B:207:ILE:HD11	2:B:503:VAL:CG2	2.03	0.83
2:B:682:GLN:HA	14:N:154:ARG:NH2	1.92	0.83
6:F:74:ILE:O	7:G:95:LEU:HD12	1.79	0.83
15:O:181:ARG:HH11	15:O:181:ARG:CB	1.89	0.83
18:R:199:LYS:NZ	18:R:204:GLU:HA	1.93	0.83
16:P:397:LYS:HZ1	18:R:85:ARG:HH11	1.01	0.83
18:R:199:LYS:CE	18:R:203:SER:C	2.52	0.83
1:A:473:GLY:HA2	2:B:1072:GLY:HA2	1.60	0.82
1:A:544:VAL:HG13	17:Q:32:GLY:O	1.79	0.82
1:A:966:LEU:CD2	1:A:997:PHE:CZ	2.62	0.82
1:A:756:LYS:HD3	9:I:85:LYS:HZ2	1.37	0.82
1:A:1297:PHE:CE2	9:I:60:LEU:HD22	2.13	0.82
16:P:323:ASN:HA	16:P:350:THR:HA	1.61	0.82
17:Q:15:CYS:HB3	17:Q:16:PRO:HA	1.60	0.82
1:A:435:ASN:O	1:A:439:ASP:C	2.21	0.82
1:A:506:THR:CA	1:A:579:ARG:O	2.26	0.82
1:A:429:THR:HG21	18:R:406:LYS:NZ	1.93	0.82
1:A:478:TYR:CG	2:B:1048:SER:O	2.33	0.82
1:A:535:GLN:NE2	17:Q:26:ARG:CD	2.34	0.82
1:A:672:ASP:CG	2:B:777:SER:HB3	2.04	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ARG:O	2:B:649:MET:HA	1.79	0.82
2:B:894:LYS:O	2:B:896:GLN:N	2.11	0.82
1:A:615:ARG:NH1	2:B:929:ARG:NE	2.28	0.82
16:P:397:LYS:HE3	18:R:85:ARG:CZ	2.10	0.82
16:P:398:ALA:HB2	18:R:87:VAL:HA	1.61	0.82
1:A:435:ASN:CB	1:A:442:LYS:HB3	2.08	0.82
1:A:615:ARG:NH2	2:B:929:ARG:HG2	1.94	0.82
2:B:889:GLY:CA	12:L:54:ARG:O	2.28	0.82
3:C:334:THR:CG2	11:K:44:ARG:HB3	2.09	0.82
16:P:397:LYS:HE2	18:R:85:ARG:HE	1.41	0.82
17:Q:351:ASN:CB	17:Q:369:TRP:CZ2	2.62	0.82
18:R:317:LEU:CD1	18:R:367:ILE:CD1	2.58	0.82
2:B:776:ILE:HB	2:B:1026:ILE:HD13	1.60	0.82
2:B:850:THR:N	12:L:60:ARG:HH22	1.78	0.82
16:P:185:GLN:CB	18:R:195:LEU:HB3	2.10	0.82
16:P:368:HIS:HB3	16:P:411:LYS:HZ2	1.45	0.82
13:M:102:SER:HB3	13:M:105:SER:CA	2.09	0.82
16:P:394:VAL:HG11	18:R:144:VAL:CG2	2.10	0.82
18:R:248:LYS:HG2	18:R:298:GLN:CD	2.05	0.82
1:A:407:GLN:HB3	1:A:409:ASP:H	1.43	0.82
6:F:73:ALA:HA	6:F:143:PHE:O	1.80	0.82
2:B:49:PHE:CE2	2:B:194:PHE:CZ	2.68	0.81
17:Q:188:ALA:HB1	17:Q:384:GLN:HG3	1.61	0.81
18:R:252:GLY:O	18:R:256:GLU:HB2	1.79	0.81
1:A:824:THR:O	2:B:1023:ARG:N	2.12	0.81
2:B:864:ASP:HB3	17:Q:412:LYS:HE3	1.62	0.81
16:P:397:LYS:HE2	18:R:85:ARG:CD	2.04	0.81
1:A:535:GLN:HE21	17:Q:26:ARG:HD3	1.44	0.81
1:A:545:SER:CB	17:Q:34:VAL:HG23	2.08	0.81
2:B:566:TYR:HB3	13:M:74:ASN:OD1	1.79	0.81
2:B:975:HIS:ND1	14:N:169:GLU:HG3	1.96	0.81
6:F:72:LYS:CB	6:F:142:SER:CA	2.24	0.81
16:P:472:ARG:NE	18:R:200:THR:CG2	2.43	0.81
17:Q:20:TRP:HZ3	17:Q:22:ILE:HG22	0.65	0.81
18:R:206:ARG:H	18:R:206:ARG:HE	1.26	0.81
18:R:206:ARG:NH2	18:R:211:ARG:HH11	1.78	0.81
1:A:828:CYS:HB3	2:B:1027:TYR:HB2	1.60	0.81
2:B:610:TYR:HE1	2:B:658:LEU:HD11	1.44	0.81
18:R:426:VAL:HG12	18:R:428:SER:H	1.45	0.81
1:A:422:ARG:NH1	18:R:412:ARG:CZ	2.42	0.81
6:F:70:LYS:HG2	7:G:95:LEU:HG	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:LYS:HD3	6:F:142:SER:HB3	1.61	0.81
15:O:248:LEU:CD1	15:O:598:PHE:HD2	1.52	0.81
16:P:185:GLN:HG3	18:R:190:SER:CB	2.10	0.81
1:A:1603:MET:HE2	1:A:1615:TYR:HD2	1.39	0.81
14:N:87:TYR:CB	14:N:141:GLU:HA	1.93	0.81
1:A:984:GLY:N	1:A:994:GLU:OE2	2.13	0.81
1:A:1180:ASN:OD1	6:F:87:LYS:CD	2.25	0.81
1:A:1276:THR:OG1	9:I:45:LEU:HD13	1.77	0.81
2:B:29:PRO:HB2	2:B:177:PRO:HG2	1.62	0.81
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.60	0.81
1:A:547:ILE:HD11	17:Q:26:ARG:CZ	1.90	0.81
2:B:567:SER:O	14:N:140:SER:HB3	1.81	0.81
2:B:679:GLN:CD	14:N:157:ARG:N	2.39	0.81
3:C:272:LYS:CB	14:N:175:TYR:CE1	2.64	0.81
15:O:240:ILE:HG22	15:O:380:SER:HB2	1.58	0.81
17:Q:198:ILE:HG21	17:Q:388:THR:CG2	2.11	0.81
18:R:251:TRP:HE3	18:R:307:LYS:HE3	1.31	0.81
1:A:1575:ILE:CB	9:I:122:ARG:NH1	2.44	0.81
7:G:24:VAL:HG11	7:G:126:GLN:NE2	1.95	0.81
15:O:376:TYR:CE1	15:O:419:LYS:HE2	2.15	0.81
17:Q:20:TRP:CE3	17:Q:22:ILE:HG23	2.15	0.81
1:A:1482:LYS:HD2	2:B:307:GLU:OE1	1.81	0.80
2:B:794:ASP:OD1	2:B:911:PRO:HD2	1.81	0.80
15:O:342:HIS:CE1	15:O:346:GLN:HE21	1.98	0.80
17:Q:188:ALA:CB	17:Q:384:GLN:HB3	2.10	0.80
1:A:954:GLY:CA	1:A:1205:PHE:CB	2.59	0.80
1:A:40:ASN:HD21	18:R:355:THR:HG22	1.44	0.80
1:A:990:ILE:O	1:A:992:PRO:N	2.14	0.80
14:N:87:TYR:HA	14:N:141:GLU:HA	0.81	0.80
15:O:235:GLU:O	15:O:238:ILE:HD12	1.81	0.80
1:A:425:ASN:ND2	18:R:406:LYS:HZ2	1.78	0.80
1:A:1329:ILE:CG2	1:A:1456:PHE:CZ	2.64	0.80
2:B:75:ASP:HB3	2:B:440:PHE:CD2	2.15	0.80
2:B:208:VAL:HG23	2:B:401:GLU:HG2	1.64	0.80
2:B:1003:ALA:O	14:N:170:HIS:CA	2.29	0.80
14:N:87:TYR:CE2	14:N:141:GLU:OE1	2.34	0.80
16:P:472:ARG:CZ	18:R:200:THR:CG2	2.58	0.80
1:A:477:ASN:HA	2:B:1047:ARG:NH1	1.95	0.80
1:A:478:TYR:O	1:A:479:ALA:HB2	1.79	0.80
1:A:721:LYS:NZ	8:H:91:ASP:HA	1.96	0.80
1:A:1657:LEU:HB2	6:F:133:VAL:HB	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:184:SER:CB	18:R:198:LEU:CB	2.39	0.80
15:O:201:LYS:HD2	15:O:239:SER:OG	1.82	0.80
16:P:390:GLN:O	18:R:149:LYS:HB3	1.80	0.80
16:P:436:ILE:O	18:R:141:TRP:O	2.00	0.80
1:A:862:THR:HG22	9:I:67:VAL:CG1	2.10	0.80
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.21	0.80
1:A:407:GLN:CB	1:A:409:ASP:H	1.94	0.80
1:A:719:ILE:HG12	8:H:97:MET:HG2	1.62	0.80
1:A:1575:ILE:CA	9:I:122:ARG:NH1	2.43	0.80
2:B:681:ILE:HB	14:N:154:ARG:CG	2.12	0.80
16:P:349:GLY:CA	18:R:153:ASN:O	2.30	0.80
1:A:1330:VAL:CG2	1:A:1455:ARG:NE	2.44	0.80
3:C:272:LYS:HA	14:N:175:TYR:CE2	2.14	0.80
7:G:141:SER:HB2	15:O:142:ILE:CD1	1.95	0.80
16:P:473:HIS:CD2	18:R:1:MET:CB	2.10	0.80
1:A:862:THR:HA	9:I:67:VAL:CB	2.12	0.80
2:B:551:ILE:HA	2:B:648:ARG:O	1.82	0.80
2:B:796:ARG:HD2	10:J:8:PHE:HA	1.62	0.80
7:G:159:LYS:H	15:O:105:ASN:HD21	0.80	0.80
1:A:581:ILE:HD12	1:A:637:PHE:CE1	2.17	0.79
1:A:1038:ILE:HD11	1:A:1050:TYR:HA	1.64	0.79
1:A:1120:TYR:O	5:E:207:ARG:NH2	2.12	0.79
2:B:25:PHE:O	10:J:62:ARG:HD2	1.83	0.79
1:A:990:ILE:CD1	1:A:995:TYR:CA	2.60	0.79
16:P:321:LYS:H	16:P:321:LYS:HD3	1.46	0.79
17:Q:371:GLU:HG3	18:R:231:LEU:HD12	1.62	0.79
1:A:40:ASN:CG	18:R:355:THR:CG2	2.55	0.79
1:A:1310:LYS:HD3	1:A:1310:LYS:H	1.45	0.79
2:B:49:PHE:CE2	2:B:194:PHE:HZ	2.01	0.79
2:B:143:TRP:CB	2:B:446:MET:HE3	2.00	0.79
18:R:347:ASP:O	18:R:351:GLU:HB2	1.81	0.79
1:A:472:MET:HG3	2:B:1073:GLU:OE1	1.82	0.79
3:C:272:LYS:N	14:N:175:TYR:CE1	2.35	0.79
16:P:397:LYS:HZ1	18:R:85:ARG:CD	1.79	0.79
16:P:434:ARG:H	18:R:145:SER:HA	1.44	0.79
17:Q:17:SER:O	17:Q:29:CYS:CB	2.30	0.79
18:R:317:LEU:CD1	18:R:367:ILE:HD13	2.12	0.79
16:P:198:ASP:HB3	16:P:205:TYR:O	1.79	0.79
17:Q:351:ASN:CA	17:Q:369:TRP:HH2	1.93	0.79
1:A:476:VAL:HG22	2:B:1070:ARG:N	1.97	0.79
1:A:1314:GLN:CD	1:A:1446:ARG:CD	2.56	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ILE:HG23	2:B:71:LYS:NZ	1.84	0.79
2:B:1089:GLN:CD	2:B:1093:LEU:HD13	2.07	0.79
16:P:185:GLN:CA	18:R:196:GLU:O	2.28	0.79
17:Q:188:ALA:CB	17:Q:384:GLN:HG3	2.12	0.79
17:Q:356:VAL:HG11	18:R:208:TYR:HD1	1.45	0.79
6:F:72:LYS:C	6:F:143:PHE:H	1.91	0.79
7:G:144:HIS:HD2	15:O:146:SER:HA	1.42	0.79
17:Q:356:VAL:CG1	18:R:212:HIS:CE1	2.66	0.79
1:A:425:ASN:ND2	18:R:406:LYS:NZ	2.30	0.79
1:A:671:GLN:OE1	2:B:952:HIS:HB2	1.83	0.79
1:A:721:LYS:HB3	8:H:96:VAL:HB	1.64	0.79
14:N:88:LYS:N	14:N:140:SER:O	2.15	0.79
1:A:1049:MET:HG3	1:A:1053:ASP:N	1.97	0.79
2:B:532:HIS:NE2	2:B:723:LYS:NZ	2.31	0.79
3:C:272:LYS:CA	14:N:175:TYR:CD1	2.44	0.79
13:M:102:SER:C	13:M:105:SER:N	2.40	0.79
16:P:775:TRP:H	17:Q:109:GLN:HE22	1.28	0.79
1:A:399:LEU:HD23	1:A:423:LEU:HD23	1.63	0.78
1:A:547:ILE:HG13	17:Q:26:ARG:HH22	1.48	0.78
3:C:103:LEU:O	10:J:6:ARG:NE	2.12	0.78
6:F:66:ARG:NH2	7:G:90:LEU:HD13	1.98	0.78
2:B:143:TRP:CZ2	2:B:446:MET:HA	2.18	0.78
1:A:40:ASN:CG	18:R:355:THR:HG22	2.08	0.78
1:A:1650:GLY:C	1:A:1652:GLY:N	2.38	0.78
2:B:1093:LEU:CG	2:B:1094:ASN:OD1	2.29	0.78
1:A:407:GLN:HE21	1:A:407:GLN:N	1.78	0.78
1:A:1657:LEU:HD23	7:G:104:LEU:HB3	1.65	0.78
6:F:66:ARG:HH22	7:G:90:LEU:CD1	1.94	0.78
17:Q:356:VAL:HG13	18:R:212:HIS:HE1	1.48	0.78
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.17	0.78
1:A:862:THR:HA	9:I:67:VAL:HA	1.65	0.78
1:A:1298:ASP:HA	1:A:1468:LYS:HZ3	1.49	0.78
2:B:145:VAL:HG11	2:B:441:LYS:CG	2.09	0.78
3:C:253:PRO:CD	14:N:180:PHE:HD1	1.90	0.78
16:P:434:ARG:HG2	18:R:143:THR:CB	2.13	0.78
18:R:317:LEU:HD12	18:R:367:ILE:CD1	2.13	0.78
1:A:83:VAL:HG11	1:A:427:PHE:CZ	2.19	0.78
1:A:88:PRO:HG3	1:A:434:VAL:HG12	1.65	0.78
1:A:403:LEU:HD11	1:A:419:ILE:HG21	0.85	0.78
1:A:862:THR:HA	9:I:67:VAL:CA	2.13	0.78
1:A:1049:MET:CG	1:A:1052:GLY:CA	2.62	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ASP:CB	2:B:440:PHE:CZ	2.66	0.78
2:B:119:ARG:NH2	12:L:53:HIS:CE1	2.52	0.78
2:B:346:ASP:CG	13:M:113:ILE:HG23	2.07	0.78
2:B:679:GLN:CG	14:N:156:PRO:HA	2.14	0.78
1:A:478:TYR:O	1:A:479:ALA:CB	2.29	0.78
1:A:996:TYR:CE2	2:B:530:PRO:HG3	2.19	0.78
15:O:461:VAL:HG13	15:O:467:MET:HE1	1.65	0.78
18:R:177:LEU:HD22	18:R:185:LYS:HG2	1.66	0.78
1:A:1049:MET:HG2	1:A:1052:GLY:CA	2.13	0.78
2:B:184:LYS:HB3	2:B:735:HIS:ND1	1.99	0.78
2:B:566:TYR:HD2	13:M:73:SER:HG	1.21	0.78
16:P:443:ASP:C	18:R:3:GLU:HB2	2.09	0.78
1:A:435:ASN:C	1:A:439:ASP:O	2.27	0.78
1:A:1032:VAL:CG2	1:A:1050:TYR:CD1	2.67	0.77
1:A:1600:ARG:NE	1:A:1616:GLU:OE1	2.16	0.77
17:Q:351:ASN:HA	17:Q:369:TRP:CH2	2.19	0.77
15:O:376:TYR:CG	15:O:419:LYS:HE2	2.19	0.77
1:A:547:ILE:HD13	17:Q:26:ARG:NH1	1.98	0.77
1:A:566:SER:CB	15:O:235:GLU:OE1	2.28	0.77
1:A:984:GLY:HA3	1:A:994:GLU:CD	2.09	0.77
1:A:1484:LEU:CD2	2:B:304:ASP:HB3	2.14	0.77
2:B:679:GLN:CG	14:N:155:VAL:O	2.32	0.77
15:O:186:SER:O	15:O:190:ILE:HG22	1.85	0.77
18:R:199:LYS:HE3	18:R:203:SER:C	2.08	0.77
2:B:207:ILE:HG12	2:B:503:VAL:HG21	1.61	0.77
2:B:878:GLU:OE2	2:B:909:ARG:NH1	2.17	0.77
2:B:143:TRP:CH2	2:B:446:MET:HA	2.19	0.77
16:P:245:ILE:HG12	16:P:269:PHE:HB2	1.66	0.77
16:P:405:TYR:CE1	16:P:414:ILE:HG23	2.19	0.77
1:A:878:ARG:CB	9:I:67:VAL:HG11	2.05	0.77
1:A:990:ILE:CD1	1:A:994:GLU:C	2.57	0.77
15:O:396:MET:HE1	15:O:433:LYS:C	2.08	0.77
2:B:73:ILE:HD12	2:B:425:ILE:HG23	1.67	0.77
2:B:743:ARG:NH2	10:J:60:PHE:CE2	2.52	0.77
15:O:155:SER:HA	15:O:158:LEU:HD12	1.67	0.77
17:Q:358:PRO:CB	18:R:206:ARG:NH1	2.47	0.77
1:A:407:GLN:H	1:A:407:GLN:NE2	1.79	0.77
17:Q:12:THR:OG1	17:Q:33:HIS:ND1	2.17	0.77
2:B:46:ILE:HA	2:B:164:MET:SD	2.25	0.77
2:B:49:PHE:CB	2:B:164:MET:HE3	2.14	0.77
7:G:144:HIS:CD2	15:O:146:SER:OG	2.38	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:159:LYS:HB2	15:O:105:ASN:ND2	1.95	0.77
15:O:235:GLU:O	15:O:238:ILE:CD1	2.33	0.77
16:P:397:LYS:HZ3	18:R:85:ARG:CD	1.80	0.77
1:A:990:ILE:HG13	1:A:995:TYR:CA	2.14	0.77
2:B:1096:SER:O	2:B:1097:ASP:HB3	1.84	0.77
1:A:953:GLU:O	1:A:1205:PHE:CG	2.38	0.76
2:B:49:PHE:CB	2:B:164:MET:CE	2.62	0.76
2:B:415:GLU:OE2	2:B:474:SER:OG	2.02	0.76
15:O:435:SER:OG	15:O:438:GLN:HG3	1.84	0.76
1:A:991:LYS:N	1:A:994:GLU:CG	2.30	0.76
2:B:207:ILE:HD11	2:B:503:VAL:HG11	1.66	0.76
2:B:1003:ALA:O	14:N:170:HIS:HB3	1.85	0.76
15:O:477:PHE:HE2	15:O:525:MET:HE1	1.50	0.76
16:P:200:THR:HG21	16:P:280:ARG:NH1	1.99	0.76
2:B:30:LYS:C	2:B:176:SER:HB2	2.11	0.76
2:B:527:PHE:CD2	2:B:666:PRO:HB3	2.19	0.76
1:A:478:TYR:HA	2:B:1048:SER:C	2.10	0.76
2:B:346:ASP:N	13:M:113:ILE:HG12	1.99	0.76
17:Q:358:PRO:C	18:R:206:ARG:HH12	1.92	0.76
1:A:382:GLN:HE21	1:A:456:VAL:HG22	1.50	0.76
1:A:1484:LEU:HD23	2:B:304:ASP:CB	2.15	0.76
8:H:80:ARG:HG3	11:K:108:TYR:CZ	2.21	0.76
16:P:24:SER:CB	18:R:318:ILE:HD11	2.14	0.76
1:A:475:ARG:NH2	2:B:1061:LYS:CG	2.49	0.76
3:C:142:ARG:CZ	10:J:67:GLU:OE2	2.33	0.76
3:C:315:PHE:CE2	11:K:139:ILE:HD12	2.20	0.76
7:G:144:HIS:CG	15:O:146:SER:CB	2.69	0.76
16:P:436:ILE:H	18:R:143:THR:N	1.84	0.76
1:A:493:ASN:HB3	1:A:654:ASP:OD1	1.85	0.76
1:A:1657:LEU:N	6:F:133:VAL:O	2.17	0.76
2:B:205:MET:HE1	2:B:500:PHE:O	1.85	0.76
2:B:563:SER:CB	13:M:73:SER:HB3	2.16	0.76
16:P:598:LEU:HD23	16:P:601:ARG:HD2	1.68	0.76
2:B:1089:GLN:CG	2:B:1093:LEU:CD1	2.59	0.76
1:A:409:ASP:OD1	1:A:410:LYS:N	2.19	0.76
1:A:1204:THR:HG21	9:I:97:HIS:HB3	1.66	0.76
2:B:202:LEU:HD11	2:B:499:HIS:HB3	1.67	0.76
6:F:70:LYS:O	6:F:74:ILE:N	2.19	0.76
1:A:435:ASN:CB	1:A:442:LYS:HB2	2.11	0.76
15:O:200:ASN:HD22	17:Q:14:ASN:C	1.92	0.76
1:A:581:ILE:HD12	1:A:637:PHE:CZ	2.21	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:HG3	6:F:78:GLN:CD	2.11	0.75
15:O:62:ASP:HB3	15:O:67:ASP:OD2	1.86	0.75
17:Q:22:ILE:HD11	17:Q:24:ASP:OD2	1.86	0.75
18:R:414:PHE:HA	18:R:417:ILE:HG22	1.66	0.75
16:P:197:ARG:CD	16:P:261:VAL:N	2.49	0.75
16:P:398:ALA:CB	18:R:87:VAL:HA	2.16	0.75
18:R:180:CYS:O	18:R:185:LYS:HE3	1.86	0.75
2:B:49:PHE:HB2	2:B:164:MET:HE1	1.66	0.75
2:B:527:PHE:CZ	2:B:666:PRO:N	2.54	0.75
7:G:144:HIS:CD2	15:O:146:SER:N	2.55	0.75
16:P:698:LYS:HE2	17:Q:124:ARG:HH21	1.50	0.75
1:A:1299:ASN:OD1	1:A:1467:GLY:C	2.28	0.75
17:Q:22:ILE:CG1	17:Q:24:ASP:OD2	2.34	0.75
1:A:953:GLU:CG	1:A:1205:PHE:CE2	2.69	0.75
2:B:551:ILE:HG23	2:B:648:ARG:H	1.48	0.75
15:O:248:LEU:HD11	15:O:598:PHE:CD2	1.86	0.75
1:A:670:ILE:CG1	2:B:783:MET:CE	2.65	0.75
1:A:990:ILE:CG1	1:A:994:GLU:HB2	2.16	0.75
1:A:1298:ASP:O	1:A:1301:GLU:N	2.20	0.75
3:C:253:PRO:HD2	14:N:180:PHE:HB3	0.78	0.75
16:P:443:ASP:HB3	18:R:3:GLU:CB	2.17	0.75
1:A:408:LYS:HB2	1:A:411:VAL:HB	1.68	0.75
1:A:474:LYS:H	2:B:1070:ARG:HG3	1.51	0.75
2:B:527:PHE:CZ	2:B:666:PRO:CB	2.70	0.75
7:G:143:SER:HB2	15:O:104:ILE:CB	2.15	0.75
1:A:472:MET:HE2	1:A:472:MET:CA	2.15	0.75
1:A:543:LEU:C	17:Q:34:VAL:O	2.30	0.75
15:O:376:TYR:OH	15:O:588:LEU:CD2	2.35	0.74
16:P:438:TRP:HD1	18:R:141:TRP:CZ2	1.98	0.74
1:A:1313:LEU:CG	1:A:1462:PHE:HZ	1.99	0.74
16:P:390:GLN:HB2	18:R:151:PRO:C	2.13	0.74
17:Q:351:ASN:C	17:Q:369:TRP:HH2	1.95	0.74
1:A:474:LYS:NZ	2:B:1096:SER:CB	2.49	0.74
2:B:518:ARG:NH2	2:B:537:SER:O	2.21	0.74
1:A:425:ASN:ND2	18:R:405:ILE:CG2	2.50	0.74
1:A:670:ILE:CG1	2:B:783:MET:HE3	2.18	0.74
1:A:984:GLY:CA	1:A:994:GLU:OE2	2.36	0.74
1:A:991:LYS:CB	1:A:993:GLN:CB	2.62	0.74
1:A:999:CYS:HA	2:B:712:SER:OG	1.86	0.74
1:A:1049:MET:HG2	1:A:1052:GLY:O	1.84	0.74
2:B:1005:TYR:CE2	14:N:170:HIS:CG	2.75	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:384:ASP:HB3	16:P:389:TRP:HB3	1.69	0.74
17:Q:3:THR:O	17:Q:20:TRP:HB3	1.87	0.74
17:Q:417:PHE:HZ	18:R:270:PHE:CD1	2.05	0.74
1:A:406:LEU:HB3	1:A:408:LYS:H	1.53	0.74
1:A:1322:ILE:CG2	1:A:1454:HIS:ND1	2.24	0.74
2:B:25:PHE:O	10:J:62:ARG:CD	2.35	0.74
2:B:679:GLN:HG2	14:N:157:ARG:CA	2.14	0.74
18:R:199:LYS:HE2	18:R:203:SER:C	2.11	0.74
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.69	0.74
13:M:102:SER:CB	13:M:105:SER:N	2.49	0.74
15:O:379:ARG:HA	15:O:379:ARG:NH1	1.99	0.74
17:Q:22:ILE:HD12	17:Q:24:ASP:CG	2.11	0.74
17:Q:198:ILE:HG21	17:Q:388:THR:HG23	1.69	0.74
1:A:1487:ASN:OD1	2:B:305:ARG:NH2	2.21	0.74
3:C:100:ARG:NH2	10:J:3:VAL:O	2.20	0.74
16:P:389:TRP:CA	18:R:151:PRO:HA	2.17	0.74
17:Q:410:ARG:HA	17:Q:413:LEU:HB3	1.69	0.74
1:A:425:ASN:CG	18:R:406:LYS:NZ	2.46	0.74
1:A:615:ARG:HH21	2:B:781:TYR:HD2	1.36	0.74
1:A:921:PRO:HD3	8:H:19:ARG:HG2	1.68	0.74
1:A:952:LEU:CD2	1:A:1004:GLU:HG3	2.07	0.74
7:G:142:ALA:CB	15:O:102:SER:O	2.35	0.74
16:P:480:VAL:HB	16:P:492:LEU:HD21	1.68	0.74
1:A:566:SER:HB2	15:O:235:GLU:OE2	1.73	0.74
1:A:588:LEU:CD2	2:B:1087:LEU:HD13	2.18	0.74
1:A:990:ILE:C	1:A:994:GLU:HB2	2.12	0.74
3:C:322:LYS:CE	11:K:129:ASP:OD1	2.35	0.74
15:O:579:LEU:CA	15:O:582:ARG:HB3	2.11	0.74
1:A:472:MET:HA	1:A:472:MET:CE	2.16	0.73
2:B:1003:ALA:O	14:N:170:HIS:CB	2.36	0.73
15:O:373:LEU:HB3	15:O:374:PRO:HD3	1.69	0.73
1:A:399:LEU:CD2	1:A:423:LEU:HD23	2.18	0.73
1:A:824:THR:CB	2:B:1023:ARG:HB2	2.11	0.73
1:A:862:THR:C	9:I:67:VAL:HA	2.13	0.73
2:B:497:ILE:HG12	2:B:699:ILE:HD13	1.68	0.73
7:G:241:ARG:NH1	15:O:189:PHE:HB2	1.95	0.73
16:P:436:ILE:HB	18:R:143:THR:CA	2.17	0.73
17:Q:22:ILE:CD1	17:Q:26:ARG:CZ	2.65	0.73
18:R:5:PRO:HD2	18:R:217:THR:OG1	1.86	0.73
1:A:40:ASN:OD1	18:R:355:THR:HG22	1.88	0.73
1:A:436:ALA:C	1:A:439:ASP:N	2.32	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASN:HD22	2:B:441:LYS:HE3	1.53	0.73
7:G:143:SER:CB	15:O:104:ILE:CG2	2.17	0.73
1:A:1204:THR:CG2	9:I:97:HIS:HB3	2.17	0.73
2:B:152:LEU:HB3	2:B:443:LYS:HE3	0.73	0.73
16:P:200:THR:HG21	16:P:280:ARG:HH11	1.54	0.73
1:A:878:ARG:CG	9:I:67:VAL:CG1	2.55	0.73
1:A:1329:ILE:HG22	1:A:1456:PHE:CZ	2.22	0.73
2:B:73:ILE:HB	2:B:425:ILE:HD12	1.70	0.73
15:O:243:GLU:CB	15:O:332:LEU:HD13	2.17	0.73
15:O:245:GLN:HA	15:O:245:GLN:HE21	1.51	0.73
1:A:435:ASN:O	1:A:439:ASP:CA	2.37	0.73
1:A:998:HIS:NE2	2:B:711:GLN:CG	2.50	0.73
1:A:1298:ASP:CG	1:A:1468:LYS:NZ	2.46	0.73
2:B:401:GLU:HG3	2:B:402:VAL:N	2.03	0.73
6:F:72:LYS:O	6:F:143:PHE:N	2.20	0.73
16:P:357:LEU:HG	18:R:24:ILE:HD11	1.69	0.73
1:A:403:LEU:CD1	1:A:419:ILE:HD13	2.18	0.73
1:A:1262:LEU:HD21	1:A:1497:ILE:HG12	1.69	0.73
2:B:346:ASP:OD2	13:M:114:LYS:N	2.22	0.73
2:B:399:HIS:O	2:B:400:GLN:CG	2.35	0.73
7:G:143:SER:CB	15:O:104:ILE:CB	2.66	0.73
1:A:399:LEU:CD2	1:A:423:LEU:CD2	2.67	0.73
1:A:481:ARG:O	2:B:1045:GLN:O	2.06	0.73
2:B:894:LYS:HG3	12:L:54:ARG:CZ	2.15	0.73
2:B:1092:LEU:O	2:B:1096:SER:CB	2.36	0.73
1:A:1310:LYS:HB3	1:A:1464:ASP:O	1.88	0.73
16:P:389:TRP:CZ2	18:R:147:GLN:HA	2.23	0.73
16:P:446:ASP:OD2	16:P:448:THR:HG22	1.89	0.73
1:A:436:ALA:O	1:A:440:SER:CA	2.37	0.73
2:B:184:LYS:HD3	2:B:735:HIS:NE2	2.04	0.73
2:B:527:PHE:CE1	2:B:666:PRO:CA	2.72	0.73
2:B:1151:ILE:HG23	7:G:21:LYS:HG3	1.70	0.73
18:R:206:ARG:HH21	18:R:211:ARG:HH11	1.34	0.73
1:A:497:VAL:HG22	1:A:635:MET:HE1	1.69	0.72
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.24	0.72
1:A:1658:ALA:HA	6:F:131:PRO:O	1.88	0.72
6:F:72:LYS:HD2	6:F:142:SER:HB3	0.76	0.72
16:P:322:GLY:O	16:P:350:THR:OG1	2.07	0.72
2:B:25:PHE:CD2	10:J:59:LYS:HG3	2.24	0.72
2:B:985:ILE:C	14:N:160:VAL:HG23	2.14	0.72
17:Q:15:CYS:CB	17:Q:16:PRO:CA	2.62	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:113:LYS:HG3	17:Q:134:LYS:HZ1	1.54	0.72
17:Q:288:GLU:O	17:Q:290:THR:OG1	2.06	0.72
18:R:373:LEU:HD12	18:R:411:VAL:HG21	1.70	0.72
1:A:670:ILE:HG12	2:B:783:MET:HE3	1.70	0.72
1:A:986:PHE:CE2	2:B:958:MET:HE2	2.24	0.72
2:B:26:ILE:O	10:J:62:ARG:CZ	2.36	0.72
2:B:566:TYR:CE2	13:M:70:SER:HA	2.24	0.72
1:A:953:GLU:HG2	1:A:1205:PHE:HE2	1.54	0.72
2:B:143:TRP:HB3	2:B:446:MET:SD	2.29	0.72
16:P:197:ARG:NE	16:P:261:VAL:N	2.34	0.72
16:P:436:ILE:O	18:R:141:TRP:CD2	2.43	0.72
2:B:345:SER:HA	13:M:113:ILE:CG1	2.17	0.72
16:P:214:LEU:HB3	16:P:220:THR:HB	1.71	0.72
1:A:1329:ILE:HB	1:A:1456:PHE:HE2	1.54	0.72
17:Q:12:THR:OG1	17:Q:33:HIS:CE1	2.42	0.72
1:A:474:LYS:HZ2	2:B:1092:LEU:CA	1.97	0.72
1:A:629:ASP:CA	2:B:926:VAL:HG21	2.19	0.72
2:B:527:PHE:CE1	2:B:666:PRO:N	2.58	0.72
1:A:1329:ILE:HG21	1:A:1456:PHE:CZ	2.24	0.72
2:B:683:ASN:H	14:N:154:ARG:NH2	1.86	0.72
1:A:629:ASP:O	2:B:926:VAL:HG21	1.87	0.72
2:B:843:ASP:OD2	12:L:58:LYS:NZ	2.23	0.72
2:B:1121:GLY:O	15:O:152:GLN:NE2	2.23	0.72
15:O:234:ILE:HG23	15:O:237:ILE:CG1	2.06	0.72
16:P:656:HIS:H	16:P:656:HIS:CD2	2.06	0.72
18:R:5:PRO:CD	18:R:217:THR:HG21	2.19	0.72
2:B:184:LYS:HD3	2:B:735:HIS:CD2	2.25	0.72
15:O:216:LEU:HD13	15:O:342:HIS:CG	2.25	0.72
16:P:662:LEU:HB3	16:P:665:ASN:ND2	2.05	0.72
18:R:4:VAL:CG1	18:R:214:VAL:HG22	2.20	0.72
1:A:990:ILE:CD1	1:A:995:TYR:N	2.52	0.71
1:A:1310:LYS:HD3	1:A:1310:LYS:N	2.05	0.71
1:A:1554:GLY:HA2	5:E:183:PRO:HD2	1.72	0.71
3:C:231:PRO:HB2	3:C:270:ALA:HB1	1.72	0.71
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.72	0.71
16:P:348:HIS:NE2	18:R:154:LYS:HD3	2.04	0.71
16:P:436:ILE:HG23	18:R:141:TRP:C	2.09	0.71
17:Q:418:PRO:HD2	18:R:233:TYR:OH	1.90	0.71
1:A:952:LEU:HD22	1:A:1004:GLU:CG	2.09	0.71
1:A:1660:VAL:O	7:G:102:GLU:CG	2.37	0.71
2:B:182:GLN:O	10:J:69:ARG:NE	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:186:TYR:N	18:R:196:GLU:O	2.23	0.71
16:P:434:ARG:HB3	18:R:143:THR:HB	1.69	0.71
17:Q:351:ASN:HA	17:Q:369:TRP:CZ2	2.24	0.71
1:A:984:GLY:HA3	1:A:994:GLU:OE2	1.89	0.71
15:O:200:ASN:CA	17:Q:14:ASN:HB2	2.15	0.71
2:B:1072:GLY:C	2:B:1075:GLU:CG	2.51	0.71
15:O:383:TYR:HD1	15:O:606:MET:HE3	1.54	0.71
16:P:184:SER:CA	18:R:198:LEU:CB	2.67	0.71
17:Q:288:GLU:HG3	17:Q:297:ARG:HH12	1.55	0.71
1:A:40:ASN:OD1	18:R:355:THR:HG23	1.89	0.71
1:A:999:CYS:CA	2:B:712:SER:HB3	2.15	0.71
2:B:1089:GLN:NE2	2:B:1093:LEU:HD13	2.05	0.71
3:C:296:ASN:OD1	3:C:297:HIS:N	2.24	0.71
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.72	0.71
1:A:953:GLU:O	1:A:1205:PHE:CD1	2.43	0.71
2:B:1069:ILE:HD12	2:B:1069:ILE:N	2.06	0.71
15:O:66:ASN:HD22	15:O:66:ASN:N	1.89	0.71
16:P:438:TRP:CD1	18:R:141:TRP:CE2	2.79	0.71
1:A:524:ILE:O	1:A:554:ARG:NH1	2.24	0.71
2:B:898:LEU:N	12:L:46:VAL:HG21	2.06	0.71
2:B:1002:LYS:CD	14:N:166:LEU:C	2.60	0.71
3:C:31:TRP:CH2	11:K:127:LEU:HD12	2.26	0.71
15:O:348:THR:CG2	15:O:351:SER:HB3	2.19	0.71
15:O:517:LEU:HA	15:O:525:MET:HE3	1.72	0.71
16:P:532:GLU:HA	16:P:554:ASN:HD22	1.55	0.71
18:R:173:MET:HG3	18:R:188:PHE:CZ	2.25	0.71
1:A:543:LEU:CB	17:Q:34:VAL:O	2.38	0.71
1:A:83:VAL:CG1	1:A:427:PHE:CZ	2.73	0.71
2:B:207:ILE:CD1	2:B:503:VAL:HG22	2.21	0.71
2:B:345:SER:HA	13:M:113:ILE:HD11	1.72	0.71
2:B:527:PHE:CE1	2:B:666:PRO:CD	2.73	0.71
2:B:1165:ASN:N	2:B:1165:ASN:OD1	2.24	0.71
3:C:272:LYS:HA	14:N:175:TYR:CG	2.24	0.71
16:P:22:GLY:HA2	18:R:139:GLU:OE2	1.89	0.71
16:P:364:GLU:O	16:P:373:LEU:HB2	1.91	0.71
1:A:581:ILE:HG13	1:A:585:ASP:CG	2.15	0.70
1:A:1482:LYS:HD3	2:B:304:ASP:OD1	1.90	0.70
15:O:245:GLN:CD	15:O:379:ARG:HB2	2.16	0.70
1:A:435:ASN:CG	1:A:442:LYS:HB3	2.16	0.70
1:A:1309:SER:HB2	1:A:1310:LYS:HD3	1.71	0.70
1:A:1657:LEU:HD22	7:G:104:LEU:HD12	1.70	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:LEU:HD13	3:C:299:ILE:HD11	1.72	0.70
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.73	0.70
16:P:375:PHE:CE1	16:P:380:MET:HG3	2.26	0.70
17:Q:183:LYS:O	17:Q:187:THR:OG1	2.08	0.70
18:R:6:ILE:CD1	18:R:213:ILE:HG22	2.16	0.70
1:A:475:ARG:NH2	2:B:1061:LYS:HG3	2.06	0.70
13:M:102:SER:O	13:M:105:SER:OG	2.08	0.70
16:P:390:GLN:CA	18:R:150:GLN:O	2.39	0.70
1:A:474:LYS:O	2:B:1070:ARG:CG	2.39	0.70
1:A:507:TYR:CE1	1:A:509:GLU:HA	2.26	0.70
1:A:862:THR:CG2	9:I:67:VAL:HG12	2.21	0.70
1:A:990:ILE:HA	1:A:994:GLU:CD	2.15	0.70
2:B:1049:THR:HG23	2:B:1050:GLY:H	1.56	0.70
18:R:5:PRO:CD	18:R:217:THR:CG2	2.67	0.70
1:A:629:ASP:HA	2:B:926:VAL:CG2	2.21	0.70
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.24	0.70
2:B:1072:GLY:CA	2:B:1075:GLU:CG	2.63	0.70
7:G:144:HIS:CD2	15:O:145:SER:C	2.69	0.70
14:N:87:TYR:CB	14:N:141:GLU:CA	2.65	0.70
16:P:345:ASP:OD1	16:P:345:ASP:N	2.23	0.70
16:P:658:LYS:HB3	16:P:660:LYS:H	1.55	0.70
1:A:506:THR:CG2	1:A:579:ARG:C	2.59	0.70
2:B:679:GLN:HG2	14:N:157:ARG:H	0.87	0.70
14:N:87:TYR:CA	14:N:141:GLU:CA	2.45	0.70
1:A:921:PRO:HD2	8:H:19:ARG:HG3	1.73	0.70
2:B:75:ASP:CA	2:B:440:PHE:CE2	2.74	0.70
2:B:894:LYS:HG2	12:L:47:ARG:NE	2.07	0.70
2:B:894:LYS:HA	12:L:54:ARG:NE	2.06	0.70
16:P:197:ARG:CD	16:P:261:VAL:H	2.04	0.70
16:P:659:LEU:H	16:P:659:LEU:HD13	1.55	0.70
17:Q:22:ILE:CD1	17:Q:26:ARG:HE	2.04	0.70
2:B:143:TRP:CZ2	2:B:446:MET:CB	2.75	0.70
2:B:207:ILE:HD11	2:B:503:VAL:CG1	2.20	0.70
7:G:142:ALA:HB3	15:O:102:SER:O	1.92	0.70
1:A:613:THR:CG2	2:B:913:ILE:HG21	2.21	0.70
2:B:527:PHE:CE2	2:B:666:PRO:CA	2.62	0.70
2:B:548:LYS:CE	2:B:695:ASN:OD1	2.40	0.70
1:A:921:PRO:CD	8:H:19:ARG:HG2	2.22	0.70
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.74	0.70
1:A:489:ASN:HB2	11:K:95:HIS:CD2	2.27	0.69
2:B:65:VAL:HG23	2:B:417:ILE:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TRP:CG	2:B:446:MET:CE	2.65	0.69
2:B:999:GLN:HG2	14:N:166:LEU:HD13	1.73	0.69
2:B:1069:ILE:HD12	2:B:1069:ILE:H	1.57	0.69
16:P:292:LEU:HD11	16:P:343:LEU:HG	1.72	0.69
1:A:65:CYS:SG	19:A:2001:ZN:ZN	1.81	0.69
1:A:99:ARG:O	1:A:109:ARG:NH2	2.24	0.69
1:A:399:LEU:HD23	1:A:423:LEU:CD2	2.21	0.69
1:A:1313:LEU:HG	1:A:1462:PHE:HE1	1.49	0.69
2:B:203:ILE:CG2	2:B:405:GLY:CA	2.71	0.69
1:A:475:ARG:NE	2:B:1061:LYS:HB2	2.06	0.69
1:A:1313:LEU:CD2	1:A:1462:PHE:CZ	2.72	0.69
2:B:212:ASN:ND2	2:B:361:HIS:HB2	2.08	0.69
2:B:848:ILE:HG22	12:L:60:ARG:NH1	2.07	0.69
16:P:382:GLU:OE1	18:R:146:SER:OG	2.10	0.69
16:P:405:TYR:HB2	16:P:416:LEU:HD12	1.73	0.69
17:Q:188:ALA:CB	17:Q:384:GLN:HG2	2.09	0.69
1:A:686:PHE:HZ	8:H:121:LEU:HD11	1.56	0.69
1:A:862:THR:CA	9:I:67:VAL:HA	2.21	0.69
2:B:399:HIS:C	2:B:400:GLN:CG	2.65	0.69
16:P:584:ARG:O	16:P:588:SER:HB2	1.91	0.69
1:A:828:CYS:CB	2:B:1027:TYR:HB2	2.21	0.69
15:O:376:TYR:CD1	15:O:419:LYS:CE	2.74	0.69
16:P:218:VAL:HG13	16:P:246:LYS:H	1.57	0.69
2:B:679:GLN:HG3	14:N:155:VAL:C	2.16	0.69
17:Q:8:PRO:HG2	17:Q:19:LEU:HD23	1.75	0.69
18:R:186:LEU:C	18:R:186:LEU:HD13	2.17	0.69
1:A:507:TYR:HE1	1:A:509:GLU:HA	1.56	0.69
2:B:143:TRP:CZ2	2:B:446:MET:HB2	2.28	0.69
2:B:212:ASN:HD21	2:B:361:HIS:HB2	1.56	0.69
3:C:31:TRP:HH2	11:K:127:LEU:HD12	1.58	0.69
15:O:202:ASN:CB	17:Q:31:TYR:OH	2.34	0.69
15:O:248:LEU:CG	15:O:598:PHE:CE2	2.74	0.69
15:O:376:TYR:CD1	15:O:419:LYS:CD	2.76	0.69
16:P:412:ASN:OD1	16:P:412:ASN:N	2.24	0.69
1:A:507:TYR:CD1	1:A:508:PRO:C	2.70	0.69
1:A:953:GLU:CB	1:A:1205:PHE:CE2	2.75	0.69
2:B:404:LEU:O	2:B:407:PHE:N	2.23	0.69
2:B:850:THR:N	12:L:60:ARG:NH2	2.40	0.69
16:P:302:VAL:HG21	16:P:362:ARG:HD2	1.75	0.69
17:Q:186:CYS:O	18:R:208:TYR:OH	2.10	0.69
18:R:201:SER:O	18:R:205:VAL:HG22	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:GLN:CG	14:N:157:ARG:CA	2.70	0.69
4:D:99:LEU:HB3	4:D:100:PRO:CD	2.22	0.69
16:P:301:GLN:HG3	16:P:361:LYS:H	1.57	0.69
16:P:302:VAL:HG11	16:P:362:ARG:HH11	1.57	0.69
16:P:389:TRP:HA	18:R:151:PRO:HA	1.74	0.69
16:P:428:GLU:HB2	16:P:435:ARG:HH12	1.58	0.69
16:P:472:ARG:NE	18:R:200:THR:HG23	2.07	0.69
1:A:862:THR:O	9:I:66:VAL:O	2.10	0.69
1:A:480:ALA:HB1	2:B:1046:VAL:HG23	1.74	0.68
2:B:475:GLY:O	2:B:476:LEU:HB2	1.92	0.68
2:B:887:LEU:HB2	12:L:56:LEU:O	1.93	0.68
6:F:75:PRO:HG2	6:F:78:GLN:CB	2.08	0.68
15:O:233:LEU:O	15:O:236:LYS:HB2	1.94	0.68
16:P:24:SER:OG	18:R:318:ILE:HG13	1.93	0.68
16:P:232:ASN:N	16:P:232:ASN:OD1	2.27	0.68
16:P:389:TRP:HZ2	18:R:147:GLN:HA	1.57	0.68
2:B:143:TRP:CD1	2:B:446:MET:SD	2.84	0.68
6:F:70:LYS:CG	7:G:95:LEU:HG	2.22	0.68
17:Q:22:ILE:HG13	17:Q:24:ASP:OD2	1.92	0.68
1:A:502:ALA:O	1:A:580:HIS:HB3	1.93	0.68
1:A:646:GLU:OE2	2:B:1086:PHE:HD2	1.75	0.68
1:A:1330:VAL:CG2	1:A:1455:ARG:NH1	2.56	0.68
2:B:266:LYS:CD	2:B:473:GLN:O	2.40	0.68
2:B:864:ASP:HB3	17:Q:412:LYS:NZ	2.08	0.68
3:C:230:LEU:CD1	3:C:231:PRO:HD2	2.13	0.68
2:B:551:ILE:CG2	2:B:647:SER:CA	2.72	0.68
6:F:70:LYS:HG2	7:G:95:LEU:CD2	2.23	0.68
16:P:193:LEU:HD12	16:P:251:SER:H	1.59	0.68
16:P:717:LYS:NZ	20:P:903:SO4:O1	2.27	0.68
1:A:406:LEU:HB2	1:A:408:LYS:HZ2	1.57	0.68
1:A:470:HIS:CD2	2:B:1058:GLN:OE1	2.43	0.68
2:B:62:ASN:OD1	2:B:102:VAL:HG23	1.93	0.68
2:B:1072:GLY:C	2:B:1075:GLU:H	2.02	0.68
3:C:41:GLU:OE2	11:K:138:LYS:CE	2.41	0.68
18:R:359:MET:N	18:R:359:MET:SD	2.67	0.68
2:B:209:GLN:HG2	2:B:210:ARG:N	2.07	0.68
15:O:237:ILE:HD12	15:O:237:ILE:H	1.59	0.68
17:Q:414:TYR:HE1	18:R:240:ILE:HG23	1.55	0.68
1:A:472:MET:CE	2:B:1076:ARG:HD3	2.24	0.68
2:B:985:ILE:CB	14:N:160:VAL:CG2	2.67	0.68
16:P:473:HIS:CD2	18:R:1:MET:CG	2.77	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:341:ARG:CZ	17:Q:369:TRP:NE1	2.54	0.68
17:Q:418:PRO:CG	18:R:233:TYR:OH	2.42	0.68
1:A:466:LEU:HD11	2:B:1181:VAL:HG21	1.74	0.68
1:A:671:GLN:OE1	2:B:952:HIS:CB	2.42	0.68
15:O:237:ILE:HD12	15:O:237:ILE:N	2.08	0.68
16:P:53:ASP:OD2	16:P:54:ALA:N	2.27	0.68
3:C:125:LYS:O	3:C:130:ASN:ND2	2.27	0.68
7:G:144:HIS:CD2	15:O:146:SER:CB	2.77	0.68
15:O:248:LEU:HD12	15:O:598:PHE:HE2	0.87	0.68
17:Q:418:PRO:HG2	18:R:233:TYR:OH	1.93	0.68
1:A:475:ARG:CB	2:B:1059:PRO:HB2	2.24	0.67
1:A:991:LYS:HB3	1:A:993:GLN:CB	2.23	0.67
1:A:1660:VAL:HG22	7:G:103:LYS:O	1.93	0.67
16:P:197:ARG:CG	16:P:261:VAL:O	2.42	0.67
1:A:83:VAL:CG1	1:A:427:PHE:CE2	2.77	0.67
1:A:408:LYS:HA	1:A:411:VAL:CB	2.25	0.67
1:A:1314:GLN:HE22	1:A:1446:ARG:NE	1.91	0.67
3:C:127:THR:H	3:C:130:ASN:HB2	1.59	0.67
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.76	0.67
1:A:1310:LYS:H	1:A:1310:LYS:CD	2.08	0.67
1:A:1326:GLU:OE1	1:A:1454:HIS:C	2.34	0.67
1:A:1655:ASP:OD2	6:F:137:TYR:OH	2.10	0.67
6:F:66:ARG:HH21	7:G:90:LEU:CD1	2.06	0.67
15:O:200:ASN:CB	17:Q:14:ASN:CA	2.53	0.67
17:Q:193:PHE:CE2	18:R:208:TYR:CE2	2.82	0.67
7:G:242:VAL:HG21	15:O:183:ILE:HG23	1.74	0.67
16:P:573:GLU:HB2	17:Q:499:LYS:HZ3	1.59	0.67
18:R:199:LYS:HD3	18:R:204:GLU:HB3	1.76	0.67
2:B:527:PHE:CE2	2:B:666:PRO:HB3	2.29	0.67
6:F:72:LYS:HA	6:F:142:SER:CB	2.13	0.67
13:M:102:SER:O	13:M:105:SER:CB	2.42	0.67
18:R:202:THR:C	18:R:205:VAL:HG23	2.19	0.67
1:A:721:LYS:HZ3	8:H:90:ALA:C	2.00	0.67
1:A:878:ARG:HB3	9:I:67:VAL:HG12	1.68	0.67
2:B:531:VAL:O	2:B:716:MET:HG3	1.95	0.67
2:B:985:ILE:CB	14:N:160:VAL:HG21	2.24	0.67
16:P:622:TYR:CZ	16:P:668:SER:HB3	2.30	0.67
18:R:161:ASN:HA	18:R:164:LYS:HD2	1.76	0.67
1:A:403:LEU:HD12	1:A:419:ILE:HD13	1.76	0.67
1:A:406:LEU:N	1:A:406:LEU:HD23	2.10	0.67
1:A:990:ILE:CG1	1:A:995:TYR:CA	2.72	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:VAL:HA	6:F:133:VAL:O	1.95	0.67
16:P:458:LYS:HD3	16:P:461:HIS:HE1	1.60	0.67
17:Q:355:VAL:HB	18:R:212:HIS:CE1	2.30	0.67
1:A:477:ASN:HA	2:B:1047:ARG:HD3	1.77	0.67
1:A:799:GLU:HG3	1:A:1062:HIS:CE1	2.30	0.67
1:A:988:SER:HB2	2:B:988:GLU:HG2	1.76	0.67
2:B:679:GLN:HG3	14:N:156:PRO:HA	1.73	0.67
15:O:373:LEU:HD12	15:O:423:TYR:CE2	2.30	0.67
17:Q:198:ILE:HD13	17:Q:390:THR:O	1.95	0.67
18:R:4:VAL:HG11	18:R:214:VAL:HG22	1.75	0.67
1:A:436:ALA:CA	1:A:439:ASP:C	2.66	0.67
1:A:545:SER:CB	17:Q:34:VAL:HG22	2.10	0.67
1:A:671:GLN:HB3	2:B:952:HIS:CD2	2.30	0.67
1:A:1484:LEU:CD2	2:B:304:ASP:CB	2.73	0.67
1:A:113:VAL:HG21	1:A:178:LEU:HD13	1.77	0.67
15:O:468:GLU:O	15:O:471:LYS:HG3	1.94	0.67
16:P:489:PHE:HD2	18:R:140:ILE:HD11	1.60	0.67
17:Q:139:LYS:HG2	17:Q:237:ILE:HG12	1.76	0.67
2:B:68:ILE:HG21	2:B:71:LYS:HZ3	0.60	0.66
3:C:272:LYS:CB	14:N:175:TYR:CD1	2.78	0.66
13:M:102:SER:CB	13:M:105:SER:CA	2.70	0.66
16:P:435:ARG:HH21	18:R:140:ILE:HG21	1.60	0.66
18:R:266:SER:O	18:R:269:ASP:N	2.28	0.66
1:A:1276:THR:CB	9:I:45:LEU:CD1	2.63	0.66
2:B:399:HIS:C	2:B:400:GLN:HG3	2.20	0.66
2:B:796:ARG:O	10:J:8:PHE:CE1	2.48	0.66
18:R:206:ARG:NH2	18:R:211:ARG:NH1	2.43	0.66
1:A:475:ARG:NH2	2:B:1061:LYS:CB	2.57	0.66
1:A:629:ASP:CA	2:B:926:VAL:CG2	2.72	0.66
2:B:202:LEU:HD22	2:B:488:ALA:CB	2.25	0.66
16:P:187:ILE:CG2	18:R:195:LEU:HD23	2.24	0.66
17:Q:378:LEU:HB3	18:R:238:THR:HG21	1.78	0.66
18:R:253:ILE:HA	18:R:256:GLU:HB3	1.76	0.66
2:B:848:ILE:HB	12:L:60:ARG:HD2	0.71	0.66
16:P:353:ASP:OD1	16:P:379:LYS:NZ	2.27	0.66
6:F:70:LYS:HG2	7:G:95:LEU:CG	2.26	0.66
15:O:383:TYR:CD1	15:O:606:MET:HE3	2.31	0.66
18:R:186:LEU:HD13	18:R:186:LEU:O	1.95	0.66
1:A:399:LEU:HD21	1:A:423:LEU:CG	2.25	0.66
1:A:611:GLU:OE2	2:B:929:ARG:NH2	2.29	0.66
1:A:998:HIS:CE1	2:B:711:GLN:HG3	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:ND2	17:Q:14:ASN:C	2.53	0.66
17:Q:196:SER:HB3	17:Q:204:ARG:HG2	1.76	0.66
15:O:375:THR:C	15:O:377:TYR:H	2.03	0.66
16:P:394:VAL:HG11	18:R:144:VAL:HG23	1.78	0.66
1:A:486:PRO:HG2	2:B:781:TYR:HA	1.78	0.66
1:A:966:LEU:CD2	1:A:997:PHE:HE1	2.09	0.66
15:O:439:ILE:HD13	15:O:487:ARG:HD3	1.76	0.66
16:P:443:ASP:HB3	18:R:3:GLU:HB3	1.77	0.66
1:A:475:ARG:C	2:B:1059:PRO:HG2	2.21	0.66
1:A:1032:VAL:CG2	1:A:1050:TYR:CE1	2.79	0.66
1:A:1032:VAL:CG2	1:A:1050:TYR:HD1	2.05	0.66
1:A:1330:VAL:CG2	1:A:1455:ARG:CD	2.73	0.66
16:P:321:LYS:HA	16:P:361:LYS:HD3	1.78	0.66
16:P:775:TRP:HE1	16:P:778:ASP:HA	1.61	0.66
17:Q:15:CYS:HB2	17:Q:16:PRO:HA	1.77	0.66
18:R:202:THR:CA	18:R:205:VAL:HG23	2.26	0.66
18:R:242:ILE:HG22	18:R:245:VAL:HG22	1.77	0.66
1:A:1330:VAL:HG23	1:A:1455:ARG:NH1	2.10	0.66
2:B:469:ASN:OD1	2:B:482:SER:HB3	1.95	0.66
3:C:294:VAL:O	3:C:297:HIS:CB	2.44	0.66
16:P:448:THR:CG2	16:P:471:MET:H	2.08	0.66
1:A:109:ARG:NH1	1:A:230:ARG:O	2.29	0.65
1:A:722:PRO:HD3	8:H:95:TYR:HA	1.76	0.65
1:A:953:GLU:HA	1:A:1205:PHE:HD2	1.52	0.65
1:A:990:ILE:CG1	1:A:994:GLU:C	2.69	0.65
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.78	0.65
4:D:99:LEU:HB3	4:D:100:PRO:HD3	1.78	0.65
17:Q:15:CYS:SG	17:Q:17:SER:CB	2.83	0.65
17:Q:208:PRO:HG2	17:Q:211:TYR:HD2	1.59	0.65
1:A:718:THR:HG23	8:H:118:PHE:HB3	1.78	0.65
1:A:824:THR:O	2:B:1023:ARG:CB	2.44	0.65
1:A:1054:ALA:O	1:A:1179:ILE:HG22	1.97	0.65
15:O:238:ILE:HD12	15:O:238:ILE:H	1.61	0.65
1:A:627:ASP:O	2:B:784:ASP:O	2.15	0.65
1:A:862:THR:HA	9:I:67:VAL:HB	1.77	0.65
1:A:995:TYR:OH	2:B:715:ASN:CG	2.39	0.65
2:B:212:ASN:ND2	2:B:361:HIS:CB	2.59	0.65
2:B:527:PHE:CE1	2:B:666:PRO:CB	2.79	0.65
2:B:894:LYS:HG2	12:L:47:ARG:HE	1.62	0.65
15:O:108:GLU:HG3	15:O:108:GLU:O	1.96	0.65
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLN:O	2:B:401:GLU:N	2.27	0.65
2:B:1072:GLY:O	2:B:1075:GLU:N	2.29	0.65
7:G:144:HIS:CE1	15:O:145:SER:CB	2.79	0.65
1:A:467:PHE:CE2	1:A:1614:SER:HB3	2.31	0.65
1:A:615:ARG:NH2	2:B:781:TYR:CD2	2.64	0.65
16:P:389:TRP:CH2	18:R:148:ASN:CA	2.76	0.65
16:P:428:GLU:HB3	18:R:142:ARG:NH1	2.11	0.65
16:P:434:ARG:CB	18:R:143:THR:HB	2.25	0.65
17:Q:188:ALA:CB	17:Q:384:GLN:CB	2.64	0.65
17:Q:208:PRO:HG2	17:Q:211:TYR:CD2	2.31	0.65
1:A:472:MET:SD	2:B:1073:GLU:CD	2.79	0.65
1:A:474:LYS:NZ	2:B:1092:LEU:HD22	1.97	0.65
15:O:428:ILE:HD11	15:O:442:VAL:HG21	1.79	0.65
1:A:824:THR:HB	2:B:1023:ARG:CB	2.13	0.65
1:A:921:PRO:CD	8:H:19:ARG:CG	2.75	0.65
2:B:345:SER:HA	13:M:113:ILE:CD1	2.27	0.65
2:B:1072:GLY:O	2:B:1075:GLU:CA	2.45	0.65
3:C:292:GLY:HA3	3:C:295:ARG:NH2	2.12	0.65
15:O:390:GLN:HG2	15:O:396:MET:HE3	1.77	0.65
1:A:1655:ASP:O	6:F:135:ARG:N	2.23	0.65
2:B:681:ILE:CB	14:N:154:ARG:HG3	2.23	0.65
2:B:990:ASP:OD1	14:N:162:LYS:NZ	2.23	0.65
16:P:656:HIS:HB2	16:P:747:LEU:O	1.97	0.65
16:P:769:GLN:HA	16:P:772:ILE:HB	1.79	0.65
17:Q:218:SER:O	17:Q:218:SER:OG	2.11	0.65
1:A:1660:VAL:C	7:G:102:GLU:HG2	2.22	0.65
2:B:328:GLN:NE2	13:M:111:PRO:O	2.29	0.65
2:B:341:SER:OG	2:B:343:ASP:OD1	2.13	0.65
3:C:328:LEU:HD23	11:K:121:LEU:HD21	1.79	0.65
15:O:387:HIS:HB2	15:O:606:MET:HE1	1.79	0.65
17:Q:26:ARG:HB3	17:Q:34:VAL:HG11	1.75	0.65
18:R:199:LYS:NZ	18:R:204:GLU:CB	2.60	0.65
2:B:49:PHE:CD2	2:B:194:PHE:HZ	2.14	0.65
2:B:152:LEU:CD2	2:B:443:LYS:HD2	2.15	0.65
2:B:1090:ASP:O	2:B:1094:ASN:HB2	1.96	0.65
6:F:73:ALA:HA	6:F:143:PHE:CG	2.32	0.65
15:O:219:ARG:NH2	15:O:360:VAL:HG22	2.12	0.65
15:O:510:VAL:HG13	15:O:517:LEU:HD11	1.79	0.65
16:P:625:ASP:O	16:P:629:ARG:CB	2.45	0.65
17:Q:189:LYS:HA	17:Q:384:GLN:HE21	1.62	0.65
17:Q:417:PHE:HZ	18:R:270:PHE:HB2	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:GLN:HB3	2:B:952:HIS:CG	2.32	0.64
1:A:825:ALA:O	2:B:1023:ARG:NH1	2.30	0.64
1:A:436:ALA:HA	1:A:440:SER:HA	1.80	0.64
1:A:1659:LYS:HG2	7:G:102:GLU:OE1	1.98	0.64
15:O:517:LEU:HA	15:O:525:MET:CE	2.27	0.64
16:P:197:ARG:HE	16:P:261:VAL:HG22	1.62	0.64
16:P:263:ILE:HG22	16:P:264:ILE:HG22	1.79	0.64
16:P:434:ARG:HG2	18:R:143:THR:HB	1.80	0.64
18:R:4:VAL:HG21	18:R:214:VAL:CG1	2.27	0.64
1:A:670:ILE:HD11	2:B:783:MET:HE2	1.79	0.64
3:C:293:ARG:HB2	3:C:295:ARG:HD3	1.80	0.64
15:O:240:ILE:HA	15:O:332:LEU:HD12	1.79	0.64
16:P:775:TRP:H	17:Q:109:GLN:NE2	1.95	0.64
18:R:317:LEU:HD13	18:R:367:ILE:CD1	2.24	0.64
1:A:40:ASN:ND2	18:R:355:THR:CG2	2.59	0.64
1:A:460:LEU:HD21	2:B:1188:GLU:HG3	1.80	0.64
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.80	0.64
6:F:70:LYS:CE	7:G:95:LEU:HD23	2.26	0.64
15:O:240:ILE:HG23	15:O:332:LEU:HG	1.78	0.64
16:P:697:GLU:OE1	16:P:697:GLU:N	2.30	0.64
17:Q:15:CYS:HB3	17:Q:17:SER:H	1.62	0.64
18:R:303:THR:HG22	18:R:304:HIS:H	1.62	0.64
1:A:476:VAL:CA	2:B:1059:PRO:HG2	2.28	0.64
2:B:531:VAL:HG13	2:B:716:MET:HA	1.78	0.64
7:G:144:HIS:NE2	15:O:146:SER:N	2.46	0.64
15:O:376:TYR:CG	15:O:419:LYS:CE	2.80	0.64
16:P:736:ILE:HD11	17:Q:254:LEU:HD13	1.80	0.64
18:R:412:ARG:NH2	18:R:439:GLU:OE2	2.31	0.64
1:A:684:ASP:OD2	8:H:20:TYR:CB	2.45	0.64
2:B:551:ILE:CG2	2:B:648:ARG:N	2.58	0.64
16:P:405:TYR:OH	16:P:414:ILE:HG12	1.97	0.64
18:R:141:TRP:H	18:R:141:TRP:CD1	2.16	0.64
18:R:202:THR:O	18:R:205:VAL:HG23	1.97	0.64
1:A:641:GLU:HB2	6:F:99:LEU:HD13	1.78	0.64
2:B:923:GLN:NE2	2:B:953:ALA:O	2.30	0.64
15:O:392:GLN:HB2	15:O:395:LEU:HD22	1.79	0.64
16:P:436:ILE:CB	18:R:143:THR:HA	2.28	0.64
17:Q:104:PHE:CZ	17:Q:156:LEU:HB2	2.33	0.64
17:Q:245:SER:HB3	17:Q:284:LEU:HB2	1.80	0.64
17:Q:374:THR:HG23	18:R:219:LEU:HD13	1.80	0.64
1:A:720:PHE:CE2	8:H:141:TYR:CE2	2.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:434:ARG:H	18:R:145:SER:CA	2.10	0.64
17:Q:8:PRO:HB2	17:Q:19:LEU:HD23	1.79	0.64
17:Q:290:THR:HB	17:Q:292:GLU:H	1.61	0.64
2:B:294:GLY:HA3	2:B:579:ALA:HB3	1.80	0.64
14:N:87:TYR:OH	14:N:141:GLU:OE1	2.16	0.64
17:Q:20:TRP:CH2	17:Q:22:ILE:HG21	2.30	0.64
17:Q:378:LEU:CD2	18:R:216:LEU:HD21	2.27	0.64
1:A:998:HIS:CD2	2:B:711:GLN:HA	2.33	0.64
2:B:848:ILE:CB	12:L:60:ARG:CD	2.39	0.64
2:B:1005:TYR:CD2	14:N:170:HIS:ND1	2.66	0.64
6:F:74:ILE:C	7:G:95:LEU:CD1	2.62	0.64
7:G:143:SER:CB	15:O:104:ILE:N	2.49	0.64
18:R:4:VAL:HG21	18:R:214:VAL:HG13	1.78	0.64
1:A:406:LEU:HB3	1:A:408:LYS:HD3	1.80	0.63
2:B:143:TRP:HE3	2:B:446:MET:HE3	1.56	0.63
3:C:229:LEU:CD2	3:C:295:ARG:O	2.42	0.63
15:O:227:PHE:HD1	15:O:363:THR:HB	1.62	0.63
16:P:700:LEU:HD12	16:P:703:PHE:HD2	1.62	0.63
1:A:684:ASP:OD1	8:H:20:TYR:HB3	1.97	0.63
2:B:1079:LEU:O	2:B:1083:GLY:N	2.31	0.63
7:G:144:HIS:CE1	15:O:145:SER:HB2	2.34	0.63
15:O:332:LEU:HD11	15:O:380:SER:CB	2.29	0.63
17:Q:283:ASN:OD1	17:Q:284:LEU:N	2.27	0.63
1:A:1263:LEU:HA	1:A:1498:ILE:CD1	2.25	0.63
2:B:30:LYS:C	2:B:176:SER:CB	2.72	0.63
3:C:253:PRO:CD	14:N:180:PHE:CG	2.46	0.63
8:H:44:VAL:HG22	8:H:48:PRO:HA	1.81	0.63
15:O:376:TYR:HB2	15:O:419:LYS:HD3	1.79	0.63
16:P:438:TRP:HZ2	18:R:297:PHE:CE1	2.15	0.63
17:Q:193:PHE:CD2	18:R:208:TYR:CE2	2.85	0.63
1:A:476:VAL:HG13	2:B:1070:ARG:HA	1.81	0.63
2:B:527:PHE:CE2	2:B:666:PRO:CB	2.82	0.63
18:R:75:GLN:HA	18:R:78:ARG:HE	1.64	0.63
18:R:180:CYS:SG	18:R:185:LYS:HG2	2.39	0.63
1:A:1482:LYS:O	2:B:308:LEU:CD2	2.38	0.63
15:O:181:ARG:HH11	15:O:181:ARG:CG	2.12	0.63
16:P:454:GLN:HA	16:P:455:LYS:HE2	1.79	0.63
2:B:50:ASN:OD1	2:B:167:SER:HB2	1.99	0.63
2:B:897:GLU:HA	12:L:46:VAL:CG2	2.29	0.63
1:A:83:VAL:HG13	1:A:427:PHE:CE2	2.34	0.63
6:F:69:LEU:O	6:F:143:PHE:CE2	2.52	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:LYS:HB3	15:O:105:ASN:OD1	1.99	0.63
15:O:376:TYR:CD1	15:O:419:LYS:HD3	2.34	0.63
1:A:472:MET:CG	2:B:1073:GLU:OE1	2.46	0.63
2:B:64:GLY:CA	2:B:242:ASP:CB	2.74	0.63
2:B:205:MET:CE	2:B:500:PHE:O	2.47	0.63
2:B:894:LYS:CG	12:L:47:ARG:NE	2.62	0.63
2:B:1072:GLY:O	2:B:1076:ARG:N	2.31	0.63
16:P:473:HIS:C	16:P:504:THR:HG23	2.24	0.63
1:A:475:ARG:O	2:B:1059:PRO:HG2	1.99	0.63
1:A:581:ILE:HD11	1:A:585:ASP:HB3	1.81	0.63
1:A:921:PRO:HD2	8:H:19:ARG:CG	2.28	0.63
2:B:373:MET:HG3	2:B:377:MET:HE3	1.79	0.63
16:P:185:GLN:NE2	18:R:197:PRO:HB3	2.14	0.63
16:P:354:PRO:HG3	18:R:31:PHE:CG	2.34	0.63
16:P:532:GLU:HB2	16:P:554:ASN:HB3	1.81	0.63
17:Q:19:LEU:HD11	17:Q:27:ARG:CB	2.27	0.63
1:A:432:ASN:OD1	1:A:443:ALA:HA	1.99	0.62
1:A:472:MET:HB3	2:B:1073:GLU:CG	2.29	0.62
1:A:1606:SER:HB2	1:A:1611:MET:HE3	1.80	0.62
2:B:143:TRP:HB3	2:B:446:MET:CE	2.25	0.62
2:B:1096:SER:O	2:B:1097:ASP:CB	2.47	0.62
15:O:245:GLN:NE2	15:O:245:GLN:HA	2.14	0.62
16:P:675:PHE:HE2	16:P:741:ILE:HG21	1.63	0.62
17:Q:6:ARG:O	17:Q:7:GLY:O	2.17	0.62
1:A:1329:ILE:CB	1:A:1456:PHE:HE2	2.12	0.62
2:B:152:LEU:CB	2:B:443:LYS:CE	2.23	0.62
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.79	0.62
17:Q:10:CYS:CB	17:Q:17:SER:H	2.13	0.62
17:Q:356:VAL:CG1	18:R:208:TYR:CE1	2.73	0.62
1:A:1055:ILE:HD13	1:A:1178:LEU:HD23	1.80	0.62
2:B:1069:ILE:O	2:B:1070:ARG:CB	2.45	0.62
15:O:181:ARG:HB2	15:O:181:ARG:NH1	2.12	0.62
16:P:197:ARG:NE	16:P:261:VAL:HG22	2.14	0.62
16:P:434:ARG:CG	18:R:143:THR:HG21	2.23	0.62
16:P:665:ASN:OD1	16:P:665:ASN:N	2.31	0.62
18:R:248:LYS:CB	18:R:298:GLN:NE2	2.61	0.62
1:A:1484:LEU:HD11	2:B:305:ARG:NE	2.14	0.62
2:B:29:PRO:O	2:B:178:TYR:N	2.29	0.62
3:C:326:GLU:CB	11:K:125:MET:HE3	2.29	0.62
6:F:72:LYS:CG	6:F:142:SER:CB	2.77	0.62
16:P:388:ASN:HB3	18:R:151:PRO:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:432:PRO:HB2	18:R:146:SER:HB2	1.81	0.62
17:Q:351:ASN:O	17:Q:369:TRP:HH2	1.82	0.62
18:R:308:PHE:HD1	18:R:309:ALA:H	1.46	0.62
1:A:1329:ILE:CB	1:A:1456:PHE:CE2	2.82	0.62
2:B:1072:GLY:O	2:B:1075:GLU:CB	2.47	0.62
6:F:66:ARG:HH21	7:G:90:LEU:HD13	1.64	0.62
16:P:278:HIS:HB2	16:P:285:MET:HE3	1.81	0.62
16:P:436:ILE:HG12	18:R:141:TRP:CE3	2.34	0.62
18:R:202:THR:CA	18:R:205:VAL:CG2	2.75	0.62
1:A:486:PRO:HG2	2:B:781:TYR:CA	2.29	0.62
1:A:825:ALA:HB3	2:B:1022:LEU:HB3	1.82	0.62
1:A:826:PHE:CD1	2:B:777:SER:CB	2.83	0.62
2:B:697:LEU:CB	2:B:702:ASN:ND2	2.59	0.62
15:O:56:VAL:HG21	15:O:99:ILE:HD12	1.82	0.62
15:O:515:ASN:HD21	15:O:547:ASN:HD21	1.47	0.62
16:P:724:LEU:HD13	17:Q:447:ALA:HB2	1.81	0.62
17:Q:8:PRO:O	17:Q:9:ILE:C	2.42	0.62
1:A:493:ASN:CB	1:A:654:ASP:OD1	2.47	0.62
1:A:506:THR:HG21	1:A:578:TYR:O	1.98	0.62
1:A:729:LYS:HD2	8:H:120:GLY:HA3	1.82	0.62
1:A:799:GLU:HG3	1:A:1062:HIS:ND1	2.14	0.62
1:A:827:THR:CG2	1:A:924:SER:HB3	2.30	0.62
2:B:45:HIS:NE2	2:B:500:PHE:HB3	2.13	0.62
2:B:64:GLY:CA	2:B:242:ASP:HB3	2.28	0.62
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.82	0.62
15:O:361:PHE:O	15:O:365:THR:HG23	1.99	0.62
1:A:1606:SER:HB3	1:A:1611:MET:HE3	1.79	0.62
1:A:1657:LEU:HB3	7:G:104:LEU:HD22	1.81	0.62
2:B:547:HIS:HB2	2:B:698:SER:HA	1.81	0.62
15:O:67:ASP:OD1	15:O:69:THR:HB	2.00	0.62
16:P:662:LEU:O	16:P:665:ASN:ND2	2.31	0.62
18:R:1:MET:HE3	18:R:2:PHE:CE1	2.35	0.62
18:R:26:TYR:HB3	18:R:169:PRO:HB3	1.81	0.62
2:B:897:GLU:HA	12:L:46:VAL:HG23	1.80	0.62
15:O:450:LEU:O	15:O:454:VAL:HG12	1.99	0.62
16:P:189:THR:O	16:P:450:ARG:NH2	2.33	0.62
17:Q:212:VAL:O	17:Q:216:GLU:HG2	1.98	0.62
18:R:171:ARG:O	18:R:174:GLU:N	2.33	0.62
1:A:477:ASN:CA	2:B:1047:ARG:HD3	2.29	0.62
2:B:1090:ASP:O	2:B:1094:ASN:N	2.33	0.62
7:G:241:ARG:CZ	15:O:189:PHE:HB3	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:305:THR:HB	18:R:308:PHE:HE1	1.64	0.62
1:A:467:PHE:CD2	1:A:1614:SER:HB2	2.34	0.61
1:A:545:SER:N	17:Q:34:VAL:CB	2.63	0.61
1:A:1049:MET:HB2	1:A:1052:GLY:HA2	1.80	0.61
1:A:1318:SER:OG	1:A:1450:ILE:HD11	2.00	0.61
2:B:143:TRP:CE3	2:B:446:MET:CE	2.82	0.61
15:O:510:VAL:CG1	15:O:543:ILE:HD12	2.30	0.61
16:P:436:ILE:O	18:R:141:TRP:CG	2.53	0.61
16:P:473:HIS:CD2	16:P:475:ARG:HD2	2.35	0.61
17:Q:198:ILE:HG21	17:Q:388:THR:HG22	1.82	0.61
1:A:438:ILE:O	1:A:457:LYS:CG	2.48	0.61
1:A:824:THR:C	2:B:1023:ARG:H	2.08	0.61
1:A:1050:TYR:CE1	1:A:1185:VAL:HG11	2.35	0.61
2:B:184:LYS:HB3	2:B:735:HIS:CG	2.35	0.61
2:B:1091:ARG:O	2:B:1096:SER:HB2	2.01	0.61
3:C:272:LYS:HG3	14:N:175:TYR:HE1	1.65	0.61
6:F:70:LYS:HA	6:F:73:ALA:HB3	1.82	0.61
15:O:374:PRO:O	15:O:376:TYR:CB	2.39	0.61
16:P:365:TRP:HB2	16:P:371:LYS:O	2.00	0.61
16:P:775:TRP:O	17:Q:113:LYS:NZ	2.33	0.61
16:P:397:LYS:NZ	18:R:85:ARG:CG	2.62	0.61
1:A:1050:TYR:CE1	1:A:1179:ILE:CG1	2.76	0.61
1:A:1314:GLN:HE22	1:A:1446:ARG:CZ	2.12	0.61
2:B:1120:ILE:HD12	15:O:117:GLN:HE21	1.61	0.61
15:O:373:LEU:CD1	15:O:423:TYR:CD2	2.84	0.61
15:O:467:MET:CG	15:O:575:SER:HA	2.30	0.61
16:P:394:VAL:CG1	18:R:144:VAL:HB	2.30	0.61
16:P:422:ILE:O	16:P:439:LYS:HB2	2.01	0.61
17:Q:351:ASN:CA	17:Q:369:TRP:CZ2	2.84	0.61
1:A:422:ARG:CZ	18:R:412:ARG:NH1	2.63	0.61
1:A:878:ARG:HG3	9:I:66:VAL:CG2	2.27	0.61
16:P:388:ASN:HB3	18:R:151:PRO:CB	2.29	0.61
16:P:389:TRP:CZ2	18:R:148:ASN:N	2.68	0.61
18:R:157:MET:HG3	18:R:162:PHE:HB2	1.81	0.61
1:A:966:LEU:HD22	1:A:997:PHE:CE1	2.36	0.61
7:G:141:SER:CB	15:O:142:ILE:HD11	2.20	0.61
15:O:581:THR:HA	15:O:584:GLN:NE2	2.15	0.61
16:P:383:ILE:HG12	16:P:390:GLN:HG2	1.81	0.61
17:Q:3:THR:HG22	17:Q:20:TRP:CB	2.29	0.61
1:A:472:MET:CG	2:B:1073:GLU:CD	2.73	0.61
2:B:683:ASN:CA	14:N:154:ARG:HH22	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:362:ARG:HB3	16:P:375:PHE:HB2	1.82	0.61
1:A:467:PHE:CD2	1:A:1614:SER:CB	2.84	0.61
1:A:1298:ASP:CA	1:A:1468:LYS:HZ3	2.14	0.61
2:B:146:ASN:ND2	2:B:441:LYS:HE3	2.15	0.61
3:C:272:LYS:HG3	14:N:175:TYR:CE1	2.36	0.61
16:P:625:ASP:O	16:P:629:ARG:HB3	2.00	0.61
17:Q:24:ASP:OD1	17:Q:26:ARG:NH1	2.31	0.61
17:Q:193:PHE:HD2	18:R:208:TYR:CD2	2.16	0.61
17:Q:503:SER:O	17:Q:507:ASN:ND2	2.33	0.61
2:B:202:LEU:HD23	2:B:202:LEU:N	2.11	0.61
2:B:203:ILE:HB	2:B:405:GLY:HA3	1.82	0.61
2:B:563:SER:HA	13:M:73:SER:CB	2.31	0.61
2:B:563:SER:HB3	13:M:73:SER:HB3	1.82	0.61
2:B:679:GLN:CD	14:N:156:PRO:C	2.65	0.61
2:B:1079:LEU:HD22	2:B:1084:THR:OG1	2.00	0.61
15:O:376:TYR:CE1	15:O:588:LEU:HD22	2.25	0.61
1:A:966:LEU:CD2	1:A:997:PHE:HZ	2.11	0.61
2:B:796:ARG:O	10:J:8:PHE:HE1	1.83	0.61
6:F:74:ILE:HG21	6:F:144:GLU:HG2	1.81	0.61
16:P:348:HIS:NE2	18:R:154:LYS:CD	2.64	0.61
16:P:397:LYS:HZ1	18:R:85:ARG:CG	2.13	0.61
1:A:1226:VAL:HG12	1:A:1227:MET:HG2	1.83	0.60
1:A:1313:LEU:HD23	1:A:1462:PHE:CZ	2.29	0.60
1:A:1314:GLN:OE1	1:A:1446:ARG:CD	2.48	0.60
2:B:995:TYR:OH	14:N:163:VAL:HG23	2.01	0.60
16:P:197:ARG:HE	16:P:261:VAL:N	1.93	0.60
16:P:198:ASP:CG	16:P:205:TYR:O	2.44	0.60
16:P:436:ILE:C	18:R:141:TRP:O	2.44	0.60
18:R:251:TRP:HE3	18:R:307:LYS:NZ	1.99	0.60
1:A:1608:SER:OG	1:A:1632:GLU:OE2	2.12	0.60
3:C:314:PHE:CD2	11:K:135:PHE:CZ	2.89	0.60
16:P:21:GLN:HB2	18:R:139:GLU:OE1	2.00	0.60
16:P:268:SER:HG	16:P:271:ILE:H	1.48	0.60
16:P:484:ARG:O	16:P:486:ALA:N	2.32	0.60
16:P:641:TRP:HZ2	16:P:656:HIS:HB3	1.67	0.60
1:A:1330:VAL:CG2	1:A:1455:ARG:HD2	2.31	0.60
2:B:143:TRP:CD2	2:B:446:MET:HE3	2.35	0.60
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.34	0.60
15:O:201:LYS:CD	15:O:239:SER:OG	2.49	0.60
1:A:474:LYS:O	2:B:1070:ARG:HG3	2.01	0.60
16:P:187:ILE:HB	16:P:188:GLN:CD	2.26	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:197:ARG:HG3	16:P:261:VAL:O	2.01	0.60
17:Q:291:ASP:OD2	17:Q:291:ASP:N	2.32	0.60
1:A:991:LYS:CB	1:A:993:GLN:OE1	2.44	0.60
1:A:1600:ARG:CG	1:A:1616:GLU:OE1	2.49	0.60
6:F:72:LYS:CA	6:F:142:SER:CB	2.59	0.60
6:F:72:LYS:NZ	6:F:140:ASP:OD2	2.21	0.60
15:O:582:ARG:O	15:O:586:ILE:HG13	2.02	0.60
1:A:413:LEU:O	1:A:416:ARG:CG	2.49	0.60
17:Q:358:PRO:HA	18:R:206:ARG:CZ	2.26	0.60
1:A:1003:ARG:NH2	2:B:530:PRO:CA	2.65	0.60
17:Q:10:CYS:HB2	17:Q:17:SER:H	1.67	0.60
1:A:438:ILE:O	1:A:457:LYS:HD3	1.96	0.60
2:B:345:SER:HA	13:M:113:ILE:HG12	1.83	0.60
2:B:923:GLN:NE2	2:B:957:ARG:HD2	2.16	0.60
2:B:1005:TYR:CZ	14:N:170:HIS:CE1	2.89	0.60
15:O:438:GLN:O	15:O:441:PHE:HB3	2.02	0.60
16:P:67:ASP:OD1	16:P:545:SER:OG	2.15	0.60
17:Q:382:GLU:HB2	18:R:241:ARG:NH1	2.17	0.60
18:R:250:LEU:HB2	18:R:270:PHE:CE2	2.37	0.60
1:A:399:LEU:HD21	1:A:423:LEU:CD2	2.30	0.60
2:B:228:SER:HB2	2:B:253:LEU:HD23	1.84	0.60
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.82	0.60
5:E:145:THR:C	5:E:147:HIS:H	2.10	0.60
7:G:242:VAL:HG21	15:O:183:ILE:CG2	2.32	0.60
15:O:376:TYR:CZ	15:O:588:LEU:CD2	2.76	0.60
16:P:319:ASP:HB2	16:P:363:ILE:HG12	1.83	0.60
1:A:613:THR:HG21	2:B:913:ILE:HG22	1.81	0.60
1:A:1329:ILE:HG22	1:A:1456:PHE:CE2	2.30	0.60
2:B:497:ILE:CG1	2:B:699:ILE:CD1	2.79	0.60
3:C:58:ASN:HA	3:C:296:ASN:HD21	0.78	0.60
3:C:326:GLU:HB2	11:K:125:MET:HE3	1.84	0.60
15:O:348:THR:HG22	15:O:351:SER:CB	2.26	0.60
16:P:426:ALA:C	16:P:433:VAL:HG11	2.27	0.60
1:A:435:ASN:HB3	1:A:442:LYS:CA	2.32	0.59
1:A:953:GLU:HB3	1:A:1205:PHE:CE2	2.37	0.59
2:B:679:GLN:CA	14:N:155:VAL:O	2.50	0.59
15:O:370:THR:OG1	15:O:371:HIS:HD2	1.84	0.59
17:Q:9:ILE:HB	17:Q:16:PRO:CB	2.26	0.59
18:R:173:MET:CG	18:R:188:PHE:HZ	2.11	0.59
1:A:489:ASN:CB	11:K:95:HIS:CD2	2.85	0.59
1:A:1650:GLY:O	1:A:1651:THR:C	2.41	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TRP:CD2	2:B:446:MET:CE	2.85	0.59
2:B:143:TRP:CZ2	2:B:446:MET:CA	2.84	0.59
2:B:207:ILE:O	2:B:207:ILE:HG22	2.02	0.59
7:G:159:LYS:CD	15:O:103:ASN:CG	2.63	0.59
15:O:602:TYR:HD2	15:O:605:LEU:HD23	1.66	0.59
16:P:473:HIS:NE2	18:R:1:MET:SD	2.74	0.59
3:C:228:ARG:HD3	14:N:173:THR:OG1	2.02	0.59
13:M:101:VAL:HG12	13:M:105:SER:OG	2.01	0.59
15:O:200:ASN:ND2	17:Q:14:ASN:CG	2.60	0.59
1:A:83:VAL:HG11	1:A:427:PHE:CE2	2.37	0.59
1:A:415:ASP:HA	1:A:418:VAL:HG12	1.84	0.59
1:A:699:CYS:O	1:A:815:ARG:NH1	2.35	0.59
1:A:1606:SER:CB	1:A:1611:MET:CE	2.79	0.59
16:P:348:HIS:CG	18:R:154:LYS:HD3	2.34	0.59
1:A:246:ASP:HB3	1:A:248:PHE:H	1.66	0.59
1:A:629:ASP:HA	2:B:926:VAL:HG23	1.84	0.59
2:B:65:VAL:CG2	2:B:417:ILE:HD12	2.32	0.59
2:B:143:TRP:CH2	2:B:446:MET:HG3	2.37	0.59
3:C:45:SER:HB2	3:C:271:ARG:NH2	2.18	0.59
7:G:241:ARG:HG2	15:O:152:GLN:OE1	2.02	0.59
16:P:631:SER:O	16:P:686:TYR:OH	2.20	0.59
1:A:422:ARG:NH1	18:R:412:ARG:HH11	1.96	0.59
1:A:618:TYR:HE1	2:B:783:MET:HB2	1.67	0.59
1:A:862:THR:HG22	9:I:67:VAL:HG11	1.83	0.59
1:A:998:HIS:CD2	2:B:712:SER:H	2.20	0.59
2:B:200:GLU:OE2	2:B:736:ARG:NH2	2.34	0.59
2:B:743:ARG:CZ	10:J:60:PHE:CZ	2.83	0.59
2:B:1090:ASP:HA	2:B:1094:ASN:CG	2.27	0.59
3:C:322:LYS:NZ	11:K:129:ASP:OD1	2.35	0.59
17:Q:369:TRP:HB3	17:Q:373:GLU:OE2	2.02	0.59
1:A:878:ARG:HG2	9:I:67:VAL:CG1	2.05	0.59
7:G:24:VAL:HA	7:G:25:THR:CA	2.25	0.59
15:O:200:ASN:ND2	17:Q:14:ASN:CB	2.65	0.59
15:O:224:GLU:OE1	15:O:224:GLU:N	2.23	0.59
16:P:626:LEU:HD11	16:P:665:ASN:HB2	1.84	0.59
1:A:474:LYS:HE3	2:B:1092:LEU:HD21	1.77	0.59
2:B:110:ASN:O	2:B:112:GLY:N	2.35	0.59
1:A:953:GLU:CB	1:A:1205:PHE:CD2	2.86	0.59
1:A:1650:GLY:O	1:A:1653:SER:N	2.35	0.59
2:B:28:PRO:HD3	10:J:62:ARG:NE	2.17	0.59
2:B:143:TRP:NE1	2:B:446:MET:HB2	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ILE:HG12	2:B:699:ILE:CD1	2.33	0.59
2:B:531:VAL:CG1	2:B:716:MET:HA	2.33	0.59
3:C:37:LYS:HG3	11:K:134:LYS:HZ2	1.68	0.59
15:O:227:PHE:CD1	15:O:363:THR:HB	2.38	0.59
15:O:240:ILE:HG23	15:O:332:LEU:CD1	2.33	0.59
17:Q:418:PRO:CD	18:R:233:TYR:OH	2.50	0.59
1:A:414:GLU:O	1:A:417:ARG:N	2.33	0.59
1:A:472:MET:HE1	2:B:1076:ARG:HD2	1.84	0.59
1:A:1606:SER:HB2	1:A:1611:MET:CE	2.33	0.59
2:B:209:GLN:O	2:B:401:GLU:HG2	2.03	0.59
2:B:538:PRO:HB2	2:B:542:LEU:HG	1.84	0.59
5:E:55:ARG:NH2	5:E:113:GLN:OE1	2.36	0.59
15:O:375:THR:O	15:O:377:TYR:N	2.35	0.59
16:P:55:LEU:HD23	18:R:227:HIS:CG	2.37	0.59
17:Q:321:ASP:O	17:Q:324:ARG:N	2.27	0.59
18:R:206:ARG:HE	18:R:206:ARG:N	1.97	0.59
1:A:436:ALA:C	1:A:439:ASP:CA	2.76	0.58
1:A:1260:LYS:HE2	1:A:1262:LEU:CD2	2.33	0.58
2:B:1069:ILE:H	2:B:1069:ILE:CD1	2.16	0.58
7:G:30:GLU:HA	7:G:32:ASN:N	2.18	0.58
8:H:80:ARG:HG3	11:K:108:TYR:OH	2.03	0.58
14:N:87:TYR:HA	14:N:141:GLU:C	2.27	0.58
15:O:607:LYS:HG3	15:O:608:GLU:N	2.17	0.58
16:P:317:ILE:HG22	16:P:363:ILE:HD13	1.84	0.58
16:P:389:TRP:HZ2	18:R:147:GLN:CA	2.16	0.58
16:P:715:TYR:CE1	16:P:733:THR:HG23	2.38	0.58
17:Q:413:LEU:CG	18:R:273:TRP:CZ2	2.74	0.58
1:A:477:ASN:O	2:B:1047:ARG:CG	2.51	0.58
1:A:1003:ARG:NH2	2:B:530:PRO:HA	2.17	0.58
1:A:1298:ASP:CG	1:A:1468:LYS:HZ3	2.11	0.58
1:A:1603:MET:HG2	1:A:1611:MET:HE1	1.85	0.58
16:P:384:ASP:OD2	16:P:387:ASN:HB2	2.03	0.58
16:P:662:LEU:HB3	16:P:665:ASN:HD21	1.67	0.58
16:P:675:PHE:CZ	16:P:742:TRP:HZ3	2.21	0.58
16:P:719:LEU:HD13	16:P:733:THR:HG21	1.85	0.58
16:P:725:VAL:HG21	17:Q:446:TYR:CD1	2.38	0.58
17:Q:436:LEU:HD12	17:Q:436:LEU:H	1.67	0.58
18:R:250:LEU:HB2	18:R:270:PHE:HE2	1.67	0.58
1:A:408:LYS:HE3	1:A:416:ARG:NH1	2.19	0.58
1:A:995:TYR:CZ	2:B:707:SER:CB	2.72	0.58
1:A:1187:ILE:HG13	2:B:1080:ILE:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1487:ASN:CG	2:B:305:ARG:HH22	2.11	0.58
2:B:75:ASP:CA	2:B:440:PHE:CZ	2.86	0.58
2:B:203:ILE:HG21	2:B:405:GLY:CA	2.33	0.58
2:B:829:ASN:OD1	2:B:829:ASN:N	2.36	0.58
12:L:38:LEU:HD12	12:L:49:LYS:HG3	1.85	0.58
16:P:479:HIS:NE2	16:P:491:SER:OG	2.24	0.58
16:P:484:ARG:HD2	16:P:488:LEU:HD12	1.85	0.58
18:R:199:LYS:HZ1	18:R:204:GLU:CA	2.13	0.58
18:R:350:SER:O	18:R:354:LEU:HB2	2.03	0.58
1:A:408:LYS:HE3	1:A:416:ARG:HH12	1.67	0.58
1:A:472:MET:HE1	2:B:1076:ARG:CD	2.34	0.58
1:A:718:THR:CG2	8:H:118:PHE:HB3	2.34	0.58
1:A:1657:LEU:CD2	7:G:104:LEU:CD1	2.61	0.58
15:O:477:PHE:CE2	15:O:525:MET:HE1	2.35	0.58
17:Q:222:PHE:HA	17:Q:492:ALA:HB1	1.86	0.58
17:Q:441:ASP:O	17:Q:445:ARG:HG2	2.02	0.58
18:R:317:LEU:HD13	18:R:367:ILE:HD13	1.85	0.58
1:A:470:HIS:HB3	2:B:1058:GLN:HE22	1.68	0.58
1:A:478:TYR:CB	2:B:1048:SER:O	2.50	0.58
1:A:581:ILE:HB	1:A:637:PHE:CE2	2.38	0.58
1:A:953:GLU:C	1:A:1205:PHE:HB3	2.27	0.58
1:A:1050:TYR:CB	1:A:1054:ALA:HA	2.33	0.58
1:A:1322:ILE:C	1:A:1454:HIS:CD2	2.82	0.58
1:A:1330:VAL:HG22	1:A:1455:ARG:CD	2.34	0.58
15:O:510:VAL:HG12	15:O:543:ILE:HD12	1.86	0.58
16:P:436:ILE:CG2	18:R:143:THR:HA	2.34	0.58
17:Q:354:LYS:HD2	17:Q:369:TRP:HZ2	1.68	0.58
1:A:545:SER:N	17:Q:34:VAL:HB	2.19	0.58
1:A:721:LYS:NZ	8:H:90:ALA:C	2.60	0.58
1:A:828:CYS:SG	2:B:1027:TYR:CB	2.92	0.58
1:A:984:GLY:HA3	1:A:994:GLU:OE1	2.02	0.58
2:B:156:ARG:NH2	2:B:455:GLU:OE1	2.24	0.58
7:G:142:ALA:HB1	15:O:102:SER:O	2.03	0.58
16:P:599:LYS:HE3	17:Q:272:GLN:HE22	1.69	0.58
16:P:659:LEU:HD12	16:P:742:TRP:CD1	2.39	0.58
17:Q:22:ILE:HD11	17:Q:26:ARG:HE	1.62	0.58
17:Q:162:ILE:HG21	17:Q:226:LEU:HD11	1.85	0.58
2:B:143:TRP:CG	2:B:446:MET:HE3	2.37	0.58
2:B:146:ASN:HD22	2:B:441:LYS:CE	2.15	0.58
14:N:69:SER:OG	14:N:70:LEU:N	2.37	0.58
15:O:219:ARG:NH2	15:O:360:VAL:CG2	2.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:374:THR:CG2	18:R:219:LEU:HD13	2.34	0.58
1:A:408:LYS:HA	1:A:411:VAL:CG2	2.34	0.58
1:A:1204:THR:HG21	9:I:97:HIS:CB	2.33	0.58
2:B:923:GLN:HG2	2:B:949:ILE:HD11	1.85	0.58
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.85	0.58
16:P:489:PHE:CD2	18:R:138:PHE:CZ	2.92	0.58
17:Q:22:ILE:HD11	17:Q:26:ARG:CD	2.33	0.58
17:Q:369:TRP:CB	17:Q:373:GLU:OE2	2.51	0.58
1:A:4:SER:HB2	1:A:573:LEU:HD22	1.85	0.58
1:A:598:ALA:HB1	1:A:601:MET:HE3	1.85	0.58
1:A:909:SER:HA	9:I:83:LYS:HZ1	1.62	0.58
1:A:1074:TYR:HE2	1:A:1159:ASP:HB3	1.68	0.58
15:O:348:THR:HG23	15:O:351:SER:H	1.68	0.58
16:P:268:SER:OG	16:P:269:PHE:N	2.36	0.58
1:A:396:ILE:HD11	1:A:426:ALA:HB1	1.84	0.58
15:O:190:ILE:HA	15:O:193:TYR:CD2	2.39	0.58
15:O:376:TYR:CZ	15:O:419:LYS:HE2	2.38	0.58
16:P:274:ILE:O	16:P:289:SER:CB	2.44	0.58
16:P:436:ILE:CA	18:R:143:THR:HG23	2.34	0.58
1:A:1298:ASP:O	1:A:1299:ASN:C	2.46	0.57
2:B:683:ASN:HA	14:N:150:TYR:CE2	2.39	0.57
11:K:49:LEU:HD23	11:K:51:THR:HG23	1.86	0.57
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.39	0.57
15:O:200:ASN:ND2	17:Q:14:ASN:OD1	2.36	0.57
16:P:348:HIS:CD2	18:R:154:LYS:CD	2.72	0.57
16:P:397:LYS:CG	18:R:85:ARG:HD3	2.34	0.57
17:Q:337:SER:HB2	17:Q:448:LYS:HD3	1.86	0.57
1:A:407:GLN:O	1:A:408:LYS:NZ	2.38	0.57
1:A:506:THR:HB	1:A:579:ARG:O	2.03	0.57
1:A:938:VAL:CG2	9:I:82:ILE:CD1	2.68	0.57
1:A:1298:ASP:CG	1:A:1468:LYS:HZ1	2.04	0.57
2:B:152:LEU:CG	2:B:443:LYS:HE3	2.27	0.57
2:B:679:GLN:HG3	14:N:156:PRO:N	2.18	0.57
2:B:796:ARG:NH2	10:J:8:PHE:O	2.37	0.57
15:O:473:PHE:HZ	15:O:509:MET:HE3	1.68	0.57
16:P:438:TRP:HZ2	18:R:297:PHE:HE1	1.51	0.57
18:R:181:THR:O	18:R:185:LYS:HG3	2.04	0.57
1:A:615:ARG:HH12	2:B:929:ARG:CD	2.17	0.57
3:C:274:THR:CB	14:N:172:ALA:HB2	2.25	0.57
13:M:10:ILE:HB	14:N:70:LEU:HB3	1.86	0.57
15:O:552:LEU:O	15:O:553:ARG:C	2.46	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:186:TYR:CZ	18:R:196:GLU:OE1	2.57	0.57
16:P:420:GLU:HA	16:P:442:LEU:O	2.03	0.57
16:P:436:ILE:N	18:R:143:THR:N	2.51	0.57
17:Q:371:GLU:HG3	18:R:231:LEU:HD11	1.85	0.57
18:R:9:THR:HB	18:R:205:VAL:HG13	1.86	0.57
1:A:422:ARG:HH12	18:R:412:ARG:NH1	1.79	0.57
1:A:476:VAL:HG22	2:B:1069:ILE:N	2.18	0.57
11:K:68:GLU:HG2	11:K:72:LEU:HD23	1.86	0.57
15:O:379:ARG:HH11	15:O:379:ARG:CA	2.09	0.57
16:P:365:TRP:HB3	16:P:372:ILE:HG22	1.86	0.57
17:Q:12:THR:HB	17:Q:33:HIS:ND1	2.18	0.57
1:A:672:ASP:CG	2:B:777:SER:CB	2.77	0.57
3:C:42:VAL:HB	11:K:138:LYS:HG3	1.86	0.57
3:C:293:ARG:N	3:C:295:ARG:CZ	2.55	0.57
15:O:219:ARG:CZ	15:O:360:VAL:HG22	2.34	0.57
16:P:317:ILE:HG13	16:P:326:ILE:HD13	1.86	0.57
16:P:357:LEU:CG	18:R:24:ILE:HD11	2.35	0.57
16:P:422:ILE:HG12	16:P:442:LEU:CD1	2.34	0.57
16:P:462:ILE:HB	16:P:483:HIS:HB3	1.87	0.57
17:Q:374:THR:HG23	18:R:219:LEU:CD1	2.35	0.57
1:A:991:LYS:N	1:A:994:GLU:CB	2.67	0.57
1:A:1032:VAL:HG21	1:A:1050:TYR:HE1	1.68	0.57
7:G:143:SER:OG	15:O:104:ILE:CG2	2.51	0.57
15:O:63:LEU:HD23	15:O:111:ARG:HD2	1.87	0.57
15:O:205:ARG:O	15:O:209:VAL:HG12	2.05	0.57
16:P:301:GLN:N	16:P:319:ASP:O	2.37	0.57
16:P:349:GLY:HA2	18:R:154:LYS:HA	1.85	0.57
17:Q:378:LEU:HD22	18:R:238:THR:OG1	2.04	0.57
1:A:672:ASP:OD1	2:B:777:SER:CB	2.53	0.57
2:B:404:LEU:O	2:B:405:GLY:C	2.47	0.57
2:B:548:LYS:O	2:B:549:CYS:C	2.47	0.57
2:B:833:PRO:HG2	2:B:836:TRP:CE2	2.40	0.57
16:P:382:GLU:OE1	18:R:146:SER:HB2	2.01	0.57
16:P:432:PRO:C	18:R:145:SER:OG	2.47	0.57
16:P:434:ARG:C	18:R:143:THR:OG1	2.47	0.57
17:Q:22:ILE:HD12	17:Q:26:ARG:NE	2.18	0.57
17:Q:351:ASN:CG	17:Q:369:TRP:CE2	2.83	0.57
1:A:995:TYR:CE2	2:B:708:ASP:CA	2.56	0.57
2:B:49:PHE:CE2	2:B:194:PHE:CE2	2.93	0.57
1:A:1032:VAL:HG22	1:A:1050:TYR:CD1	2.39	0.57
1:A:1118:VAL:HG11	5:E:199:ILE:HG13	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:200:ASN:OD1	17:Q:14:ASN:CG	2.47	0.57
15:O:359:GLY:O	15:O:363:THR:CG2	2.53	0.57
16:P:407:ARG:HH22	16:P:411:LYS:HA	1.70	0.57
2:B:203:ILE:CG2	2:B:405:GLY:HA3	2.35	0.56
16:P:712:ASP:OD1	16:P:712:ASP:N	2.38	0.56
17:Q:356:VAL:CG1	18:R:208:TYR:HD1	2.09	0.56
1:A:986:PHE:CE2	2:B:958:MET:CE	2.88	0.56
1:A:1314:GLN:NE2	1:A:1446:ARG:NE	2.49	0.56
1:A:1484:LEU:HD11	2:B:305:ARG:CD	2.35	0.56
16:P:667:ASP:OD1	16:P:667:ASP:N	2.33	0.56
17:Q:193:PHE:CE2	18:R:208:TYR:CG	2.93	0.56
17:Q:362:THR:O	17:Q:365:ASP:HB2	2.04	0.56
17:Q:410:ARG:HE	17:Q:413:LEU:HD13	1.69	0.56
18:R:6:ILE:HD13	18:R:213:ILE:HB	1.83	0.56
1:A:474:LYS:CE	2:B:1092:LEU:HD22	2.33	0.56
1:A:615:ARG:CZ	2:B:929:ARG:HE	2.16	0.56
1:A:686:PHE:CZ	8:H:121:LEU:HD11	2.40	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD12	1.70	0.56
2:B:1013:MET:SD	2:B:1026:ILE:HG12	2.45	0.56
2:B:1072:GLY:H	2:B:1075:GLU:CD	2.13	0.56
15:O:66:ASN:N	15:O:66:ASN:ND2	2.53	0.56
15:O:109:SER:OG	15:O:111:ARG:HG3	2.05	0.56
16:P:608:GLN:HA	16:P:611:ILE:HD12	1.87	0.56
17:Q:15:CYS:CB	17:Q:17:SER:N	2.59	0.56
17:Q:20:TRP:CE2	17:Q:28:THR:HB	2.39	0.56
17:Q:211:TYR:O	17:Q:214:ILE:HG22	2.05	0.56
18:R:180:CYS:SG	18:R:185:LYS:CG	2.94	0.56
1:A:436:ALA:HA	1:A:439:ASP:C	2.28	0.56
1:A:475:ARG:HH22	2:B:1061:LYS:HG3	1.67	0.56
1:A:581:ILE:HG12	1:A:582:LYS:N	2.21	0.56
1:A:615:ARG:HH12	2:B:929:ARG:NE	2.02	0.56
1:A:1275:THR:C	9:I:45:LEU:O	2.48	0.56
1:A:1482:LYS:HD3	2:B:304:ASP:CG	2.29	0.56
2:B:45:HIS:O	2:B:164:MET:HE1	2.06	0.56
16:P:358:SER:HB3	16:P:377:ARG:HD3	1.87	0.56
16:P:362:ARG:HH22	16:P:364:GLU:HG3	1.71	0.56
17:Q:417:PHE:CE2	18:R:270:PHE:CE1	2.75	0.56
1:A:408:LYS:H	1:A:408:LYS:HD3	1.70	0.56
1:A:535:GLN:HE22	17:Q:26:ARG:CG	2.17	0.56
1:A:615:ARG:HH12	2:B:929:ARG:HD3	1.71	0.56
1:A:721:LYS:NZ	8:H:91:ASP:CA	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:SER:HA	9:I:83:LYS:HE3	1.84	0.56
1:A:1310:LYS:CG	1:A:1311:GLU:OE1	2.37	0.56
1:A:1574:ALA:C	9:I:122:ARG:NH1	2.62	0.56
2:B:184:LYS:CD	2:B:735:HIS:CD2	2.89	0.56
2:B:1005:TYR:CE1	14:N:170:HIS:CE1	2.93	0.56
5:E:159:ASP:OD1	5:E:162:ARG:NH1	2.38	0.56
7:G:143:SER:OG	15:O:104:ILE:HG22	2.01	0.56
15:O:243:GLU:HB3	15:O:332:LEU:CD1	2.30	0.56
1:A:477:ASN:CG	2:B:1047:ARG:NH1	2.56	0.56
1:A:921:PRO:HD3	8:H:19:ARG:CG	2.33	0.56
5:E:145:THR:O	5:E:147:HIS:N	2.38	0.56
13:M:15:VAL:HG22	13:M:90:LEU:HB2	1.88	0.56
15:O:234:ILE:CG1	15:O:367:LEU:HD13	2.36	0.56
16:P:375:PHE:HD1	16:P:402:ILE:HD13	1.69	0.56
17:Q:152:LEU:HB3	17:Q:154:LEU:HD22	1.85	0.56
17:Q:274:ILE:HG23	17:Q:282:ARG:HH22	1.71	0.56
18:R:5:PRO:HD3	18:R:217:THR:CB	2.23	0.56
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.38	0.56
2:B:563:SER:HA	13:M:73:SER:OG	2.06	0.56
2:B:567:SER:O	14:N:140:SER:CB	2.52	0.56
1:A:435:ASN:HB3	1:A:442:LYS:C	2.29	0.56
1:A:503:VAL:CA	1:A:580:HIS:HD2	1.69	0.56
2:B:681:ILE:HB	14:N:154:ARG:CB	2.34	0.56
16:P:472:ARG:NE	18:R:200:THR:HG21	2.18	0.56
18:R:236:PHE:O	18:R:240:ILE:HG22	2.05	0.56
18:R:369:ALA:HB1	18:R:411:VAL:HG23	1.86	0.56
1:A:438:ILE:O	1:A:457:LYS:HB3	2.04	0.56
1:A:1657:LEU:CB	7:G:104:LEU:HD13	2.35	0.56
2:B:30:LYS:HG2	2:B:178:TYR:CB	2.35	0.56
2:B:30:LYS:O	2:B:176:SER:CB	2.54	0.56
2:B:49:PHE:CG	2:B:164:MET:HE3	2.40	0.56
6:F:66:ARG:HH22	7:G:90:LEU:CB	2.19	0.56
6:F:70:LYS:CD	7:G:95:LEU:CD2	2.79	0.56
15:O:243:GLU:CB	15:O:332:LEU:CD1	2.84	0.56
15:O:602:TYR:CD2	15:O:605:LEU:HD23	2.40	0.56
16:P:504:THR:HG22	16:P:505:PRO:HD2	1.88	0.56
18:R:4:VAL:CG2	18:R:214:VAL:CG1	2.79	0.56
18:R:83:HIS:O	18:R:85:ARG:N	2.39	0.56
1:A:1162:ASN:HD22	1:A:1165:LYS:HG3	1.71	0.56
1:A:1187:ILE:HG13	2:B:1080:ILE:CG2	2.36	0.56
2:B:864:ASP:CB	17:Q:412:LYS:CE	2.81	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:191:ASP:O	15:O:194:LEU:HB2	2.06	0.56
16:P:488:LEU:HB2	18:R:137:SER:OG	2.07	0.56
16:P:623:LEU:HG	16:P:678:LEU:HD12	1.88	0.56
17:Q:22:ILE:HD12	17:Q:24:ASP:OD1	2.04	0.56
18:R:173:MET:CG	18:R:188:PHE:CZ	2.87	0.56
1:A:502:ALA:HB1	1:A:530:TRP:NE1	2.21	0.55
2:B:143:TRP:HB3	2:B:446:MET:HE1	1.84	0.55
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.55
10:J:10:CYS:HB3	10:J:43:ARG:NH1	2.21	0.55
13:M:11:GLU:N	13:M:86:LYS:O	2.36	0.55
17:Q:163:SER:HA	17:Q:230:ILE:HG22	1.88	0.55
18:R:4:VAL:CG2	18:R:214:VAL:CG2	2.65	0.55
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.87	0.55
1:A:998:HIS:NE2	2:B:711:GLN:HA	2.22	0.55
1:A:1482:LYS:CE	2:B:304:ASP:CG	2.64	0.55
1:A:1499:ARG:O	1:A:1500:GLN:HB2	2.05	0.55
2:B:208:VAL:HG23	2:B:401:GLU:CG	2.35	0.55
8:H:80:ARG:NH1	11:K:108:TYR:CD1	2.74	0.55
17:Q:411:ARG:O	17:Q:415:LYS:HB2	2.05	0.55
18:R:308:PHE:HD1	18:R:309:ALA:N	2.04	0.55
1:A:721:LYS:HE2	8:H:93:TYR:O	2.06	0.55
1:A:756:LYS:HD3	9:I:85:LYS:HZ3	1.30	0.55
1:A:756:LYS:HG3	9:I:85:LYS:HZ2	1.71	0.55
1:A:821:ILE:O	1:A:825:ALA:N	2.40	0.55
1:A:1658:ALA:HA	6:F:132:LEU:HA	1.87	0.55
3:C:314:PHE:CE2	11:K:135:PHE:CE1	2.95	0.55
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.87	0.55
16:P:474:LYS:O	16:P:499:GLU:HB2	2.07	0.55
17:Q:103:LEU:HD21	17:Q:205:ILE:HG21	1.88	0.55
17:Q:227:TYR:O	17:Q:230:ILE:HG13	2.06	0.55
17:Q:287:TRP:NE1	17:Q:289:ARG:HB3	2.21	0.55
17:Q:416:ILE:CD1	18:R:273:TRP:CD1	2.90	0.55
2:B:819:ASP:CG	2:B:820:PRO:HD2	2.31	0.55
16:P:414:ILE:HB	16:P:425:GLY:C	2.32	0.55
17:Q:8:PRO:HB2	17:Q:19:LEU:CD2	2.36	0.55
2:B:985:ILE:CG1	14:N:160:VAL:HG21	2.37	0.55
15:O:376:TYR:CD2	15:O:419:LYS:HE2	2.40	0.55
15:O:468:GLU:C	15:O:470:PHE:H	2.15	0.55
16:P:473:HIS:ND1	16:P:473:HIS:O	2.37	0.55
18:R:246:GLN:HG2	18:R:247:ILE:H	1.71	0.55
1:A:476:VAL:HA	2:B:1059:PRO:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:ARG:HG2	2:B:1049:THR:N	2.21	0.55
3:C:292:GLY:HA3	3:C:295:ARG:HH22	1.71	0.55
5:E:90:VAL:HG13	5:E:120:ALA:HA	1.88	0.55
16:P:534:VAL:HA	16:P:552:LEU:O	2.06	0.55
1:A:508:PRO:CD	1:A:639:GLN:HG3	2.37	0.55
7:G:144:HIS:CE1	15:O:145:SER:HB3	2.38	0.55
15:O:219:ARG:NE	15:O:230:TRP:HE1	2.05	0.55
15:O:332:LEU:CD2	15:O:599:LEU:HD21	2.36	0.55
15:O:578:SER:O	15:O:579:LEU:HB2	2.06	0.55
16:P:435:ARG:HH21	18:R:140:ILE:CD1	2.19	0.55
18:R:158:THR:HG23	18:R:161:ASN:H	1.72	0.55
18:R:187:TYR:O	18:R:191:ILE:HG23	2.07	0.55
18:R:353:VAL:CG1	18:R:364:VAL:HB	2.36	0.55
1:A:436:ALA:CA	1:A:440:SER:HA	2.37	0.55
1:A:953:GLU:HB3	1:A:1205:PHE:CZ	2.41	0.55
1:A:1260:LYS:HE2	1:A:1262:LEU:HG	1.89	0.55
1:A:1484:LEU:CD1	2:B:305:ARG:NH1	2.56	0.55
2:B:322:ASN:HB3	2:B:325:GLN:H	1.71	0.55
3:C:139:LYS:HG2	3:C:201:GLU:HB3	1.89	0.55
15:O:169:THR:HA	15:O:172:HIS:ND1	2.22	0.55
16:P:218:VAL:HG22	16:P:246:LYS:HB3	1.89	0.55
16:P:433:VAL:C	18:R:145:SER:HA	2.31	0.55
16:P:444:PRO:HG2	16:P:449:LEU:HD11	1.89	0.55
1:A:697:TYR:CE2	11:K:92:SER:OG	2.58	0.55
1:A:966:LEU:HD22	1:A:997:PHE:CZ	2.40	0.55
1:A:990:ILE:CA	1:A:994:GLU:CB	2.64	0.55
1:A:1314:GLN:CD	1:A:1446:ARG:HH11	2.13	0.55
2:B:203:ILE:CG2	2:B:405:GLY:HA2	2.37	0.55
3:C:223:SER:HB3	10:J:12:LYS:HB2	1.87	0.55
3:C:315:PHE:CE2	11:K:139:ILE:CD1	2.89	0.55
15:O:69:THR:O	15:O:73:ILE:HG13	2.07	0.55
16:P:233:VAL:HG12	16:P:234:THR:H	1.71	0.55
17:Q:6:ARG:HA	17:Q:18:ARG:HD2	1.88	0.55
17:Q:290:THR:HB	17:Q:292:GLU:N	2.22	0.55
18:R:317:LEU:HD12	18:R:367:ILE:HD12	1.85	0.55
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.55
2:B:401:GLU:HG3	2:B:402:VAL:H	1.70	0.55
2:B:1003:ALA:C	14:N:169:GLU:H	2.15	0.55
15:O:163:ILE:HD12	15:O:207:LYS:HE3	1.89	0.55
15:O:376:TYR:HE2	15:O:377:TYR:HE2	1.44	0.55
16:P:434:ARG:CG	18:R:143:THR:HB	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:193:PHE:HE2	18:R:208:TYR:CE2	2.25	0.55
18:R:320:CYS:O	18:R:323:SER:N	2.40	0.55
1:A:503:VAL:HG23	1:A:530:TRP:CB	2.19	0.54
1:A:827:THR:HG21	1:A:924:SER:HB3	1.89	0.54
2:B:54:GLU:HG3	2:B:168:ASN:HD21	1.71	0.54
2:B:625:GLU:OE1	2:B:667:PHE:HB3	2.07	0.54
3:C:315:PHE:HE2	11:K:139:ILE:HD12	1.70	0.54
15:O:359:GLY:O	15:O:363:THR:HG22	2.08	0.54
15:O:467:MET:HG2	15:O:575:SER:HA	1.89	0.54
17:Q:24:ASP:CG	17:Q:26:ARG:HE	2.14	0.54
18:R:26:TYR:CB	18:R:169:PRO:HB3	2.37	0.54
1:A:1276:THR:HG1	9:I:45:LEU:CD1	1.94	0.54
2:B:48:SER:HB3	2:B:404:LEU:HD13	1.88	0.54
2:B:119:ARG:CZ	12:L:53:HIS:HE1	2.17	0.54
2:B:548:LYS:O	2:B:550:ARG:CZ	2.56	0.54
2:B:788:ILE:HB	2:B:948:ILE:HB	1.89	0.54
7:G:144:HIS:CE1	15:O:146:SER:OG	2.60	0.54
16:P:194:ARG:HA	16:P:209:LYS:O	2.06	0.54
16:P:315:PHE:HB3	16:P:317:ILE:CD1	2.37	0.54
16:P:389:TRP:CE3	18:R:149:LYS:O	2.60	0.54
16:P:448:THR:HG23	16:P:471:MET:H	1.71	0.54
1:A:403:LEU:HD11	1:A:419:ILE:HD13	1.88	0.54
1:A:1298:ASP:HA	1:A:1468:LYS:NZ	2.20	0.54
1:A:1641:ILE:HG23	2:B:1092:LEU:HD13	1.88	0.54
2:B:21:ARG:NH1	2:B:22:GLU:OE1	2.40	0.54
2:B:212:ASN:HD21	2:B:361:HIS:CB	2.20	0.54
3:C:33:VAL:CG1	11:K:130:VAL:HG21	2.38	0.54
7:G:24:VAL:N	7:G:128:GLN:CD	2.28	0.54
16:P:352:PHE:CE1	18:R:157:MET:HG2	2.42	0.54
16:P:468:VAL:HG22	16:P:477:TYR:HB3	1.89	0.54
16:P:592:LEU:O	16:P:596:ILE:HG22	2.06	0.54
17:Q:318:LEU:HB3	17:Q:476:ILE:HD12	1.88	0.54
18:R:161:ASN:O	18:R:164:LYS:HB2	2.07	0.54
18:R:361:ASP:C	18:R:363:GLU:H	2.14	0.54
2:B:1073:GLU:HA	2:B:1076:ARG:CB	2.38	0.54
5:E:145:THR:C	5:E:147:HIS:N	2.65	0.54
7:G:229:LEU:HD12	7:G:230:ARG:H	1.72	0.54
17:Q:196:SER:CB	17:Q:204:ARG:HG2	2.37	0.54
1:A:953:GLU:C	1:A:1205:PHE:HB2	2.24	0.54
1:A:1162:ASN:HD21	1:A:1164:LYS:HB2	1.71	0.54
1:A:1655:ASP:N	6:F:135:ARG:O	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:GLY:CA	2:B:242:ASP:HB2	2.38	0.54
2:B:550:ARG:O	2:B:648:ARG:O	2.26	0.54
2:B:550:ARG:N	2:B:650:LEU:O	2.40	0.54
7:G:154:ASN:HD21	15:O:182:MET:HE3	1.73	0.54
15:O:412:GLU:OE1	15:O:416:LYS:HD3	2.06	0.54
16:P:492:LEU:HD22	16:P:492:LEU:H	1.73	0.54
16:P:722:TRP:CD1	17:Q:264:PRO:HD3	2.42	0.54
1:A:67:LEU:HD13	1:A:71:PHE:O	2.08	0.54
1:A:671:GLN:CB	2:B:952:HIS:CD2	2.90	0.54
2:B:212:ASN:OD1	2:B:238:SER:HA	2.08	0.54
2:B:679:GLN:N	14:N:155:VAL:O	2.41	0.54
2:B:894:LYS:HG2	12:L:47:ARG:CD	2.38	0.54
6:F:72:LYS:HB3	6:F:142:SER:HA	0.59	0.54
15:O:373:LEU:HD12	15:O:423:TYR:CD2	2.43	0.54
15:O:376:TYR:CE2	15:O:377:TYR:CD2	2.93	0.54
17:Q:335:THR:HG21	17:Q:478:ARG:HG3	1.89	0.54
1:A:408:LYS:HB2	1:A:411:VAL:O	2.08	0.54
1:A:449:GLY:O	1:A:451:VAL:N	2.34	0.54
1:A:909:SER:CA	9:I:83:LYS:NZ	2.61	0.54
2:B:203:ILE:HG22	2:B:405:GLY:HA2	1.90	0.54
2:B:373:MET:O	2:B:377:MET:HG3	2.07	0.54
18:R:4:VAL:CB	18:R:214:VAL:HG22	2.38	0.54
2:B:284:SER:OG	2:B:287:GLU:HG3	2.07	0.54
2:B:317:TYR:HB3	2:B:320:LEU:HD12	1.89	0.54
3:C:315:PHE:CZ	11:K:139:ILE:HD12	2.42	0.54
11:K:48:LYS:HE2	11:K:64:GLN:NE2	2.23	0.54
16:P:221:ARG:HH12	16:P:266:GLU:HB3	1.72	0.54
16:P:659:LEU:HD12	16:P:742:TRP:NE1	2.23	0.54
16:P:711:LEU:HD21	16:P:741:ILE:HD13	1.90	0.54
17:Q:101:LYS:O	17:Q:105:LEU:HG	2.07	0.54
1:A:475:ARG:HD2	2:B:1059:PRO:O	2.07	0.54
1:A:492:THR:HG23	1:A:811:SER:OG	2.08	0.54
1:A:1262:LEU:HD23	1:A:1497:ILE:HA	1.90	0.54
1:A:1482:LYS:CD	2:B:304:ASP:CG	2.81	0.54
2:B:551:ILE:HG23	2:B:647:SER:C	2.29	0.54
2:B:679:GLN:OE1	14:N:157:ARG:HB2	2.06	0.54
2:B:1091:ARG:CZ	2:B:1095:SER:OG	2.56	0.54
3:C:97:LEU:HD11	3:C:202:ILE:HD13	1.90	0.54
16:P:436:ILE:CB	18:R:143:THR:CA	2.85	0.54
17:Q:162:ILE:HG22	17:Q:226:LEU:HD21	1.90	0.54
17:Q:505:ILE:HA	17:Q:508:ALA:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ILE:HA	8:H:97:MET:HA	1.89	0.54
1:A:1025:LYS:HZ2	2:B:1076:ARG:NH1	2.06	0.54
1:A:1297:PHE:CD2	9:I:60:LEU:HD13	2.43	0.54
1:A:1446:ARG:O	1:A:1450:ILE:HG13	2.08	0.54
1:A:1657:LEU:O	6:F:132:LEU:C	2.49	0.54
2:B:699:ILE:O	2:B:703:LEU:HG	2.08	0.54
3:C:65:ASN:O	3:C:69:ARG:HG3	2.07	0.54
3:C:67:PHE:O	3:C:71:MET:HG3	2.08	0.54
7:G:132:VAL:HG22	7:G:232:THR:HG22	1.90	0.54
2:B:42:VAL:HG21	2:B:190:ILE:HD12	1.89	0.53
2:B:894:LYS:CA	12:L:54:ARG:HE	2.18	0.53
2:B:943:ILE:CD1	10:J:44:TYR:CZ	2.68	0.53
15:O:63:LEU:CD2	15:O:111:ARG:HD2	2.38	0.53
15:O:189:PHE:CD1	15:O:190:ILE:N	2.76	0.53
2:B:574:SER:O	13:M:97:VAL:HG22	2.07	0.53
2:B:859:CYS:HB3	2:B:872:LYS:HB2	1.88	0.53
15:O:235:GLU:O	15:O:238:ILE:HD13	2.08	0.53
15:O:240:ILE:HD13	15:O:240:ILE:N	2.23	0.53
16:P:184:SER:HA	18:R:198:LEU:CB	2.29	0.53
18:R:213:ILE:HG12	18:R:242:ILE:HD13	1.90	0.53
18:R:305:THR:HB	18:R:308:PHE:CE1	2.43	0.53
1:A:1136:VAL:HG22	1:A:1174:TYR:CG	2.44	0.53
1:A:1310:LYS:HG2	1:A:1311:GLU:CG	2.38	0.53
1:A:1654:PHE:CD2	6:F:134:ILE:HG23	2.44	0.53
15:O:100:LEU:HD22	15:O:107:ILE:CD1	2.38	0.53
16:P:184:SER:N	18:R:198:LEU:HD23	1.95	0.53
16:P:197:ARG:HB3	16:P:261:VAL:O	2.08	0.53
17:Q:361:PRO:O	17:Q:364:SER:N	2.42	0.53
18:R:168:ILE:HD11	18:R:172:LYS:HE2	1.90	0.53
18:R:350:SER:HA	18:R:353:VAL:HB	1.90	0.53
2:B:551:ILE:HG21	2:B:647:SER:CA	2.18	0.53
7:G:20:HIS:O	7:G:20:HIS:ND1	2.38	0.53
17:Q:115:GLN:HB3	17:Q:190:MET:HE2	1.91	0.53
17:Q:341:ARG:NH2	17:Q:369:TRP:HE1	2.05	0.53
17:Q:385:PHE:CE1	18:R:209:ARG:HG3	2.44	0.53
2:B:16:PHE:HD2	10:J:32:GLU:OE2	1.90	0.53
2:B:38:LEU:HD11	2:B:493:PHE:CZ	2.43	0.53
2:B:38:LEU:HD11	2:B:493:PHE:HZ	1.74	0.53
2:B:1071:VAL:C	2:B:1075:GLU:HG3	2.27	0.53
3:C:215:ASP:CG	12:L:70:ARG:HH22	2.17	0.53
3:C:230:LEU:HD22	3:C:297:HIS:CE1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:21:GLN:C	18:R:139:GLU:OE2	2.49	0.53
16:P:273:ARG:HG2	16:P:291:PRO:HB3	1.90	0.53
17:Q:333:SER:HA	17:Q:336:GLU:HG2	1.89	0.53
1:A:824:THR:O	2:B:1023:ARG:HB2	2.08	0.53
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.90	0.53
2:B:985:ILE:C	14:N:160:VAL:CG2	2.80	0.53
2:B:1005:TYR:HH	10:J:44:TYR:HE2	1.46	0.53
13:M:12:ILE:HD12	14:N:67:LEU:HB2	1.90	0.53
16:P:320:ILE:HG13	16:P:323:ASN:OD1	2.07	0.53
16:P:394:VAL:HG22	16:P:434:ARG:HH11	1.73	0.53
1:A:1002:GLY:HA3	2:B:713:PRO:HD3	1.91	0.53
2:B:664:VAL:HG22	2:B:672:MET:HE1	1.91	0.53
2:B:894:LYS:HG2	12:L:54:ARG:CZ	2.38	0.53
3:C:33:VAL:HG12	11:K:130:VAL:HG21	1.90	0.53
16:P:472:ARG:HH12	18:R:203:SER:HB2	1.74	0.53
17:Q:8:PRO:CB	17:Q:19:LEU:HD23	2.39	0.53
18:R:273:TRP:O	18:R:277:ILE:HG22	2.08	0.53
9:I:96:TYR:HA	9:I:111:PHE:O	2.09	0.53
13:M:75:GLN:HB2	14:N:60:SER:HA	1.91	0.53
15:O:206:ARG:HA	15:O:209:VAL:HG12	1.91	0.53
15:O:468:GLU:C	15:O:470:PHE:N	2.65	0.53
15:O:473:PHE:HE2	15:O:516:PRO:HG3	1.73	0.53
16:P:185:GLN:CB	18:R:195:LEU:CB	2.79	0.53
16:P:265:THR:HG23	16:P:274:ILE:HG12	1.90	0.53
16:P:662:LEU:HB3	16:P:665:ASN:CG	2.33	0.53
1:A:481:ARG:HB3	2:B:1045:GLN:O	2.09	0.53
2:B:25:PHE:O	10:J:62:ARG:HD3	2.08	0.53
6:F:66:ARG:HH22	7:G:90:LEU:HD12	1.57	0.53
16:P:292:LEU:CD1	16:P:343:LEU:HG	2.39	0.53
16:P:436:ILE:HB	18:R:143:THR:CB	2.38	0.53
16:P:443:ASP:CB	18:R:3:GLU:OE2	2.52	0.53
17:Q:370:SER:O	17:Q:373:GLU:N	2.42	0.53
18:R:199:LYS:NZ	18:R:204:GLU:HB3	2.23	0.53
1:A:1025:LYS:NZ	2:B:1076:ARG:NH1	2.56	0.53
15:O:243:GLU:HA	15:O:328:LEU:HD23	1.90	0.53
18:R:352:TRP:O	18:R:356:PRO:HD3	2.08	0.53
1:A:954:GLY:N	1:A:1205:PHE:HB3	2.10	0.52
1:A:1297:PHE:CZ	1:A:1301:GLU:OE1	2.52	0.52
2:B:497:ILE:CG1	2:B:699:ILE:HD13	2.38	0.52
2:B:679:GLN:HA	14:N:155:VAL:O	2.09	0.52
2:B:1005:TYR:CD2	14:N:170:HIS:CG	2.98	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:ARG:O	2:B:1065:ARG:HG3	2.08	0.52
2:B:1092:LEU:C	2:B:1096:SER:CB	2.82	0.52
15:O:245:GLN:HG3	15:O:377:TYR:O	2.09	0.52
15:O:499:GLU:O	15:O:502:LEU:HG	2.09	0.52
16:P:436:ILE:CG2	18:R:143:THR:CA	2.87	0.52
17:Q:351:ASN:ND2	17:Q:373:GLU:OE1	2.41	0.52
18:R:252:GLY:O	18:R:256:GLU:CB	2.56	0.52
1:A:209:THR:HG21	5:E:173:SER:OG	2.09	0.52
1:A:544:VAL:HA	17:Q:34:VAL:H	1.74	0.52
2:B:134:ARG:HD2	2:B:160:GLY:HA3	1.91	0.52
2:B:894:LYS:HG2	12:L:47:ARG:HD2	1.90	0.52
15:O:376:TYR:CG	15:O:419:LYS:HD3	2.44	0.52
16:P:365:TRP:HE3	16:P:372:ILE:HG22	1.73	0.52
16:P:408:ILE:HB	16:P:453:VAL:HG21	1.91	0.52
16:P:448:THR:HG21	16:P:471:MET:H	1.74	0.52
18:R:347:ASP:O	18:R:351:GLU:CB	2.56	0.52
1:A:472:MET:CE	2:B:1076:ARG:CD	2.88	0.52
1:A:822:THR:O	2:B:1015:SER:HB2	2.09	0.52
1:A:862:THR:CA	9:I:67:VAL:HG12	2.39	0.52
2:B:762:MET:HE2	2:B:762:MET:HA	1.91	0.52
16:P:302:VAL:O	16:P:363:ILE:HD11	2.09	0.52
18:R:242:ILE:HG23	18:R:244:GLY:H	1.74	0.52
15:O:337:THR:O	15:O:341:THR:OG1	2.27	0.52
17:Q:22:ILE:HD12	17:Q:26:ARG:NH1	2.24	0.52
1:A:382:GLN:NE2	1:A:456:VAL:HG22	2.23	0.52
1:A:403:LEU:CD1	1:A:419:ILE:HG23	2.35	0.52
2:B:833:PRO:O	2:B:834:LYS:HB3	2.10	0.52
3:C:272:LYS:HA	14:N:175:TYR:CD2	2.43	0.52
7:G:30:GLU:HA	7:G:32:ASN:H	1.74	0.52
7:G:35:SER:HG	7:G:132:VAL:H	1.57	0.52
15:O:402:THR:O	15:O:406:ILE:HG13	2.09	0.52
16:P:472:ARG:NH2	18:R:200:THR:HG23	2.21	0.52
1:A:1050:TYR:CD1	1:A:1179:ILE:CG2	2.85	0.52
3:C:326:GLU:HG3	11:K:125:MET:CE	2.40	0.52
15:O:467:MET:HG3	15:O:519:PHE:CZ	2.45	0.52
16:P:184:SER:C	18:R:198:LEU:HB3	2.34	0.52
16:P:350:THR:CG2	18:R:153:ASN:OD1	2.58	0.52
16:P:436:ILE:HG12	18:R:141:TRP:CZ3	2.45	0.52
16:P:650:LEU:HD13	16:P:652:GLY:H	1.74	0.52
18:R:6:ILE:CD1	18:R:213:ILE:HG21	2.37	0.52
1:A:477:ASN:CA	2:B:1047:ARG:NH1	2.69	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:CYS:CA	2:B:712:SER:HB2	2.21	0.52
1:A:1654:PHE:CZ	6:F:89:GLU:HA	2.45	0.52
2:B:796:ARG:HB3	10:J:8:PHE:HD1	1.75	0.52
2:B:1092:LEU:CA	2:B:1096:SER:CB	2.79	0.52
15:O:518:LYS:HD3	15:O:519:PHE:CZ	2.45	0.52
18:R:410:TYR:O	18:R:413:THR:OG1	2.20	0.52
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.92	0.52
1:A:613:THR:CG2	2:B:913:ILE:CG2	2.79	0.52
1:A:878:ARG:NH2	9:I:66:VAL:O	2.37	0.52
2:B:307:GLU:OE2	2:B:311:ARG:NH1	2.43	0.52
2:B:678:PRO:O	14:N:154:ARG:HA	2.10	0.52
3:C:45:SER:CB	3:C:271:ARG:NH2	2.71	0.52
4:D:80:THR:OG1	15:O:228:GLN:HG2	2.10	0.52
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.91	0.52
15:O:248:LEU:HD23	15:O:248:LEU:O	2.10	0.52
16:P:436:ILE:HG22	18:R:143:THR:CA	2.38	0.52
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.91	0.52
2:B:527:PHE:CG	2:B:666:PRO:HB3	2.44	0.52
17:Q:116:ILE:O	17:Q:120:ILE:HG12	2.09	0.52
17:Q:414:TYR:CD1	18:R:240:ILE:HG13	2.45	0.52
18:R:171:ARG:O	18:R:174:GLU:HB3	2.09	0.52
1:A:670:ILE:HG13	2:B:783:MET:HE3	1.92	0.52
1:A:969:PHE:CE2	1:A:978:ALA:HA	2.44	0.52
1:A:1318:SER:HA	1:A:1450:ILE:CD1	2.39	0.52
2:B:22:GLU:O	2:B:26:ILE:HG13	2.10	0.52
2:B:64:GLY:HA2	2:B:242:ASP:HB2	1.90	0.52
2:B:112:GLY:HA3	2:B:893:ASN:HB3	1.91	0.52
3:C:272:LYS:HD3	14:N:179:ASP:HB3	1.91	0.52
15:O:235:GLU:CA	15:O:237:ILE:HB	2.40	0.52
15:O:374:PRO:O	15:O:376:TYR:CD2	2.63	0.52
16:P:414:ILE:HB	16:P:425:GLY:O	2.10	0.52
16:P:452:THR:HG21	16:P:508:ILE:HG22	1.92	0.52
17:Q:8:PRO:CG	17:Q:19:LEU:HD23	2.40	0.52
17:Q:22:ILE:HD12	17:Q:26:ARG:CZ	2.40	0.52
17:Q:341:ARG:HH12	17:Q:369:TRP:HE1	1.53	0.52
1:A:466:LEU:HD11	2:B:1181:VAL:CG2	2.41	0.51
1:A:475:ARG:O	2:B:1059:PRO:HD2	2.10	0.51
1:A:507:TYR:CE1	1:A:508:PRO:C	2.87	0.51
1:A:990:ILE:C	1:A:994:GLU:CB	2.82	0.51
1:A:1089:LEU:HD11	1:A:1175:MET:HE1	1.92	0.51
1:A:1603:MET:HE2	1:A:1615:TYR:CG	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.93	0.51
3:C:47:LEU:HD23	3:C:48:ASP:N	2.25	0.51
3:C:142:ARG:NH2	10:J:67:GLU:OE2	2.42	0.51
16:P:185:GLN:HB3	18:R:195:LEU:C	2.34	0.51
16:P:382:GLU:OE2	16:P:432:PRO:HG2	2.10	0.51
1:A:1657:LEU:CG	7:G:104:LEU:HD13	2.39	0.51
2:B:16:PHE:CD2	10:J:32:GLU:OE2	2.63	0.51
15:O:223:SER:O	15:O:226:GLY:N	2.35	0.51
16:P:193:LEU:CD1	16:P:251:SER:H	2.23	0.51
16:P:436:ILE:H	18:R:143:THR:H	1.59	0.51
1:A:476:VAL:CG2	2:B:1069:ILE:N	2.73	0.51
1:A:1050:TYR:CE1	1:A:1185:VAL:CG1	2.93	0.51
1:A:1575:ILE:CD1	9:I:122:ARG:NH1	2.64	0.51
1:A:1657:LEU:O	6:F:132:LEU:HA	2.09	0.51
15:O:240:ILE:HG22	15:O:380:SER:OG	2.04	0.51
16:P:317:ILE:HD11	16:P:326:ILE:HG23	1.92	0.51
16:P:426:ALA:O	16:P:433:VAL:HG11	2.10	0.51
2:B:535:ASP:CG	2:B:720:GLN:HE22	2.17	0.51
12:L:28:LYS:O	12:L:59:ALA:N	2.40	0.51
15:O:467:MET:HA	15:O:467:MET:HE2	1.91	0.51
16:P:384:ASP:HB3	16:P:389:TRP:CD1	2.45	0.51
18:R:4:VAL:HG11	18:R:214:VAL:CG2	2.40	0.51
18:R:177:LEU:HD22	18:R:185:LYS:CG	2.37	0.51
18:R:206:ARG:HH21	18:R:211:ARG:NH1	2.05	0.51
2:B:49:PHE:CD2	2:B:194:PHE:CZ	2.95	0.51
2:B:497:ILE:HG13	2:B:699:ILE:CD1	2.40	0.51
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.93	0.51
16:P:217:ALA:O	16:P:219:LEU:N	2.43	0.51
16:P:294:PHE:HB2	16:P:296:GLU:H	1.75	0.51
16:P:438:TRP:CD1	18:R:141:TRP:CH2	2.97	0.51
17:Q:351:ASN:C	17:Q:369:TRP:CH2	2.80	0.51
1:A:1276:THR:H	9:I:45:LEU:C	2.11	0.51
1:A:1450:ILE:HD12	1:A:1460:TYR:CD2	2.46	0.51
14:N:87:TYR:CE2	14:N:141:GLU:CD	2.88	0.51
15:O:240:ILE:CG2	15:O:332:LEU:HD11	2.41	0.51
17:Q:341:ARG:HH12	17:Q:369:TRP:NE1	2.05	0.51
17:Q:447:ALA:HA	17:Q:450:THR:HB	1.91	0.51
1:A:966:LEU:HD21	1:A:997:PHE:HE1	1.62	0.51
2:B:25:PHE:CZ	10:J:59:LYS:HD2	2.44	0.51
2:B:554:GLN:O	2:B:555:GLN:C	2.54	0.51
2:B:864:ASP:CB	17:Q:412:LYS:NZ	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:778:ASP:CG	16:P:779:ASP:H	2.19	0.51
17:Q:413:LEU:CD2	18:R:273:TRP:CZ2	2.94	0.51
18:R:269:ASP:N	18:R:269:ASP:OD2	2.43	0.51
1:A:40:ASN:OD1	1:A:40:ASN:N	2.44	0.51
1:A:507:TYR:HD1	1:A:509:GLU:HG2	1.76	0.51
2:B:532:HIS:NE2	2:B:723:LYS:CE	2.73	0.51
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.43	0.51
16:P:272:PHE:HE1	16:P:303:VAL:HB	1.75	0.51
16:P:420:GLU:HA	16:P:442:LEU:HD22	1.93	0.51
16:P:625:ASP:O	16:P:629:ARG:HB2	2.11	0.51
17:Q:10:CYS:HB2	17:Q:17:SER:N	2.25	0.51
17:Q:258:MET:HE2	17:Q:438:PHE:HE2	1.75	0.51
17:Q:382:GLU:HB2	18:R:241:ARG:HH11	1.75	0.51
2:B:212:ASN:ND2	2:B:361:HIS:CG	2.79	0.51
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.46	0.51
16:P:422:ILE:HG12	16:P:442:LEU:HD12	1.93	0.51
1:A:588:LEU:HD21	2:B:1087:LEU:CD1	2.31	0.51
1:A:597:LYS:HD3	2:B:1081:GLY:C	2.36	0.51
1:A:1662:ASN:C	7:G:101:SER:HB2	2.35	0.51
2:B:721:MET:HE2	2:B:721:MET:HA	1.92	0.51
15:O:144:CYS:HB2	15:O:179:PHE:CZ	2.46	0.51
16:P:442:LEU:HD13	16:P:442:LEU:N	2.26	0.51
16:P:573:GLU:HB3	17:Q:499:LYS:HD3	1.93	0.51
17:Q:188:ALA:C	17:Q:384:GLN:HG2	2.35	0.51
1:A:597:LYS:HD2	2:B:1082:HIS:CG	2.46	0.50
1:A:721:LYS:HZ1	8:H:91:ASP:HA	1.74	0.50
1:A:840:ASN:O	1:A:844:THR:HG23	2.11	0.50
17:Q:313:THR:O	17:Q:317:MET:HB2	2.11	0.50
17:Q:414:TYR:HD1	18:R:240:ILE:HG13	1.74	0.50
1:A:1573:TYR:HA	9:I:111:PHE:HE2	1.76	0.50
2:B:68:ILE:HD13	2:B:418:ASP:OD1	2.12	0.50
2:B:858:ILE:HD13	2:B:872:LYS:O	2.11	0.50
2:B:1089:GLN:HB3	2:B:1093:LEU:HD22	1.91	0.50
15:O:169:THR:O	15:O:170:VAL:C	2.54	0.50
15:O:378:THR:O	15:O:379:ARG:NH1	2.44	0.50
16:P:253:SER:HA	16:P:261:VAL:HG11	1.94	0.50
16:P:603:ARG:O	16:P:607:VAL:HG23	2.12	0.50
17:Q:406:GLN:HE21	18:R:282:SER:C	2.18	0.50
1:A:408:LYS:CD	1:A:408:LYS:N	2.73	0.50
1:A:991:LYS:CA	1:A:994:GLU:HG3	2.39	0.50
15:O:190:ILE:HD13	15:O:190:ILE:C	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:240:ILE:HG23	15:O:332:LEU:CG	2.41	0.50
15:O:507:GLN:O	15:O:511:ILE:HG23	2.12	0.50
1:A:597:LYS:HD3	2:B:1082:HIS:N	2.27	0.50
1:A:991:LYS:N	1:A:994:GLU:N	2.58	0.50
1:A:1025:LYS:NZ	2:B:1076:ARG:HH12	2.09	0.50
2:B:202:LEU:H	2:B:202:LEU:CD2	2.13	0.50
15:O:216:LEU:HD13	15:O:342:HIS:CB	2.41	0.50
15:O:591:TYR:HE2	15:O:593:PRO:HG3	1.77	0.50
16:P:656:HIS:CE1	16:P:748:GLU:HG3	2.47	0.50
16:P:767:PRO:O	16:P:771:ILE:HG12	2.11	0.50
16:P:770:ASP:HB2	17:Q:145:ASN:CG	2.36	0.50
17:Q:10:CYS:SG	17:Q:29:CYS:SG	3.07	0.50
17:Q:303:GLU:O	17:Q:306:VAL:N	2.44	0.50
17:Q:355:VAL:HB	18:R:212:HIS:HE1	1.75	0.50
17:Q:414:TYR:CE2	17:Q:419:LEU:HB3	2.45	0.50
1:A:435:ASN:CA	1:A:442:LYS:HB2	2.42	0.50
1:A:827:THR:CG2	1:A:924:SER:CB	2.90	0.50
1:A:970:LYS:HG2	1:A:973:GLU:HG2	1.92	0.50
1:A:1484:LEU:HD22	2:B:305:ARG:HH21	1.76	0.50
2:B:293:ILE:HG12	2:B:306:LEU:HD13	1.94	0.50
2:B:1005:TYR:CE2	14:N:170:HIS:CD2	2.99	0.50
10:J:1:MET:HG2	10:J:57:ILE:HB	1.93	0.50
15:O:236:LYS:N	15:O:237:ILE:CD1	2.75	0.50
16:P:658:LYS:CB	16:P:660:LYS:H	2.24	0.50
17:Q:118:TRP:CZ2	17:Q:189:LYS:HB3	2.47	0.50
1:A:597:LYS:HD2	2:B:1082:HIS:CE1	2.47	0.50
2:B:943:ILE:CD1	10:J:44:TYR:CD1	2.93	0.50
3:C:272:LYS:CA	14:N:175:TYR:CE2	2.83	0.50
9:I:91:ASN:OD1	9:I:92:GLU:N	2.45	0.50
15:O:324:GLY:O	15:O:326:LYS:N	2.44	0.50
16:P:443:ASP:HB3	18:R:3:GLU:HB2	1.93	0.50
18:R:6:ILE:CG1	18:R:213:ILE:HG22	2.40	0.50
18:R:364:VAL:HA	18:R:367:ILE:HB	1.93	0.50
1:A:414:GLU:C	1:A:416:ARG:N	2.67	0.50
2:B:531:VAL:HG13	2:B:716:MET:CA	2.41	0.50
3:C:37:LYS:HG3	11:K:134:LYS:NZ	2.27	0.50
16:P:363:ILE:HG22	16:P:374:VAL:HG22	1.93	0.50
16:P:390:GLN:O	18:R:149:LYS:CB	2.56	0.50
16:P:498:LEU:HD23	16:P:499:GLU:H	1.75	0.50
18:R:85:ARG:HH11	18:R:85:ARG:HG2	1.77	0.50
1:A:486:PRO:O	2:B:781:TYR:HD2	1.85	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:ASP:CB	1:A:1468:LYS:HZ3	2.24	0.50
1:A:1323:HIS:N	1:A:1454:HIS:NE2	2.60	0.50
2:B:656:LEU:HD22	14:N:153:VAL:CG2	2.42	0.50
2:B:682:GLN:N	14:N:154:ARG:HH21	2.03	0.50
3:C:47:LEU:HD23	3:C:48:ASP:H	1.77	0.50
15:O:515:ASN:HD21	15:O:547:ASN:ND2	2.10	0.50
1:A:395:LEU:HD11	18:R:410:TYR:CE1	2.47	0.50
1:A:476:VAL:CG2	2:B:1070:ARG:H	2.05	0.50
1:A:1575:ILE:H	9:I:122:ARG:NH1	2.03	0.50
2:B:545:PHE:CE1	2:B:649:MET:SD	3.04	0.50
16:P:435:ARG:NH2	18:R:140:ILE:HD12	2.26	0.50
16:P:768:TYR:O	16:P:771:ILE:HB	2.12	0.50
17:Q:417:PHE:HZ	18:R:270:PHE:CB	2.25	0.50
1:A:425:ASN:HD22	18:R:405:ILE:HG21	1.71	0.49
2:B:225:ARG:NH2	2:B:261:ARG:HD3	2.27	0.49
2:B:262:PHE:CD1	2:B:357:ILE:HD13	2.47	0.49
15:O:248:LEU:HB2	15:O:598:PHE:CE2	2.47	0.49
16:P:194:ARG:NH2	16:P:208:GLY:HA3	2.27	0.49
16:P:274:ILE:HD13	16:P:305:PHE:HZ	1.76	0.49
16:P:681:GLN:HA	16:P:684:GLN:HB2	1.93	0.49
17:Q:413:LEU:HA	17:Q:416:ILE:HD12	1.94	0.49
18:R:231:LEU:O	18:R:235:ILE:HG12	2.12	0.49
1:A:544:VAL:CG1	17:Q:32:GLY:O	2.57	0.49
2:B:535:ASP:N	2:B:720:GLN:OE1	2.43	0.49
2:B:679:GLN:NE2	14:N:155:VAL:O	2.45	0.49
2:B:1090:ASP:OD1	2:B:1094:ASN:ND2	2.43	0.49
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.47	0.49
16:P:441:ASP:HA	16:P:442:LEU:HD13	1.94	0.49
16:P:489:PHE:CD2	18:R:138:PHE:HZ	2.29	0.49
17:Q:188:ALA:O	17:Q:384:GLN:HG3	2.11	0.49
18:R:372:HIS:CD2	18:R:410:TYR:HB3	2.47	0.49
1:A:437:PHE:HA	1:A:455:GLY:HA3	1.93	0.49
1:A:467:PHE:CD2	1:A:1614:SER:HB3	2.46	0.49
1:A:689:ARG:HD2	8:H:79:TRP:HZ3	1.76	0.49
2:B:74:PHE:C	2:B:440:PHE:HE2	2.20	0.49
6:F:72:LYS:HD3	6:F:142:SER:CB	2.28	0.49
17:Q:137:TRP:O	17:Q:141:LEU:HB2	2.12	0.49
18:R:361:ASP:HB3	18:R:364:VAL:HG13	1.94	0.49
1:A:408:LYS:N	1:A:408:LYS:CE	2.75	0.49
1:A:720:PHE:CE1	8:H:98:TYR:HB2	2.47	0.49
1:A:966:LEU:HD21	1:A:997:PHE:CZ	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	1.93	0.49
2:B:243:GLN:CD	2:B:646:HIS:HE2	2.20	0.49
2:B:550:ARG:HG2	2:B:650:LEU:O	2.12	0.49
15:O:518:LYS:NZ	15:O:575:SER:HB2	2.27	0.49
16:P:22:GLY:HA3	18:R:139:GLU:OE2	2.05	0.49
16:P:365:TRP:CB	16:P:372:ILE:HA	2.42	0.49
17:Q:188:ALA:HB1	17:Q:384:GLN:CG	2.20	0.49
1:A:507:TYR:HE1	1:A:510:PRO:HD3	1.77	0.49
1:A:828:CYS:SG	2:B:1027:TYR:HB2	2.53	0.49
1:A:1085:LEU:HD22	6:F:84:TYR:HH	1.75	0.49
2:B:29:PRO:O	2:B:177:PRO:HB2	2.11	0.49
2:B:149:GLU:CD	2:B:441:LYS:HZ1	2.15	0.49
6:F:73:ALA:CA	6:F:143:PHE:O	2.56	0.49
15:O:376:TYR:CB	15:O:419:LYS:HD3	2.43	0.49
15:O:379:ARG:NH1	15:O:379:ARG:CA	2.73	0.49
16:P:599:LYS:HG2	17:Q:272:GLN:OE1	2.13	0.49
17:Q:417:PHE:CE2	18:R:253:ILE:HD13	2.47	0.49
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.93	0.49
1:A:1658:ALA:CA	6:F:131:PRO:O	2.58	0.49
2:B:25:PHE:CG	10:J:59:LYS:CG	2.96	0.49
2:B:743:ARG:CZ	10:J:60:PHE:HZ	2.23	0.49
2:B:1073:GLU:HA	2:B:1076:ARG:HB2	1.95	0.49
3:C:58:ASN:N	3:C:296:ASN:ND2	2.58	0.49
3:C:117:ASP:OD1	3:C:119:ASN:ND2	2.44	0.49
13:M:103:LYS:HA	13:M:106:LYS:HB2	1.93	0.49
15:O:248:LEU:CG	15:O:598:PHE:CD2	2.90	0.49
15:O:428:ILE:CD1	15:O:442:VAL:HG21	2.42	0.49
15:O:436:ARG:HG3	15:O:490:ILE:HG23	1.95	0.49
16:P:225:LEU:HD11	16:P:235:SER:HB3	1.93	0.49
16:P:446:ASP:OD2	16:P:448:THR:N	2.40	0.49
18:R:177:LEU:CD2	18:R:185:LYS:HA	2.43	0.49
1:A:410:LYS:CB	1:A:411:VAL:HG23	2.43	0.49
1:A:425:ASN:ND2	18:R:406:LYS:HZ3	2.09	0.49
1:A:514:TYR:O	6:F:115:THR:HG22	2.12	0.49
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.93	0.49
13:M:65:TYR:CE1	13:M:97:VAL:HB	2.48	0.49
15:O:474:TYR:HB3	15:O:520:CYS:SG	2.53	0.49
16:P:49:THR:O	16:P:49:THR:OG1	2.27	0.49
17:Q:10:CYS:HB3	17:Q:16:PRO:HA	1.93	0.49
1:A:629:ASP:O	2:B:926:VAL:CG2	2.55	0.49
2:B:30:LYS:O	2:B:176:SER:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ILE:CG1	2:B:503:VAL:HG22	2.13	0.49
2:B:679:GLN:OE1	14:N:157:ARG:CB	2.61	0.49
3:C:230:LEU:HD22	3:C:297:HIS:NE2	2.28	0.49
8:H:112:ILE:HD12	8:H:129:TYR:HB2	1.94	0.49
16:P:197:ARG:HD2	16:P:260:LEU:C	2.38	0.49
16:P:480:VAL:HB	16:P:492:LEU:CD2	2.40	0.49
1:A:509:GLU:CG	1:A:579:ARG:HE	2.26	0.49
1:A:1055:ILE:HD11	1:A:1174:TYR:CE1	2.48	0.49
1:A:1317:ILE:HB	1:A:1460:TYR:OH	2.13	0.49
2:B:202:LEU:CD1	2:B:499:HIS:HB3	2.40	0.49
2:B:1066:HIS:NE2	17:Q:23:ILE:HD13	2.27	0.49
7:G:24:VAL:O	7:G:128:GLN:HB3	2.04	0.49
15:O:208:LEU:O	15:O:212:THR:HG23	2.12	0.49
16:P:499:GLU:OE1	16:P:499:GLU:HA	2.13	0.49
16:P:757:GLN:HE21	16:P:758:ASN:N	2.10	0.49
17:Q:108:PHE:CZ	17:Q:156:LEU:HD22	2.47	0.49
17:Q:161:THR:OG1	17:Q:162:ILE:N	2.46	0.49
1:A:563:THR:HG22	15:O:375:THR:CG2	2.42	0.49
1:A:670:ILE:CD1	2:B:783:MET:HE2	2.42	0.49
1:A:671:GLN:HB3	2:B:952:HIS:CE1	2.48	0.49
2:B:62:ASN:OD1	2:B:102:VAL:CG2	2.60	0.49
2:B:143:TRP:CZ2	2:B:446:MET:HG3	2.47	0.49
2:B:162:PRO:HG2	2:B:465:LEU:HD12	1.95	0.49
2:B:338:PHE:CE1	2:B:353:VAL:HG22	2.47	0.49
6:F:66:ARG:HH22	7:G:90:LEU:HB3	1.77	0.49
15:O:336:LEU:HD13	15:O:602:TYR:CE1	2.48	0.49
16:P:197:ARG:HD2	16:P:261:VAL:O	2.12	0.49
16:P:226:HIS:CE1	16:P:234:THR:HG22	2.48	0.49
18:R:361:ASP:O	18:R:363:GLU:N	2.40	0.49
1:A:477:ASN:C	2:B:1049:THR:HA	2.38	0.48
2:B:203:ILE:HG22	2:B:405:GLY:CA	2.42	0.48
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.94	0.48
16:P:420:GLU:HG2	16:P:441:ASP:HB2	1.95	0.48
17:Q:152:LEU:HD12	17:Q:154:LEU:HD11	1.95	0.48
17:Q:414:TYR:HE2	17:Q:419:LEU:HB3	1.78	0.48
1:A:563:THR:HG22	15:O:375:THR:HG22	1.95	0.48
1:A:1657:LEU:CD2	7:G:104:LEU:HB3	2.38	0.48
2:B:68:ILE:HD13	2:B:71:LYS:NZ	2.29	0.48
10:J:6:ARG:HD2	10:J:11:GLY:O	2.13	0.48
15:O:361:PHE:CE2	15:O:365:THR:HG21	2.48	0.48
16:P:59:ILE:HG22	16:P:60:VAL:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:206:ARG:N	18:R:206:ARG:NE	2.60	0.48
1:A:68:ASP:O	1:A:70:LYS:N	2.46	0.48
1:A:597:LYS:HB3	2:B:1082:HIS:CD2	2.42	0.48
2:B:25:PHE:CE2	10:J:59:LYS:HG3	2.48	0.48
16:P:264:ILE:HG12	16:P:265:THR:N	2.27	0.48
16:P:443:ASP:CB	18:R:3:GLU:CB	2.90	0.48
17:Q:7:GLY:HA3	17:Q:8:PRO:HD2	1.44	0.48
18:R:273:TRP:CZ3	18:R:274:MET:HE2	2.48	0.48
1:A:472:MET:CA	1:A:472:MET:CE	2.86	0.48
1:A:747:ILE:HD13	1:A:748:ASN:H	1.77	0.48
1:A:1200:MET:HE1	1:A:1569:VAL:HG12	1.95	0.48
3:C:326:GLU:CG	11:K:125:MET:HE3	2.43	0.48
15:O:198:PHE:CZ	15:O:236:LYS:HG3	2.48	0.48
16:P:21:GLN:HB2	18:R:139:GLU:CD	2.38	0.48
1:A:472:MET:HG3	2:B:1073:GLU:CD	2.34	0.48
1:A:1053:ASP:C	1:A:1055:ILE:HG12	2.36	0.48
2:B:211:ARG:NH2	2:B:646:HIS:O	2.47	0.48
2:B:1092:LEU:C	2:B:1096:SER:HB2	2.37	0.48
15:O:581:THR:HA	15:O:584:GLN:CD	2.38	0.48
16:P:733:THR:HA	16:P:736:ILE:HG22	1.95	0.48
18:R:186:LEU:C	18:R:186:LEU:CD1	2.86	0.48
1:A:1329:ILE:HG21	1:A:1456:PHE:CD2	2.40	0.48
5:E:48:ASP:OD1	5:E:50:MET:HB3	2.13	0.48
7:G:158:LYS:CB	15:O:105:ASN:OD1	2.61	0.48
15:O:181:ARG:CG	15:O:181:ARG:NH1	2.77	0.48
15:O:224:GLU:H	15:O:224:GLU:CD	2.17	0.48
16:P:186:TYR:OH	18:R:196:GLU:OE1	2.29	0.48
2:B:212:ASN:CG	2:B:361:HIS:CG	2.92	0.48
3:C:293:ARG:O	3:C:295:ARG:HD3	2.14	0.48
6:F:70:LYS:CG	7:G:95:LEU:CD2	2.90	0.48
16:P:315:PHE:HB2	16:P:365:TRP:HH2	1.78	0.48
16:P:399:TRP:HZ3	18:R:291:ARG:O	1.92	0.48
16:P:476:ILE:HD12	16:P:508:ILE:HD11	1.96	0.48
16:P:762:ARG:HG3	17:Q:139:LYS:HE3	1.95	0.48
1:A:478:TYR:CE1	2:B:1049:THR:HB	2.49	0.48
1:A:826:PHE:CE1	2:B:777:SER:OG	2.66	0.48
1:A:869:PRO:HG2	1:A:872:ASP:HB2	1.96	0.48
1:A:1162:ASN:ND2	1:A:1165:LYS:HG3	2.29	0.48
1:A:1297:PHE:HD2	9:I:60:LEU:HD13	1.75	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.13	0.48
1:A:1322:ILE:CB	1:A:1454:HIS:CD2	2.85	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:VAL:HG21	5:E:142:VAL:CG2	2.43	0.48
2:B:28:PRO:CD	10:J:62:ARG:NE	2.76	0.48
2:B:1047:ARG:HD3	2:B:1049:THR:O	2.14	0.48
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.62	0.48
5:E:131:THR:HG21	5:E:191:LYS:CE	2.44	0.48
7:G:23:GLN:O	7:G:25:THR:N	2.46	0.48
7:G:137:ILE:HG13	7:G:227:GLY:O	2.13	0.48
7:G:139:ILE:HD13	15:O:145:SER:OG	2.14	0.48
15:O:199:PRO:HB2	15:O:208:LEU:HD23	1.95	0.48
15:O:521:ASN:O	15:O:525:MET:HG2	2.12	0.48
16:P:277:VAL:HG23	16:P:286:VAL:HG12	1.95	0.48
1:A:19:LEU:HD11	2:B:1190:SER:HB2	1.96	0.48
1:A:410:LYS:CB	1:A:411:VAL:CG2	2.91	0.48
1:A:505:LEU:O	1:A:580:HIS:HA	2.14	0.48
1:A:826:PHE:CD2	1:A:827:THR:N	2.82	0.48
1:A:934:LYS:HG2	2:B:955:PRO:HG2	1.96	0.48
2:B:54:GLU:HG3	2:B:168:ASN:ND2	2.29	0.48
2:B:202:LEU:N	2:B:202:LEU:CD2	2.76	0.48
2:B:413:LEU:O	2:B:417:ILE:HG13	2.14	0.48
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.95	0.48
5:E:54:GLN:HB2	5:E:57:MET:HE2	1.95	0.48
15:O:342:HIS:HE1	15:O:346:GLN:HE21	1.58	0.48
15:O:477:PHE:CE2	15:O:481:CYS:SG	3.07	0.48
18:R:9:THR:O	18:R:13:PHE:HD2	1.97	0.48
18:R:273:TRP:HZ3	18:R:274:MET:HE2	1.78	0.48
1:A:1603:MET:SD	1:A:1612:LYS:HA	2.54	0.48
2:B:1005:TYR:CE2	14:N:170:HIS:ND1	2.82	0.48
3:C:239:ILE:HG23	3:C:243:SER:HB3	1.96	0.48
16:P:290:GLU:HG3	16:P:291:PRO:O	2.14	0.48
16:P:300:LEU:HA	16:P:320:ILE:HG22	1.96	0.48
16:P:427:SER:HA	16:P:433:VAL:HB	1.95	0.48
16:P:770:ASP:HB2	17:Q:145:ASN:OD1	2.14	0.48
1:A:1260:LYS:CE	1:A:1262:LEU:HD21	2.44	0.47
2:B:475:GLY:O	2:B:476:LEU:CB	2.59	0.47
6:F:73:ALA:CA	6:F:143:PHE:CG	2.91	0.47
15:O:518:LYS:HZ3	15:O:575:SER:HB2	1.77	0.47
18:R:4:VAL:HG21	18:R:214:VAL:CB	2.40	0.47
1:A:477:ASN:HA	2:B:1047:ARG:CD	2.42	0.47
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.95	0.47
1:A:999:CYS:SG	2:B:712:SER:HB3	2.54	0.47
1:A:1050:TYR:HB3	1:A:1054:ALA:CA	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:ASP:O	1:A:1300:ASN:N	2.47	0.47
2:B:152:LEU:HD22	2:B:443:LYS:CE	2.43	0.47
12:L:45:ALA:O	12:L:47:ARG:N	2.46	0.47
13:M:102:SER:C	13:M:105:SER:CB	2.72	0.47
15:O:48:SER:O	15:O:49:ALA:C	2.57	0.47
16:P:333:PHE:CD2	16:P:334:ASN:HB2	2.49	0.47
1:A:718:THR:HG21	8:H:118:PHE:O	2.14	0.47
1:A:1604:GLU:CD	1:A:1621:PHE:HE1	2.21	0.47
2:B:53:THR:HG21	2:B:104:ILE:HD12	1.95	0.47
2:B:1090:ASP:CA	2:B:1093:LEU:HB3	2.36	0.47
14:N:111:VAL:HG13	14:N:122:ALA:HB2	1.96	0.47
15:O:386:PHE:HB2	15:O:594:TYR:CE2	2.49	0.47
16:P:257:ARG:HG3	16:P:411:LYS:HZ1	1.78	0.47
17:Q:22:ILE:HD11	17:Q:26:ARG:CG	2.44	0.47
18:R:15:GLN:OE1	18:R:181:THR:HG23	2.14	0.47
18:R:82:ARG:HD2	18:R:82:ARG:O	2.14	0.47
18:R:162:PHE:HA	18:R:165:ILE:HD12	1.95	0.47
1:A:641:GLU:HB2	6:F:99:LEU:CD1	2.44	0.47
1:A:862:THR:O	9:I:67:VAL:HA	2.14	0.47
1:A:991:LYS:HA	1:A:992:PRO:N	2.29	0.47
2:B:415:GLU:OE2	2:B:472:SER:HB2	2.13	0.47
2:B:1005:TYR:HH	10:J:44:TYR:HD2	1.52	0.47
16:P:185:GLN:HE22	18:R:197:PRO:HB3	1.78	0.47
16:P:227:LEU:HD13	16:P:227:LEU:H	1.78	0.47
17:Q:287:TRP:CE2	17:Q:289:ARG:HB3	2.50	0.47
18:R:11:ARG:H	18:R:11:ARG:HG3	1.53	0.47
1:A:456:VAL:HG13	2:B:1188:GLU:OE1	2.14	0.47
1:A:508:PRO:HD2	1:A:639:GLN:HG3	1.95	0.47
1:A:999:CYS:N	2:B:712:SER:HB3	2.28	0.47
2:B:975:HIS:CE1	14:N:169:GLU:HG3	2.49	0.47
2:B:1151:ILE:HG12	7:G:21:LYS:HZ3	1.77	0.47
13:M:102:SER:CA	13:M:105:SER:H	2.28	0.47
15:O:124:LYS:HD3	15:O:127:GLU:OE2	2.13	0.47
15:O:245:GLN:O	15:O:248:LEU:N	2.40	0.47
15:O:383:TYR:HB3	15:O:606:MET:HE3	1.96	0.47
16:P:68:THR:HG23	16:P:214:LEU:HA	1.95	0.47
17:Q:250:GLN:OE1	17:Q:271:LYS:HD2	2.15	0.47
18:R:361:ASP:C	18:R:363:GLU:N	2.73	0.47
1:A:425:ASN:HD21	18:R:406:LYS:NZ	2.11	0.47
1:A:454:PRO:HG2	1:A:462:LYS:HZ2	1.79	0.47
1:A:486:PRO:CD	2:B:928:SER:OG	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HD13	1:A:748:ASN:N	2.29	0.47
1:A:1574:ALA:HB1	9:I:121:PHE:HA	1.95	0.47
3:C:222:VAL:C	3:C:224:THR:H	2.20	0.47
4:D:46:GLU:OE1	4:D:47:LYS:HE2	2.15	0.47
15:O:66:ASN:CG	15:O:111:ARG:NH1	2.72	0.47
15:O:376:TYR:CD1	15:O:419:LYS:HG2	2.49	0.47
16:P:390:GLN:C	18:R:149:LYS:HB3	2.38	0.47
17:Q:356:VAL:CB	18:R:208:TYR:HD1	2.27	0.47
1:A:410:LYS:HB3	1:A:411:VAL:HG22	1.96	0.47
1:A:436:ALA:HA	1:A:440:SER:CA	2.44	0.47
1:A:476:VAL:HG11	2:B:1071:VAL:HG23	1.96	0.47
1:A:507:TYR:CD1	1:A:509:GLU:HG2	2.50	0.47
1:A:720:PHE:N	8:H:96:VAL:O	2.46	0.47
1:A:1049:MET:HG3	1:A:1053:ASP:H	1.76	0.47
1:A:1317:ILE:CG2	1:A:1460:TYR:CZ	2.96	0.47
2:B:182:GLN:HE22	10:J:69:ARG:CB	2.08	0.47
2:B:208:VAL:CG2	2:B:401:GLU:CG	2.92	0.47
2:B:338:PHE:CZ	2:B:357:ILE:HD12	2.49	0.47
2:B:1047:ARG:CD	2:B:1049:THR:O	2.60	0.47
3:C:247:PHE:HE1	3:C:289:VAL:HG21	1.80	0.47
6:F:93:ILE:HA	6:F:93:ILE:HD13	1.70	0.47
7:G:144:HIS:HB3	15:O:146:SER:HB3	1.97	0.47
15:O:206:ARG:HA	15:O:209:VAL:CG1	2.45	0.47
15:O:376:TYR:CE2	15:O:419:LYS:HE2	2.50	0.47
16:P:388:ASN:HB3	18:R:151:PRO:HB3	1.97	0.47
16:P:422:ILE:HG12	16:P:442:LEU:HD11	1.96	0.47
16:P:443:ASP:CB	18:R:3:GLU:HB3	2.43	0.47
18:R:198:LEU:HD12	18:R:199:LYS:HB2	1.95	0.47
1:A:1484:LEU:HD11	2:B:305:ARG:HD3	1.97	0.47
2:B:470:LEU:HD21	2:B:476:LEU:HD12	1.97	0.47
2:B:841:ASP:OD1	2:B:842:GLU:N	2.40	0.47
3:C:292:GLY:CA	3:C:295:ARG:HH22	2.27	0.47
7:G:156:SER:OG	15:O:146:SER:HA	2.13	0.47
15:O:91:LYS:HG3	15:O:92:ASN:N	2.28	0.47
16:P:56:ASP:OD1	16:P:554:ASN:ND2	2.48	0.47
16:P:381:ILE:HA	16:P:391:THR:O	2.14	0.47
16:P:421:ILE:CG2	16:P:423:ILE:HG13	2.44	0.47
17:Q:165:LEU:HD13	17:Q:190:MET:HE1	1.95	0.47
17:Q:371:GLU:HG3	18:R:231:LEU:CG	2.45	0.47
1:A:407:GLN:C	1:A:409:ASP:H	2.23	0.47
1:A:1032:VAL:HG22	1:A:1050:TYR:HD1	1.75	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.97	0.47
2:B:551:ILE:CG2	2:B:647:SER:C	2.87	0.47
4:D:33:THR:HG23	4:D:96:PHE:HD1	1.80	0.47
16:P:290:GLU:OE2	16:P:291:PRO:HD2	2.15	0.47
17:Q:414:TYR:CE1	18:R:240:ILE:HG23	2.44	0.47
17:Q:417:PHE:CZ	18:R:270:PHE:HB2	2.47	0.47
1:A:990:ILE:CB	1:A:994:GLU:HB3	2.07	0.47
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.15	0.47
6:F:69:LEU:HG	6:F:143:PHE:HE2	1.80	0.47
15:O:240:ILE:CG2	15:O:332:LEU:CD1	2.93	0.47
15:O:243:GLU:HG2	15:O:332:LEU:HB2	1.97	0.47
16:P:330:PRO:HG3	16:P:342:GLN:CG	2.45	0.47
17:Q:193:PHE:HE2	18:R:208:TYR:CZ	2.32	0.47
17:Q:197:GLU:HG3	17:Q:388:THR:O	2.14	0.47
1:A:721:LYS:HB3	8:H:96:VAL:CB	2.40	0.46
1:A:1482:LYS:HD3	2:B:304:ASP:HA	1.97	0.46
1:A:1655:ASP:CB	6:F:135:ARG:HB3	2.38	0.46
2:B:1103:VAL:HG22	2:B:1176:VAL:HG22	1.97	0.46
16:P:272:PHE:HB2	16:P:300:LEU:HD11	1.97	0.46
16:P:626:LEU:HD22	16:P:626:LEU:HA	1.59	0.46
17:Q:235:GLY:HA3	17:Q:287:TRP:CD1	2.50	0.46
18:R:30:ARG:NE	18:R:168:ILE:HD12	2.30	0.46
1:A:407:GLN:C	1:A:408:LYS:NZ	2.73	0.46
2:B:265:ARG:NH2	2:B:339:GLN:OE1	2.48	0.46
2:B:407:PHE:HE2	2:B:647:SER:OG	1.98	0.46
2:B:448:ARG:HA	2:B:451:MET:HE3	1.97	0.46
2:B:812:ALA:HA	2:B:815:ARG:HD3	1.96	0.46
2:B:848:ILE:CA	12:L:60:ARG:CD	2.72	0.46
2:B:943:ILE:HD13	10:J:44:TYR:CE1	2.47	0.46
15:O:409:ALA:HB3	15:O:412:GLU:HG3	1.97	0.46
16:P:350:THR:CG2	18:R:153:ASN:CG	2.88	0.46
16:P:438:TRP:HE1	18:R:297:PHE:HZ	1.63	0.46
16:P:443:ASP:OD2	18:R:3:GLU:OE2	2.33	0.46
16:P:704:LEU:HD23	17:Q:258:MET:HE1	1.96	0.46
18:R:6:ILE:CG1	18:R:213:ILE:CG2	2.93	0.46
18:R:402:ASN:O	18:R:406:LYS:HG2	2.15	0.46
1:A:474:LYS:NZ	2:B:1096:SER:HB2	2.30	0.46
1:A:1440:ASN:HA	1:A:1443:GLN:HB2	1.96	0.46
2:B:397:THR:HA	2:B:400:GLN:OE1	2.14	0.46
2:B:549:CYS:SG	2:B:649:MET:CB	3.03	0.46
6:F:72:LYS:CG	6:F:142:SER:CA	2.91	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:468:GLU:O	15:O:470:PHE:N	2.49	0.46
16:P:366:PHE:HE2	16:P:433:VAL:H	1.64	0.46
16:P:437:SER:CB	18:R:140:ILE:HD13	2.45	0.46
17:Q:9:ILE:CG1	17:Q:10:CYS:N	2.50	0.46
17:Q:274:ILE:HG23	17:Q:282:ARG:NH2	2.29	0.46
17:Q:309:TYR:O	17:Q:313:THR:OG1	2.20	0.46
18:R:257:ILE:HG21	18:R:266:SER:HA	1.96	0.46
1:A:472:MET:CB	2:B:1073:GLU:OE1	2.64	0.46
1:A:986:PHE:HD2	2:B:958:MET:HE2	1.75	0.46
2:B:890:ASP:HB3	2:B:896:GLN:OE1	2.16	0.46
5:E:67:GLU:CD	5:E:67:GLU:H	2.23	0.46
5:E:93:MET:CG	5:E:120:ALA:HB1	2.46	0.46
11:K:55:SER:OG	11:K:57:ASP:OD1	2.28	0.46
15:O:521:ASN:HD22	15:O:524:VAL:H	1.63	0.46
16:P:350:THR:HG23	18:R:153:ASN:CG	2.40	0.46
16:P:408:ILE:HD12	16:P:464:LEU:HD13	1.97	0.46
16:P:770:ASP:OD2	17:Q:141:LEU:HG	2.15	0.46
17:Q:250:GLN:HB3	17:Q:267:TYR:OH	2.15	0.46
18:R:199:LYS:NZ	18:R:204:GLU:CA	2.62	0.46
1:A:475:ARG:HD3	2:B:1060:VAL:O	2.16	0.46
1:A:720:PHE:HB2	8:H:96:VAL:HG12	1.97	0.46
2:B:894:LYS:CG	12:L:47:ARG:CD	2.94	0.46
15:O:240:ILE:HG22	15:O:332:LEU:HD11	1.96	0.46
15:O:390:GLN:NE2	15:O:433:LYS:H	2.13	0.46
16:P:187:ILE:CG2	18:R:195:LEU:CD2	2.92	0.46
16:P:438:TRP:CG	18:R:141:TRP:HZ2	2.30	0.46
18:R:222:LEU:HD23	18:R:226:ARG:NH2	2.31	0.46
1:A:589:MET:HE1	1:A:614:LEU:HD13	1.98	0.46
1:A:1118:VAL:CG1	5:E:199:ILE:HG13	2.44	0.46
2:B:401:GLU:C	2:B:402:VAL:HG23	2.41	0.46
2:B:774:ALA:HB1	2:B:1026:ILE:HD11	1.97	0.46
2:B:990:ASP:OD2	14:N:159:ASP:HB3	2.16	0.46
6:F:70:LYS:HD2	7:G:94:PRO:HB2	1.45	0.46
9:I:23:VAL:O	9:I:39:LYS:NZ	2.49	0.46
11:K:49:LEU:HG	11:K:54:THR:HG21	1.98	0.46
15:O:234:ILE:HG21	15:O:367:LEU:HB3	1.96	0.46
15:O:407:SER:HB3	15:O:420:SER:HB2	1.96	0.46
16:P:265:THR:HG1	16:P:305:PHE:HE1	1.61	0.46
16:P:389:TRP:HH2	18:R:148:ASN:HA	1.77	0.46
16:P:428:GLU:O	18:R:142:ARG:NH1	2.46	0.46
16:P:444:PRO:CG	16:P:449:LEU:HD11	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:22:ILE:HD13	17:Q:26:ARG:CZ	2.45	0.46
18:R:177:LEU:HD21	18:R:185:LYS:HA	1.98	0.46
1:A:258:GLU:HA	1:A:261:ILE:HD12	1.96	0.46
2:B:25:PHE:CG	10:J:59:LYS:HG2	2.51	0.46
2:B:49:PHE:CD2	2:B:164:MET:HE3	2.51	0.46
6:F:74:ILE:N	7:G:95:LEU:HD11	2.30	0.46
15:O:93:LEU:HD23	15:O:132:THR:CG2	2.46	0.46
16:P:321:LYS:HB2	16:P:321:LYS:NZ	2.31	0.46
16:P:574:TRP:CH2	17:Q:495:LYS:HD2	2.51	0.46
17:Q:358:PRO:O	18:R:206:ARG:NH1	2.49	0.46
1:A:68:ASP:C	1:A:70:LYS:H	2.24	0.46
1:A:1484:LEU:CD2	2:B:304:ASP:HB2	2.46	0.46
2:B:427:GLN:HA	2:B:430:MET:HE3	1.98	0.46
2:B:679:GLN:OE1	14:N:157:ARG:CA	2.63	0.46
2:B:848:ILE:CG1	12:L:60:ARG:HD2	2.36	0.46
3:C:71:MET:HE1	3:C:302:VAL:HG21	1.97	0.46
3:C:176:SER:O	3:C:180:ALA:HB2	2.16	0.46
3:C:293:ARG:O	3:C:295:ARG:CD	2.64	0.46
16:P:54:ALA:HA	16:P:55:LEU:HD12	1.98	0.46
16:P:56:ASP:O	16:P:57:LEU:HD13	2.16	0.46
16:P:197:ARG:CD	16:P:261:VAL:O	2.64	0.46
16:P:417:THR:OG1	16:P:451:ILE:HB	2.16	0.46
17:Q:351:ASN:ND2	17:Q:369:TRP:CE2	2.83	0.46
18:R:323:SER:OG	18:R:324:MET:N	2.46	0.46
1:A:406:LEU:CB	1:A:408:LYS:HZ2	2.27	0.46
1:A:1574:ALA:HB3	9:I:122:ARG:HG2	1.97	0.46
2:B:292:ILE:HB	2:B:306:LEU:HD11	1.98	0.46
2:B:679:GLN:HG2	14:N:156:PRO:CA	2.33	0.46
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.97	0.46
2:B:1049:THR:CG2	2:B:1050:GLY:N	2.63	0.46
10:J:36:LEU:HD13	10:J:47:ARG:HB3	1.98	0.46
15:O:74:ILE:O	15:O:78:VAL:HG13	2.16	0.46
16:P:197:ARG:CB	16:P:261:VAL:O	2.63	0.46
16:P:254:ILE:HG21	16:P:368:HIS:CE1	2.50	0.46
16:P:326:ILE:HG21	16:P:385:PHE:CE1	2.51	0.46
17:Q:137:TRP:CH2	17:Q:141:LEU:HD13	2.51	0.46
17:Q:311:MET:HE3	17:Q:311:MET:HB3	1.89	0.46
18:R:365:TRP:HB3	18:R:418:CYS:HB2	1.98	0.46
1:A:407:GLN:C	1:A:409:ASP:N	2.74	0.46
1:A:582:LYS:O	1:A:585:ASP:HB2	2.16	0.46
1:A:1049:MET:CB	1:A:1052:GLY:N	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ILE:CD1	2:B:302:LEU:HB3	2.46	0.46
2:B:822:THR:HB	2:B:823:GLN:HG3	1.98	0.46
9:I:89:CYS:SG	9:I:91:ASN:HB2	2.56	0.46
15:O:245:GLN:NE2	15:O:379:ARG:CB	2.74	0.46
15:O:388:VAL:HG13	15:O:389:SER:N	2.31	0.46
16:P:350:THR:HB	18:R:155:GLN:HA	1.98	0.46
17:Q:109:GLN:CD	17:Q:137:TRP:HE1	2.24	0.46
17:Q:193:PHE:HD2	18:R:208:TYR:CE2	2.31	0.46
1:A:1237:GLN:H	1:A:1544:ASN:HB2	1.81	0.45
2:B:119:ARG:CZ	12:L:53:HIS:NE2	2.79	0.45
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.51	0.45
3:C:228:ARG:HH22	14:N:175:TYR:HE2	1.62	0.45
6:F:70:LYS:CE	7:G:95:LEU:CD2	2.82	0.45
16:P:580:ASN:HB2	17:Q:506:LYS:HE2	1.98	0.45
17:Q:375:LEU:HD21	18:R:231:LEU:HD23	1.98	0.45
18:R:236:PHE:CZ	18:R:253:ILE:HB	2.51	0.45
1:A:476:VAL:N	2:B:1059:PRO:HG2	2.31	0.45
1:A:489:ASN:CB	11:K:95:HIS:HD2	2.29	0.45
1:A:1053:ASP:O	1:A:1055:ILE:CG1	2.55	0.45
3:C:58:ASN:C	3:C:296:ASN:ND2	2.72	0.45
3:C:228:ARG:CD	14:N:173:THR:OG1	2.64	0.45
15:O:69:THR:HG22	15:O:70:GLN:N	2.31	0.45
16:P:224:THR:HG21	16:P:237:GLU:HA	1.99	0.45
18:R:312:TYR:O	18:R:316:SER:OG	2.22	0.45
1:A:466:LEU:HD21	2:B:1181:VAL:HG22	1.98	0.45
1:A:514:TYR:CD1	6:F:115:THR:O	2.70	0.45
2:B:54:GLU:OE2	2:B:168:ASN:ND2	2.46	0.45
2:B:1047:ARG:HG2	2:B:1049:THR:H	1.81	0.45
3:C:228:ARG:HG3	3:C:299:ILE:HB	1.98	0.45
16:P:296:GLU:HB3	16:P:298:ASP:OD1	2.16	0.45
16:P:408:ILE:HG23	16:P:413:GLY:C	2.41	0.45
17:Q:193:PHE:HA	17:Q:219:ILE:HD11	1.97	0.45
17:Q:356:VAL:HG21	18:R:208:TYR:CE1	2.51	0.45
17:Q:359:ASP:OD2	17:Q:359:ASP:N	2.47	0.45
17:Q:378:LEU:HD11	18:R:235:ILE:HD13	1.96	0.45
17:Q:416:ILE:HD13	18:R:273:TRP:CD1	2.50	0.45
18:R:1:MET:HG3	18:R:2:PHE:CD1	2.51	0.45
18:R:23:TYR:HA	18:R:173:MET:HE3	1.99	0.45
1:A:184:LYS:HA	1:A:187:GLU:HG2	1.98	0.45
1:A:403:LEU:HD13	1:A:419:ILE:HG23	1.98	0.45
1:A:535:GLN:HE22	17:Q:26:ARG:HG2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:VAL:HG23	7:G:103:LYS:H	1.82	0.45
2:B:203:ILE:CB	2:B:405:GLY:HA3	2.46	0.45
2:B:697:LEU:CB	2:B:702:ASN:CG	2.85	0.45
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.98	0.45
5:E:7:ARG:O	5:E:11:ARG:HG3	2.17	0.45
15:O:578:SER:O	15:O:579:LEU:CB	2.64	0.45
16:P:498:LEU:HD23	16:P:499:GLU:O	2.16	0.45
17:Q:104:PHE:HZ	17:Q:156:LEU:HB2	1.77	0.45
1:A:1603:MET:HE3	1:A:1603:MET:HB3	1.79	0.45
2:B:894:LYS:HA	12:L:54:ARG:HE	1.77	0.45
16:P:61:VAL:HB	16:P:551:ALA:HB3	1.97	0.45
16:P:198:ASP:OD1	16:P:204:ALA:HB1	2.17	0.45
16:P:428:GLU:HB2	16:P:435:ARG:NH1	2.30	0.45
1:A:474:LYS:NZ	2:B:1092:LEU:CA	2.67	0.45
1:A:1600:ARG:HB2	1:A:1616:GLU:OE2	2.17	0.45
16:P:24:SER:CB	18:R:318:ILE:CD1	2.89	0.45
16:P:196:TYR:HA	16:P:207:SER:O	2.16	0.45
16:P:198:ASP:OD1	16:P:204:ALA:CB	2.64	0.45
16:P:384:ASP:CB	16:P:389:TRP:HB3	2.43	0.45
16:P:728:GLN:HB3	16:P:731:LEU:HB3	1.97	0.45
17:Q:204:ARG:HG3	17:Q:205:ILE:HG13	1.99	0.45
17:Q:286:LEU:CD2	17:Q:300:ASN:HB3	2.47	0.45
1:A:719:ILE:HG12	8:H:97:MET:CG	2.40	0.45
2:B:1003:ALA:C	14:N:170:HIS:HB3	2.41	0.45
5:E:78:LEU:HD13	5:E:107:THR:HB	1.98	0.45
7:G:17:ILE:C	7:G:19:LYS:H	2.25	0.45
16:P:394:VAL:HG22	16:P:434:ARG:NH1	2.32	0.45
16:P:454:GLN:HE22	16:P:536:ASP:H	1.65	0.45
17:Q:153:LYS:HE2	17:Q:153:LYS:HB3	1.57	0.45
17:Q:310:PHE:O	17:Q:314:ILE:HG13	2.16	0.45
1:A:615:ARG:HH22	2:B:929:ARG:CG	2.14	0.45
2:B:145:VAL:CG2	2:B:440:PHE:O	2.65	0.45
2:B:679:GLN:OE1	14:N:157:ARG:HA	2.16	0.45
3:C:222:VAL:HB	3:C:224:THR:H	1.81	0.45
15:O:433:LYS:HZ2	15:O:609:TYR:HE1	1.63	0.45
16:P:189:THR:HB	16:P:247:ILE:HG23	1.98	0.45
16:P:246:LYS:HB3	16:P:246:LYS:HE3	1.59	0.45
16:P:252:GLU:OE1	16:P:253:SER:N	2.35	0.45
16:P:596:ILE:HD12	16:P:596:ILE:O	2.16	0.45
17:Q:123:MET:HE2	17:Q:184:TRP:CZ2	2.51	0.45
17:Q:435:GLN:H	17:Q:435:GLN:HG3	1.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:295:PRO:HB3	18:R:296:PRO:HD2	1.97	0.45
1:A:89:LEU:HD11	2:B:1192:MET:HB3	1.97	0.45
1:A:407:GLN:CB	1:A:409:ASP:N	2.73	0.45
1:A:653:THR:OG1	1:A:654:ASP:OD1	2.35	0.45
2:B:190:ILE:HG13	2:B:191:GLY:N	2.32	0.45
2:B:403:LEU:HD11	2:B:411:MET:HE3	1.99	0.45
2:B:548:LYS:O	2:B:550:ARG:NH1	2.50	0.45
13:M:65:TYR:HE1	13:M:97:VAL:HB	1.81	0.45
16:P:193:LEU:HD12	16:P:250:ALA:HA	1.99	0.45
17:Q:188:ALA:C	17:Q:384:GLN:CG	2.89	0.45
17:Q:385:PHE:CZ	18:R:209:ARG:HG3	2.52	0.45
1:A:545:SER:HB2	17:Q:34:VAL:HG21	0.50	0.45
1:A:581:ILE:CD1	1:A:637:PHE:CZ	2.97	0.45
16:P:21:GLN:O	16:P:25:LEU:HB2	2.17	0.45
16:P:198:ASP:N	16:P:206:ALA:HA	2.32	0.45
16:P:425:GLY:O	16:P:426:ALA:HB2	2.17	0.45
16:P:675:PHE:HZ	16:P:742:TRP:HZ3	1.61	0.45
1:A:474:LYS:HZ2	2:B:1096:SER:HB2	1.82	0.44
1:A:598:ALA:CB	1:A:601:MET:HE3	2.47	0.44
1:A:996:TYR:CE1	2:B:525:TRP:CE3	3.05	0.44
1:A:1154:LEU:O	1:A:1158:SER:HB2	2.17	0.44
1:A:1297:PHE:CD2	9:I:60:LEU:HD22	2.51	0.44
1:A:1574:ALA:HB3	9:I:122:ARG:HB3	1.99	0.44
1:A:1655:ASP:O	6:F:134:ILE:HA	2.17	0.44
2:B:45:HIS:CE1	2:B:205:MET:HE2	2.52	0.44
7:G:158:LYS:HB3	15:O:105:ASN:CG	2.42	0.44
16:P:366:PHE:HZ	16:P:433:VAL:HG12	1.82	0.44
16:P:435:ARG:NH2	18:R:140:ILE:CD1	2.80	0.44
16:P:478:MET:HE2	16:P:497:VAL:HG13	1.97	0.44
16:P:533:LEU:H	16:P:554:ASN:HB2	1.82	0.44
16:P:627:GLY:C	16:P:628:TYR:HD1	2.26	0.44
18:R:299:THR:CG2	18:R:305:THR:HA	2.46	0.44
1:A:408:LYS:HG3	1:A:416:ARG:HE	1.72	0.44
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.98	0.44
2:B:923:GLN:HG2	2:B:949:ILE:CD1	2.47	0.44
2:B:1153:ILE:HA	2:B:1153:ILE:HD13	1.79	0.44
13:M:26:PHE:CE1	13:M:98:SER:HB2	2.51	0.44
17:Q:484:ALA:O	17:Q:488:LEU:HG	2.17	0.44
17:Q:494:SER:HB2	17:Q:497:GLN:H	1.82	0.44
18:R:236:PHE:CE2	18:R:253:ILE:HD12	2.52	0.44
1:A:257:ASN:OD1	1:A:258:GLU:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASP:CG	2:B:781:TYR:OH	2.61	0.44
1:A:878:ARG:NH2	9:I:66:VAL:C	2.75	0.44
1:A:1055:ILE:CD1	1:A:1178:LEU:HD23	2.44	0.44
1:A:1063:MET:HE1	1:A:1174:TYR:CD2	2.52	0.44
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.52	0.44
2:B:699:ILE:HG22	2:B:700:LEU:HD12	1.98	0.44
2:B:833:PRO:HG2	2:B:836:TRP:CZ2	2.52	0.44
3:C:326:GLU:HG3	11:K:125:MET:HE3	2.00	0.44
16:P:62:LYS:HE2	16:P:550:TYR:OH	2.17	0.44
16:P:198:ASP:HB2	16:P:206:ALA:HA	1.99	0.44
16:P:210:THR:HB	16:P:226:HIS:NE2	2.32	0.44
17:Q:374:THR:O	17:Q:377:PHE:HB3	2.17	0.44
1:A:535:GLN:HA	1:A:546:LEU:HG	1.99	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.44	0.44
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.17	0.44
5:E:177:ARG:HD3	5:E:215:MET:HB2	2.00	0.44
15:O:506:PHE:CG	15:O:528:PHE:HZ	2.35	0.44
16:P:263:ILE:HG21	16:P:276:SER:C	2.42	0.44
16:P:433:VAL:HG22	16:P:434:ARG:O	2.17	0.44
16:P:632:ILE:O	16:P:636:GLU:HG3	2.17	0.44
18:R:187:TYR:CE2	18:R:191:ILE:HG21	2.52	0.44
1:A:543:LEU:CA	17:Q:34:VAL:O	2.66	0.44
1:A:1260:LYS:HE2	1:A:1262:LEU:CG	2.47	0.44
2:B:42:VAL:HG21	2:B:190:ILE:HB	2.00	0.44
2:B:894:LYS:CG	12:L:47:ARG:HD2	2.47	0.44
16:P:290:GLU:HB3	16:P:342:GLN:HG2	1.99	0.44
16:P:532:GLU:HB2	16:P:554:ASN:CB	2.46	0.44
17:Q:221:PRO:HA	17:Q:225:GLN:HB2	1.99	0.44
17:Q:351:ASN:OD1	17:Q:369:TRP:CZ2	2.69	0.44
18:R:5:PRO:HD2	18:R:217:THR:HG21	1.94	0.44
18:R:217:THR:HG22	18:R:239:LEU:HD21	2.00	0.44
18:R:353:VAL:HG13	18:R:364:VAL:HB	1.98	0.44
1:A:909:SER:HA	9:I:83:LYS:HZ3	1.70	0.44
1:A:1156:LYS:C	1:A:1158:SER:H	2.25	0.44
1:A:1330:VAL:HG23	1:A:1455:ARG:HD2	2.00	0.44
2:B:1001:ALA:O	14:N:168:LEU:HD23	2.17	0.44
15:O:376:TYR:OH	15:O:377:TYR:CE2	2.66	0.44
15:O:515:ASN:N	15:O:516:PRO:HD3	2.33	0.44
16:P:323:ASN:HB3	16:P:350:THR:HB	1.98	0.44
17:Q:137:TRP:HE3	17:Q:140:ILE:HD11	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:317:LEU:HD13	18:R:367:ILE:HD11	2.00	0.44
1:A:477:ASN:CG	2:B:1049:THR:OG1	2.61	0.44
1:A:863:ASN:HB2	9:I:66:VAL:O	2.17	0.44
1:A:986:PHE:HE2	2:B:958:MET:CE	2.30	0.44
1:A:1248:ASP:OD1	1:A:1517:ARG:NH1	2.49	0.44
1:A:1323:HIS:HE1	1:A:1453:HIS:HB3	1.81	0.44
1:A:1575:ILE:CD1	9:I:122:ARG:CZ	2.95	0.44
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	2.00	0.44
2:B:548:LYS:HG2	2:B:695:ASN:O	2.18	0.44
2:B:894:LYS:CG	12:L:54:ARG:NH1	2.81	0.44
3:C:230:LEU:CD1	3:C:299:ILE:HD11	2.44	0.44
9:I:11:LEU:H	9:I:37:TYR:HH	1.64	0.44
11:K:80:ILE:HD13	11:K:105:ILE:HD11	1.98	0.44
13:M:102:SER:HB3	13:M:105:SER:HB3	0.45	0.44
15:O:200:ASN:CB	17:Q:14:ASN:O	2.65	0.44
16:P:362:ARG:NH2	16:P:364:GLU:HG3	2.31	0.44
16:P:472:ARG:N	16:P:504:THR:HG21	2.33	0.44
1:A:530:TRP:CZ2	1:A:607:VAL:HG21	2.53	0.44
1:A:581:ILE:HD11	1:A:585:ASP:CB	2.48	0.44
1:A:697:TYR:OH	11:K:102:ASN:HB3	2.17	0.44
1:A:721:LYS:HD2	8:H:90:ALA:HB1	2.00	0.44
1:A:912:VAL:HA	1:A:913:PRO:HA	1.84	0.44
2:B:535:ASP:OD1	2:B:720:GLN:NE2	2.49	0.44
2:B:623:ASP:OD2	2:B:648:ARG:NH2	2.40	0.44
2:B:1090:ASP:O	2:B:1094:ASN:CB	2.64	0.44
14:N:94:ASP:HB3	14:N:99:LEU:HG	2.00	0.44
15:O:129:PRO:O	15:O:130:PRO:C	2.59	0.44
16:P:274:ILE:HD13	16:P:305:PHE:CZ	2.53	0.44
16:P:331:LYS:HA	16:P:331:LYS:HD3	1.72	0.44
16:P:399:TRP:O	16:P:419:ARG:NH2	2.51	0.44
16:P:656:HIS:CD2	16:P:656:HIS:N	2.79	0.44
17:Q:195:ALA:O	17:Q:196:SER:C	2.60	0.44
18:R:76:LYS:O	18:R:80:ARG:HG3	2.17	0.44
2:B:78:PRO:O	2:B:79:LEU:HB3	2.17	0.44
15:O:243:GLU:OE1	15:O:243:GLU:HA	2.17	0.44
16:P:574:TRP:HB3	16:P:578:PHE:CE2	2.53	0.44
17:Q:128:GLU:O	17:Q:132:VAL:HG23	2.17	0.44
18:R:250:LEU:HB3	18:R:274:MET:HE3	2.00	0.44
1:A:37:VAL:HG12	1:A:38:LEU:HG	2.00	0.43
1:A:697:TYR:CD2	11:K:92:SER:HB3	2.53	0.43
1:A:1575:ILE:CG1	9:I:122:ARG:CZ	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:PRO:HD2	3:C:255:VAL:HG21	1.99	0.43
7:G:163:PRO:HG2	7:G:166:TRP:CD1	2.52	0.43
16:P:229:ARG:HG3	16:P:231:ASN:H	1.82	0.43
16:P:363:ILE:HG23	16:P:374:VAL:HG13	2.00	0.43
17:Q:140:ILE:HG22	17:Q:236:MET:HG2	2.00	0.43
18:R:19:LEU:HB3	18:R:188:PHE:CD1	2.52	0.43
18:R:75:GLN:HA	18:R:78:ARG:NE	2.32	0.43
18:R:80:ARG:O	18:R:83:HIS:HB3	2.18	0.43
18:R:138:PHE:CE1	18:R:140:ILE:HD11	2.53	0.43
1:A:403:LEU:HD12	1:A:403:LEU:HA	1.71	0.43
1:A:1003:ARG:HH22	2:B:530:PRO:HA	1.84	0.43
15:O:189:PHE:HA	15:O:192:THR:HG23	2.00	0.43
16:P:194:ARG:HG2	16:P:209:LYS:O	2.18	0.43
16:P:238:LEU:HD22	16:P:284:VAL:H	1.84	0.43
16:P:363:ILE:O	16:P:363:ILE:HD12	2.18	0.43
16:P:413:GLY:HA2	16:P:426:ALA:HB2	1.99	0.43
16:P:428:GLU:HB3	18:R:142:ARG:HH11	1.81	0.43
16:P:584:ARG:O	16:P:588:SER:CB	2.62	0.43
16:P:751:SER:O	16:P:753:PHE:N	2.51	0.43
17:Q:355:VAL:HG12	18:R:212:HIS:ND1	2.32	0.43
18:R:4:VAL:HG22	18:R:214:VAL:HA	1.99	0.43
18:R:299:THR:HG21	18:R:305:THR:HA	2.00	0.43
1:A:414:GLU:O	1:A:416:ARG:N	2.52	0.43
1:A:475:ARG:O	2:B:1059:PRO:CG	2.66	0.43
1:A:478:TYR:CZ	2:B:1049:THR:HB	2.53	0.43
1:A:684:ASP:OD2	8:H:20:TYR:CA	2.66	0.43
2:B:26:ILE:HD11	10:J:58:GLU:HG2	2.00	0.43
2:B:849:GLY:C	12:L:60:ARG:NH2	2.44	0.43
3:C:292:GLY:CA	3:C:295:ARG:NH2	2.80	0.43
7:G:159:LYS:HD2	15:O:103:ASN:ND2	2.28	0.43
15:O:198:PHE:CD2	15:O:199:PRO:HD2	2.53	0.43
16:P:361:LYS:HA	16:P:375:PHE:O	2.18	0.43
16:P:369:PHE:O	16:P:369:PHE:HD1	2.01	0.43
16:P:394:VAL:HG11	18:R:144:VAL:HG21	1.95	0.43
16:P:686:TYR:O	16:P:691:VAL:HG11	2.17	0.43
17:Q:19:LEU:CD1	17:Q:27:ARG:CB	2.94	0.43
17:Q:137:TRP:CE3	17:Q:140:ILE:HD11	2.53	0.43
17:Q:502:ILE:HA	17:Q:505:ILE:HG22	1.99	0.43
18:R:171:ARG:C	18:R:174:GLU:H	2.27	0.43
1:A:545:SER:OG	17:Q:26:ARG:NH2	2.50	0.43
1:A:581:ILE:CG1	1:A:585:ASP:OD2	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ASP:O	2:B:916:LYS:HE2	2.17	0.43
1:A:833:LEU:C	1:A:944:MET:HE3	2.43	0.43
1:A:862:THR:HG22	9:I:67:VAL:HG12	1.81	0.43
6:F:70:LYS:HA	7:G:94:PRO:HG3	1.83	0.43
15:O:56:VAL:CG2	15:O:99:ILE:HD12	2.48	0.43
15:O:200:ASN:HB2	17:Q:14:ASN:HB3	1.70	0.43
16:P:319:ASP:HB2	16:P:363:ILE:CG1	2.48	0.43
16:P:507:GLY:O	16:P:539:VAL:HA	2.19	0.43
16:P:705:HIS:ND1	20:P:902:SO4:O4	2.51	0.43
17:Q:106:LYS:O	17:Q:110:PHE:HB3	2.18	0.43
18:R:18:LYS:HA	18:R:78:ARG:HD3	2.00	0.43
18:R:76:LYS:HA	18:R:79:ARG:HB2	2.01	0.43
18:R:348:LYS:HE2	18:R:352:TRP:HE1	1.83	0.43
1:A:36:THR:HG22	1:A:45:VAL:HG21	2.00	0.43
1:A:407:GLN:HB3	1:A:409:ASP:N	2.23	0.43
1:A:477:ASN:CB	2:B:1047:ARG:NH1	2.81	0.43
1:A:1003:ARG:HH22	2:B:530:PRO:C	2.20	0.43
2:B:209:GLN:CG	2:B:210:ARG:H	2.08	0.43
3:C:253:PRO:N	14:N:180:PHE:CB	2.72	0.43
7:G:24:VAL:CA	7:G:25:THR:HA	2.32	0.43
15:O:374:PRO:C	15:O:376:TYR:CB	2.60	0.43
15:O:376:TYR:CD1	15:O:376:TYR:O	2.70	0.43
16:P:474:LYS:CD	16:P:474:LYS:H	2.30	0.43
16:P:487:ASN:O	18:R:138:PHE:CZ	2.67	0.43
16:P:730:GLU:O	16:P:734:LYS:HB2	2.19	0.43
17:Q:234:CYS:SG	17:Q:284:LEU:HB3	2.57	0.43
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.18	0.43
1:A:921:PRO:CD	8:H:19:ARG:HG3	2.42	0.43
1:A:1484:LEU:HD22	2:B:305:ARG:NH2	2.34	0.43
2:B:46:ILE:HG13	2:B:192:GLY:HA2	1.99	0.43
2:B:57:ASP:OD1	2:B:57:ASP:N	2.52	0.43
16:P:389:TRP:C	18:R:151:PRO:HA	2.43	0.43
16:P:397:LYS:NZ	18:R:85:ARG:HG2	2.31	0.43
16:P:412:ASN:O	16:P:426:ALA:HB1	2.18	0.43
18:R:5:PRO:CD	18:R:217:THR:HB	2.16	0.43
1:A:486:PRO:CG	2:B:781:TYR:O	2.67	0.43
1:A:1063:MET:HB3	1:A:1063:MET:HE2	1.66	0.43
1:A:1269:LYS:HB2	1:A:1269:LYS:HE3	1.89	0.43
1:A:1463:ASP:HB2	1:A:1469:TRP:CE2	2.52	0.43
2:B:30:LYS:HG2	2:B:178:TYR:HB2	2.00	0.43
2:B:75:ASP:HA	2:B:440:PHE:CZ	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:PHE:H	2:B:955:PRO:HD2	1.83	0.43
7:G:143:SER:CB	15:O:104:ILE:HB	2.48	0.43
12:L:32:ALA:HB3	12:L:55:ILE:HG23	2.01	0.43
16:P:438:TRP:HD1	18:R:141:TRP:CH2	2.35	0.43
16:P:472:ARG:CD	18:R:200:THR:CG2	2.96	0.43
17:Q:366:TYR:CD1	18:R:215:THR:HG23	2.53	0.43
17:Q:369:TRP:CA	17:Q:373:GLU:OE2	2.66	0.43
1:A:475:ARG:CD	2:B:1059:PRO:O	2.67	0.43
9:I:26:SER:O	9:I:39:LYS:HB2	2.19	0.43
15:O:76:ASN:O	15:O:80:LEU:HD13	2.18	0.43
15:O:444:SER:O	15:O:448:SER:HB3	2.18	0.43
16:P:187:ILE:HG22	18:R:195:LEU:HD23	1.98	0.43
16:P:361:LYS:HG3	16:P:376:ASP:HB3	2.01	0.43
16:P:697:GLU:HG2	16:P:698:LYS:H	1.84	0.43
16:P:760:ILE:O	16:P:764:LEU:HG	2.18	0.43
17:Q:105:LEU:HD13	17:Q:141:LEU:HD11	1.99	0.43
17:Q:239:PHE:CG	17:Q:240:LYS:N	2.86	0.43
17:Q:255:LYS:O	17:Q:259:GLN:HB2	2.18	0.43
18:R:180:CYS:SG	18:R:185:LYS:HG3	2.59	0.43
1:A:827:THR:HG21	1:A:924:SER:CB	2.49	0.43
1:A:828:CYS:HG	2:B:1027:TYR:CB	2.30	0.43
1:A:991:LYS:CB	1:A:994:GLU:HG3	2.48	0.43
1:A:998:HIS:C	2:B:712:SER:OG	2.59	0.43
1:A:1313:LEU:O	1:A:1317:ILE:HD12	2.18	0.43
1:A:1484:LEU:HB3	2:B:305:ARG:NH2	2.34	0.43
2:B:404:LEU:C	2:B:406:GLY:N	2.66	0.43
2:B:551:ILE:CG2	2:B:648:ARG:H	2.22	0.43
15:O:107:ILE:O	15:O:109:SER:N	2.47	0.43
15:O:218:LEU:HD12	15:O:221:TYR:CZ	2.54	0.43
15:O:376:TYR:CG	15:O:376:TYR:O	2.70	0.43
17:Q:4:PHE:HE1	17:Q:18:ARG:HH11	1.67	0.43
17:Q:160:SER:HA	17:Q:163:SER:HB2	2.00	0.43
17:Q:366:TYR:CE1	18:R:215:THR:HG23	2.54	0.43
17:Q:375:LEU:HD23	17:Q:375:LEU:HA	1.88	0.43
17:Q:378:LEU:HD22	18:R:235:ILE:HA	2.01	0.43
17:Q:406:GLN:HA	17:Q:409:ALA:HB3	2.00	0.43
18:R:25:ASN:O	18:R:29:ARG:HB2	2.19	0.43
1:A:697:TYR:CE2	11:K:92:SER:CB	3.01	0.43
2:B:681:ILE:HB	14:N:154:ARG:HB2	2.01	0.43
2:B:848:ILE:N	12:L:60:ARG:NE	2.67	0.43
15:O:202:ASN:OD1	15:O:202:ASN:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:235:GLU:C	15:O:237:ILE:HB	2.44	0.43
16:P:193:LEU:HD12	16:P:251:SER:N	2.31	0.43
17:Q:132:VAL:O	17:Q:136:ILE:HG13	2.19	0.43
18:R:426:VAL:C	18:R:428:SER:N	2.76	0.43
1:A:629:ASP:CA	2:B:926:VAL:HG23	2.46	0.42
2:B:48:SER:HB3	2:B:404:LEU:CD1	2.49	0.42
2:B:77:LYS:NZ	2:B:439:ASN:HA	2.33	0.42
2:B:345:SER:CA	13:M:113:ILE:HG12	2.48	0.42
7:G:29:ASP:OD1	7:G:30:GLU:N	2.52	0.42
7:G:35:SER:OG	7:G:132:VAL:N	2.46	0.42
9:I:34:LYS:HA	9:I:34:LYS:HD3	1.86	0.42
16:P:265:THR:HG21	16:P:303:VAL:HG21	2.01	0.42
16:P:472:ARG:NH1	18:R:203:SER:HB2	2.33	0.42
17:Q:177:TYR:OH	17:Q:252:LEU:N	2.52	0.42
18:R:248:LYS:O	18:R:250:LEU:N	2.49	0.42
18:R:248:LYS:C	18:R:250:LEU:H	2.27	0.42
1:A:489:ASN:HB3	11:K:95:HIS:CD2	2.54	0.42
1:A:908:VAL:C	9:I:83:LYS:HZ1	2.27	0.42
1:A:1120:TYR:C	5:E:207:ARG:HH22	2.17	0.42
1:A:1172:LEU:O	1:A:1176:ARG:HG2	2.19	0.42
2:B:45:HIS:CD2	2:B:500:PHE:HD1	2.37	0.42
2:B:49:PHE:HE2	2:B:194:PHE:CZ	2.30	0.42
2:B:550:ARG:H	2:B:650:LEU:H	1.66	0.42
2:B:893:ASN:O	2:B:895:PHE:HD1	2.01	0.42
13:M:8:SER:O	14:N:71:PRO:HA	2.19	0.42
16:P:300:LEU:N	16:P:300:LEU:HD23	2.34	0.42
16:P:330:PRO:HG3	16:P:342:GLN:HG3	2.00	0.42
18:R:234:LYS:O	18:R:238:THR:OG1	2.33	0.42
1:A:4:SER:HB2	1:A:573:LEU:CD2	2.49	0.42
1:A:449:GLY:C	1:A:451:VAL:H	2.22	0.42
1:A:475:ARG:NH2	2:B:1061:LYS:HD2	2.34	0.42
1:A:722:PRO:HD2	8:H:95:TYR:HD1	1.83	0.42
1:A:1053:ASP:OD2	5:E:204:THR:CG2	2.67	0.42
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	2.01	0.42
2:B:527:PHE:CD1	2:B:666:PRO:CB	2.99	0.42
2:B:574:SER:HB3	13:M:67:ASP:OD2	2.20	0.42
2:B:809:VAL:HG13	2:B:901:VAL:HB	2.01	0.42
2:B:883:GLU:HG3	2:B:906:ARG:HB2	2.01	0.42
16:P:438:TRP:NE1	18:R:297:PHE:HZ	2.16	0.42
17:Q:6:ARG:HA	17:Q:18:ARG:CD	2.50	0.42
17:Q:410:ARG:HA	17:Q:413:LEU:CB	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:O	2:B:1068:GLY:CA	2.47	0.42
1:A:953:GLU:CA	1:A:1205:PHE:CG	2.85	0.42
1:A:1089:LEU:CD1	1:A:1175:MET:HE1	2.48	0.42
1:A:1313:LEU:CG	1:A:1462:PHE:CE1	2.73	0.42
1:A:1657:LEU:CB	7:G:104:LEU:HD22	2.47	0.42
2:B:563:SER:CA	13:M:73:SER:HB3	2.48	0.42
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.01	0.42
15:O:56:VAL:HG23	15:O:57:LYS:N	2.35	0.42
15:O:96:LEU:O	15:O:100:LEU:HG	2.20	0.42
15:O:379:ARG:NH1	15:O:382:GLN:HE22	2.17	0.42
15:O:468:GLU:HG2	15:O:469:ARG:N	2.34	0.42
16:P:473:HIS:CG	16:P:475:ARG:HD2	2.54	0.42
16:P:619:GLU:OE2	16:P:670:ALA:N	2.52	0.42
16:P:659:LEU:H	16:P:659:LEU:CD1	2.27	0.42
18:R:8:LEU:H	18:R:8:LEU:HD22	1.83	0.42
1:A:83:VAL:HG13	1:A:427:PHE:CZ	2.52	0.42
1:A:1325:LEU:HD21	1:A:1474:LEU:HD11	2.00	0.42
3:C:229:LEU:C	3:C:293:ARG:HD2	2.44	0.42
3:C:315:PHE:HE2	11:K:139:ILE:CD1	2.30	0.42
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.84	0.42
15:O:453:TYR:CE2	15:O:473:PHE:HB2	2.54	0.42
16:P:321:LYS:HD3	16:P:321:LYS:N	2.25	0.42
16:P:390:GLN:N	18:R:150:GLN:O	2.52	0.42
16:P:434:ARG:CG	18:R:143:THR:CB	2.90	0.42
16:P:675:PHE:HZ	16:P:742:TRP:CZ3	2.36	0.42
17:Q:262:LEU:HD23	17:Q:262:LEU:HA	1.84	0.42
17:Q:344:THR:HG22	17:Q:436:LEU:HD13	2.01	0.42
18:R:306:ALA:O	18:R:307:LYS:C	2.62	0.42
1:A:83:VAL:HG21	1:A:427:PHE:CZ	2.55	0.42
1:A:410:LYS:HB3	1:A:411:VAL:CG2	2.50	0.42
1:A:474:LYS:HZ2	2:B:1092:LEU:CD2	2.08	0.42
1:A:826:PHE:CG	1:A:827:THR:N	2.88	0.42
1:A:878:ARG:HH11	9:I:66:VAL:HG21	1.63	0.42
1:A:1263:LEU:HD12	1:A:1498:ILE:HD11	2.02	0.42
2:B:682:GLN:HA	14:N:154:ARG:CZ	2.46	0.42
2:B:799:GLY:O	2:B:911:PRO:HG3	2.20	0.42
3:C:61:THR:HA	3:C:298:PHE:CZ	2.55	0.42
3:C:274:THR:HG21	14:N:171:PHE:HA	1.60	0.42
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.35	0.42
15:O:199:PRO:HD3	15:O:211:TYR:CG	2.54	0.42
16:P:273:ARG:NH1	16:P:288:SER:OG	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:607:VAL:HB	16:P:731:LEU:HD13	2.01	0.42
18:R:253:ILE:HG12	18:R:257:ILE:HG13	2.02	0.42
1:A:410:LYS:HB2	1:A:411:VAL:HG23	2.01	0.42
1:A:436:ALA:O	1:A:440:SER:HA	2.15	0.42
1:A:475:ARG:NH2	2:B:1061:LYS:CD	2.82	0.42
1:A:564:PRO:CD	15:O:370:THR:O	2.68	0.42
1:A:711:LYS:HA	11:K:104:ARG:NH2	2.35	0.42
1:A:977:MET:HE1	1:A:991:LYS:HD2	2.01	0.42
1:A:1657:LEU:O	6:F:132:LEU:CA	2.68	0.42
3:C:116:VAL:HG11	3:C:125:LYS:HE3	2.01	0.42
3:C:170:GLU:HA	3:C:171:PRO:HD3	1.84	0.42
7:G:160:ASN:OD1	7:G:160:ASN:N	2.52	0.42
13:M:101:VAL:CG1	13:M:105:SER:OG	2.66	0.42
15:O:234:ILE:HA	15:O:234:ILE:HD13	1.74	0.42
16:P:366:PHE:CZ	16:P:433:VAL:HG12	2.54	0.42
16:P:427:SER:HB2	16:P:429:SER:O	2.19	0.42
16:P:648:SER:HA	16:P:757:GLN:NE2	2.35	0.42
17:Q:120:ILE:HA	17:Q:125:PHE:HB2	2.01	0.42
17:Q:351:ASN:O	17:Q:355:VAL:HG23	2.19	0.42
1:A:670:ILE:CG1	2:B:783:MET:HE2	2.49	0.42
2:B:436:MET:HE1	2:B:448:ARG:HD3	2.02	0.42
2:B:897:GLU:HA	12:L:46:VAL:HG21	2.01	0.42
3:C:105:PRO:HG3	10:J:6:ARG:CZ	2.50	0.42
4:D:82:LEU:O	4:D:86:ILE:HG23	2.20	0.42
15:O:376:TYR:CG	15:O:419:LYS:CD	3.03	0.42
15:O:396:MET:HE1	15:O:433:LYS:HB2	2.02	0.42
15:O:400:LEU:O	15:O:404:ILE:HG13	2.19	0.42
16:P:187:ILE:HG23	18:R:195:LEU:CD2	2.50	0.42
16:P:443:ASP:O	18:R:3:GLU:CA	2.66	0.42
16:P:663:LEU:HD12	16:P:664:GLU:N	2.34	0.42
1:A:414:GLU:O	1:A:415:ASP:C	2.63	0.42
1:A:990:ILE:CA	1:A:994:GLU:OE1	2.26	0.42
2:B:656:LEU:HD21	2:B:689:VAL:HG12	2.02	0.42
2:B:697:LEU:HD13	2:B:702:ASN:HA	2.02	0.42
11:K:93:ILE:HA	11:K:94:PRO:HD2	1.75	0.42
15:O:77:GLN:HG2	15:O:88:ILE:HB	2.01	0.42
15:O:236:LYS:HD3	15:O:236:LYS:HA	1.73	0.42
15:O:364:LEU:HB3	15:O:385:MET:HE3	2.02	0.42
16:P:465:VAL:HG13	16:P:480:VAL:HG13	2.01	0.42
17:Q:152:LEU:HA	17:Q:152:LEU:HD13	1.67	0.42
17:Q:257:VAL:HG13	17:Q:262:LEU:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:502:ILE:O	17:Q:506:LYS:HB2	2.20	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.84	0.42
1:A:498:PRO:HA	1:A:499:PRO:HD3	1.81	0.42
1:A:550:SER:OG	1:A:553:GLN:HG3	2.19	0.42
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.42
1:A:874:GLU:OE2	1:A:878:ARG:HD2	2.20	0.42
1:A:1318:SER:HA	1:A:1450:ILE:HD13	2.00	0.42
2:B:196:VAL:HG21	2:B:465:LEU:HB3	2.02	0.42
2:B:394:PRO:O	2:B:400:GLN:NE2	2.48	0.42
3:C:230:LEU:O	3:C:293:ARG:HA	2.20	0.42
15:O:66:ASN:ND2	15:O:111:ARG:CZ	2.83	0.42
17:Q:103:LEU:HD21	17:Q:205:ILE:HD13	2.00	0.42
17:Q:409:ALA:O	17:Q:413:LEU:CB	2.58	0.42
1:A:1:MET:HE2	7:G:110:ASP:OD1	2.20	0.41
1:A:68:ASP:C	1:A:70:LYS:N	2.77	0.41
1:A:407:GLN:O	1:A:408:LYS:HE2	2.19	0.41
1:A:1260:LYS:HE2	1:A:1262:LEU:HD21	2.01	0.41
1:A:1310:LYS:HG2	1:A:1311:GLU:OE1	2.07	0.41
2:B:800:TYR:OH	2:B:908:ARG:CZ	2.65	0.41
15:O:390:GLN:CG	15:O:396:MET:HE3	2.45	0.41
16:P:484:ARG:HB2	16:P:488:LEU:HB3	2.02	0.41
17:Q:498:LEU:O	17:Q:502:ILE:HG23	2.20	0.41
18:R:150:GLN:H	18:R:150:GLN:HG2	1.26	0.41
1:A:82:PRO:HD3	1:A:393:SER:OG	2.20	0.41
1:A:474:LYS:CE	2:B:1096:SER:OG	2.63	0.41
1:A:581:ILE:CG1	1:A:582:LYS:N	2.83	0.41
2:B:145:VAL:HG21	2:B:440:PHE:O	2.20	0.41
2:B:1005:TYR:CE2	14:N:170:HIS:CE1	3.08	0.41
3:C:314:PHE:HD2	11:K:135:PHE:CE2	2.38	0.41
15:O:548:ASN:O	15:O:552:LEU:HG	2.21	0.41
16:P:64:LEU:CD2	16:P:64:LEU:H	2.33	0.41
16:P:535:VAL:HG13	16:P:552:LEU:HD12	2.01	0.41
16:P:740:ILE:O	16:P:744:LEU:HG	2.19	0.41
16:P:762:ARG:HG3	17:Q:139:LYS:NZ	2.35	0.41
17:Q:192:TYR:CD1	17:Q:193:PHE:CD1	3.08	0.41
17:Q:282:ARG:HG2	17:Q:302:ALA:HB1	2.02	0.41
17:Q:329:LYS:O	17:Q:332:LEU:N	2.53	0.41
17:Q:341:ARG:NH1	17:Q:369:TRP:CD1	2.87	0.41
18:R:158:THR:OG1	18:R:159:TYR:N	2.53	0.41
18:R:220:LEU:N	18:R:235:ILE:HG21	2.36	0.41
18:R:421:LYS:HG3	18:R:422:GLY:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.95	0.41
1:A:501:PHE:CD1	2:B:1046:VAL:HG21	2.55	0.41
1:A:1180:ASN:N	1:A:1180:ASN:HD22	2.18	0.41
1:A:1538:VAL:HG21	5:E:142:VAL:HG22	2.01	0.41
2:B:1151:ILE:HG23	7:G:21:LYS:CG	2.47	0.41
15:O:78:VAL:HA	15:O:88:ILE:HG22	2.00	0.41
16:P:263:ILE:HB	16:P:275:GLU:O	2.21	0.41
16:P:397:LYS:CD	18:R:85:ARG:HD3	2.49	0.41
16:P:489:PHE:CD2	18:R:140:ILE:HD11	2.48	0.41
16:P:607:VAL:O	16:P:611:ILE:HG13	2.21	0.41
17:Q:287:TRP:HE1	17:Q:289:ARG:HB3	1.86	0.41
18:R:6:ILE:HG21	18:R:210:THR:HG22	2.02	0.41
18:R:264:SER:O	18:R:265:SER:C	2.62	0.41
18:R:268:LEU:HD11	18:R:316:SER:OG	2.20	0.41
2:B:49:PHE:HB3	2:B:164:MET:SD	2.60	0.41
2:B:61:LEU:HA	2:B:61:LEU:HD23	1.75	0.41
2:B:995:TYR:HE1	14:N:162:LYS:HA	1.85	0.41
2:B:1002:LYS:C	14:N:168:LEU:HD23	2.45	0.41
15:O:219:ARG:CZ	15:O:360:VAL:CG2	2.98	0.41
15:O:235:GLU:HA	15:O:237:ILE:HB	2.01	0.41
15:O:244:LEU:HD23	15:O:244:LEU:O	2.20	0.41
16:P:378:SER:HB2	16:P:379:LYS:HD2	2.03	0.41
16:P:454:GLN:HB3	16:P:465:VAL:HG23	2.02	0.41
17:Q:6:ARG:HA	17:Q:18:ARG:HG3	2.02	0.41
17:Q:289:ARG:C	17:Q:290:THR:HG1	2.28	0.41
18:R:209:ARG:H	18:R:209:ARG:HD3	1.85	0.41
18:R:436:LYS:HA	18:R:439:GLU:HB2	2.02	0.41
1:A:711:LYS:HA	11:K:104:ARG:HH22	1.84	0.41
1:A:826:PHE:HE1	2:B:952:HIS:CE1	2.39	0.41
1:A:878:ARG:HG2	9:I:66:VAL:CG2	2.23	0.41
1:A:1622:LEU:HD21	2:B:1189:LEU:HD22	2.01	0.41
2:B:1005:TYR:CZ	14:N:170:HIS:NE2	2.87	0.41
3:C:246:ARG:HD2	3:C:284:GLU:OE2	2.21	0.41
11:K:95:HIS:HB3	11:K:98:GLU:HG2	2.03	0.41
15:O:169:THR:O	15:O:172:HIS:N	2.52	0.41
15:O:182:MET:HE2	15:O:183:ILE:HG13	2.03	0.41
16:P:241:PRO:C	16:P:242:ILE:HG13	2.44	0.41
16:P:389:TRP:CZ2	18:R:147:GLN:CA	2.95	0.41
17:Q:15:CYS:CB	17:Q:17:SER:H	2.30	0.41
17:Q:26:ARG:CB	17:Q:34:VAL:HG11	2.43	0.41
17:Q:318:LEU:HD12	17:Q:318:LEU:HA	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:355:VAL:CG1	18:R:212:HIS:ND1	2.83	0.41
1:A:481:ARG:N	2:B:1045:GLN:O	2.53	0.41
1:A:506:THR:HG22	1:A:580:HIS:N	2.31	0.41
1:A:507:TYR:CD1	1:A:509:GLU:N	2.89	0.41
1:A:1055:ILE:HD13	1:A:1178:LEU:CD2	2.48	0.41
1:A:1484:LEU:HD23	2:B:304:ASP:HB2	2.01	0.41
1:A:1573:TYR:HA	9:I:111:PHE:CE2	2.55	0.41
2:B:550:ARG:HA	2:B:550:ARG:HD3	1.81	0.41
2:B:679:GLN:NE2	14:N:156:PRO:O	2.53	0.41
12:L:33:GLU:HG3	12:L:53:HIS:ND1	2.36	0.41
15:O:372:VAL:HG22	15:O:381:ILE:HD13	2.03	0.41
16:P:65:LEU:HD21	16:P:226:HIS:CE1	2.55	0.41
16:P:347:LEU:HD12	16:P:347:LEU:N	2.35	0.41
17:Q:156:LEU:HD23	17:Q:156:LEU:HA	1.84	0.41
18:R:19:LEU:HB3	18:R:188:PHE:HD1	1.86	0.41
18:R:362:ALA:CB	18:R:421:LYS:HB3	2.38	0.41
1:A:514:TYR:CE1	6:F:115:THR:O	2.74	0.41
1:A:721:LYS:HZ2	8:H:91:ASP:HA	1.80	0.41
1:A:938:VAL:HG22	9:I:82:ILE:HD11	1.93	0.41
1:A:1322:ILE:C	1:A:1454:HIS:NE2	2.79	0.41
2:B:186:GLU:OE2	2:B:731:VAL:HB	2.20	0.41
2:B:469:ASN:OD1	2:B:482:SER:CB	2.67	0.41
4:D:37:LEU:HD23	4:D:37:LEU:HA	1.88	0.41
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.84	0.41
16:P:448:THR:HG21	16:P:471:MET:HB2	2.03	0.41
17:Q:26:ARG:H	17:Q:26:ARG:HG3	1.57	0.41
17:Q:136:ILE:HG12	17:Q:243:PHE:CZ	2.56	0.41
18:R:219:LEU:HD23	18:R:219:LEU:HA	1.83	0.41
1:A:413:LEU:HD13	1:A:416:ARG:HG3	2.03	0.41
1:A:684:ASP:OD2	8:H:21:ASN:N	2.51	0.41
1:A:1329:ILE:HB	1:A:1456:PHE:CE2	2.41	0.41
5:E:26:ARG:O	5:E:75:MET:HE1	2.20	0.41
10:J:49:MET:HE3	10:J:49:MET:HB3	1.79	0.41
11:K:50:LEU:O	11:K:54:THR:HG23	2.20	0.41
14:N:85:HIS:C	14:N:141:GLU:OE2	2.63	0.41
15:O:505:PHE:CD2	15:O:505:PHE:C	2.99	0.41
16:P:301:GLN:CD	16:P:360:TRP:HA	2.45	0.41
16:P:304:ASP:HB2	16:P:363:ILE:O	2.20	0.41
16:P:458:LYS:HD3	16:P:461:HIS:CE1	2.46	0.41
16:P:577:LEU:O	17:Q:506:LYS:NZ	2.47	0.41
16:P:712:ASP:O	16:P:715:TYR:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:762:ARG:NE	16:P:762:ARG:HA	2.34	0.41
1:A:67:LEU:HB2	1:A:72:CYS:HB2	2.02	0.41
1:A:315:ILE:HG13	1:A:319:GLU:HB2	2.03	0.41
1:A:382:GLN:HE21	1:A:456:VAL:CG2	2.28	0.41
1:A:406:LEU:CB	1:A:408:LYS:H	2.29	0.41
1:A:634:ASN:OD1	2:B:1069:ILE:HG12	2.21	0.41
1:A:1000:MET:HG2	2:B:520:LEU:HD23	2.02	0.41
1:A:1025:LYS:HD2	1:A:1025:LYS:HA	1.85	0.41
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.03	0.41
2:B:149:GLU:OE1	2:B:441:LYS:HE2	2.15	0.41
2:B:238:SER:OG	2:B:361:HIS:ND1	2.48	0.41
2:B:262:PHE:CE1	2:B:357:ILE:HD13	2.56	0.41
2:B:279:ALA:HB2	2:B:326:VAL:HG12	2.03	0.41
3:C:314:PHE:HE2	11:K:135:PHE:CD1	2.39	0.41
7:G:50:ALA:HA	7:G:113:PHE:CD2	2.56	0.41
7:G:144:HIS:NE2	15:O:145:SER:CA	2.84	0.41
7:G:159:LYS:HB3	15:O:105:ASN:ND2	2.12	0.41
9:I:20:PRO:C	9:I:22:ALA:H	2.29	0.41
11:K:54:THR:HG22	11:K:62:SER:H	1.86	0.41
15:O:232:LEU:HD12	15:O:232:LEU:HA	1.74	0.41
15:O:430:ARG:NH2	15:O:596:PRO:HD3	2.36	0.41
15:O:592:PHE:HA	15:O:593:PRO:HD3	1.90	0.41
16:P:56:ASP:HB2	16:P:554:ASN:OD1	2.21	0.41
16:P:432:PRO:HB2	18:R:146:SER:CB	2.49	0.41
16:P:475:ARG:HG2	18:R:1:MET:HE2	1.35	0.41
16:P:596:ILE:HD13	17:Q:272:GLN:OE1	2.20	0.41
17:Q:26:ARG:HD2	17:Q:34:VAL:HG11	2.02	0.41
17:Q:375:LEU:HA	17:Q:378:LEU:HD12	2.01	0.41
17:Q:509:CYS:O	17:Q:513:MET:HB2	2.20	0.41
18:R:15:GLN:O	18:R:18:LYS:HB2	2.21	0.41
18:R:173:MET:O	18:R:176:PRO:HD2	2.20	0.41
18:R:430:LEU:O	18:R:434:GLN:HG3	2.21	0.41
1:A:436:ALA:N	1:A:439:ASP:O	2.54	0.41
1:A:680:LEU:O	1:A:728:GLY:HA3	2.20	0.41
1:A:703:GLU:HG2	11:K:50:LEU:HD13	2.02	0.41
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.21	0.41
1:A:1600:ARG:NH2	1:A:1617:THR:HG1	2.10	0.41
2:B:152:LEU:HA	2:B:443:LYS:HE3	1.94	0.41
2:B:206:LEU:O	2:B:402:VAL:HG13	2.21	0.41
2:B:415:GLU:CD	2:B:472:SER:CB	2.94	0.41
3:C:236:LEU:HD11	3:C:290:LYS:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:PRO:HG2	9:I:119:TYR:CE2	2.56	0.41
16:P:317:ILE:CG1	16:P:326:ILE:HD13	2.49	0.41
17:Q:140:ILE:O	17:Q:143:THR:HG22	2.21	0.41
17:Q:178:THR:HG21	17:Q:227:TYR:OH	2.21	0.41
17:Q:245:SER:HB3	17:Q:284:LEU:HD13	2.03	0.41
17:Q:384:GLN:C	17:Q:387:PRO:HD2	2.46	0.41
17:Q:408:ILE:HD11	17:Q:412:LYS:HE3	2.02	0.41
18:R:303:THR:HA	18:R:358:PHE:HZ	1.85	0.41
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.88	0.40
1:A:413:LEU:HD22	1:A:413:LEU:HA	1.78	0.40
1:A:634:ASN:CG	2:B:1069:ILE:HG12	2.46	0.40
1:A:878:ARG:NE	9:I:66:VAL:C	2.79	0.40
1:A:1056:ASP:OD2	1:A:1057:ILE:N	2.54	0.40
1:A:1326:GLU:HB3	1:A:1455:ARG:NH1	2.36	0.40
2:B:527:PHE:CG	2:B:666:PRO:HG3	2.34	0.40
2:B:1002:LYS:O	14:N:168:LEU:HD23	2.21	0.40
7:G:166:TRP:HZ3	7:G:225:ILE:HD13	1.87	0.40
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.86	0.40
15:O:115:LEU:O	15:O:119:ILE:HG13	2.21	0.40
15:O:124:LYS:O	15:O:127:GLU:HB2	2.22	0.40
15:O:383:TYR:CE2	15:O:597:LEU:HD13	2.56	0.40
16:P:389:TRP:CZ2	18:R:149:LYS:N	2.79	0.40
16:P:500:ILE:HB	16:P:501:PRO:CD	2.51	0.40
18:R:408:ILE:HG23	18:R:435:LEU:HD13	2.03	0.40
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.86	0.40
1:A:407:GLN:HB3	1:A:409:ASP:CG	2.46	0.40
1:A:487:ASP:HB2	1:A:615:ARG:HB3	2.02	0.40
1:A:615:ARG:NH1	2:B:929:ARG:CD	2.82	0.40
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.68	0.40
1:A:1024:THR:HG22	1:A:1190:SER:CB	2.50	0.40
1:A:1613:MET:HG2	1:A:1618:THR:HG23	2.03	0.40
2:B:152:LEU:CD2	2:B:443:LYS:HE3	2.51	0.40
2:B:1004:GLY:HA2	14:N:168:LEU:HD22	2.03	0.40
2:B:1091:ARG:O	2:B:1096:SER:N	2.55	0.40
6:F:72:LYS:HD2	6:F:142:SER:CA	2.44	0.40
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.02	0.40
14:N:127:ASP:OD2	14:N:129:ALA:HB2	2.21	0.40
15:O:505:PHE:O	15:O:509:MET:HG2	2.21	0.40
16:P:185:GLN:NE2	18:R:197:PRO:CB	2.82	0.40
17:Q:10:CYS:CB	17:Q:17:SER:N	2.83	0.40
17:Q:158:MET:HA	17:Q:161:THR:HG23	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:173:MET:HB3	18:R:188:PHE:CZ	2.56	0.40
18:R:271:LEU:HD13	18:R:312:TYR:CB	2.51	0.40
1:A:323:ILE:O	1:A:327:VAL:HG23	2.22	0.40
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.56	0.40
2:B:498:SER:OG	2:B:723:LYS:HD3	2.22	0.40
2:B:736:ARG:NH1	2:B:738:ASP:OD1	2.54	0.40
6:F:75:PRO:CG	6:F:78:GLN:CB	2.82	0.40
15:O:107:ILE:CD1	15:O:115:LEU:HD23	2.51	0.40
16:P:377:ARG:H	16:P:377:ARG:HG3	1.64	0.40
16:P:428:GLU:CB	16:P:435:ARG:HH12	2.31	0.40
18:R:304:HIS:CE1	18:R:306:ALA:HA	2.56	0.40
1:A:408:LYS:HD3	1:A:408:LYS:N	2.33	0.40
1:A:581:ILE:HD12	1:A:637:PHE:CD1	2.57	0.40
1:A:1074:TYR:CE2	1:A:1159:ASP:HB3	2.54	0.40
1:A:1276:THR:HB	9:I:45:LEU:CD1	2.47	0.40
1:A:1574:ALA:HB3	9:I:122:ARG:CB	2.52	0.40
2:B:25:PHE:CD2	10:J:59:LYS:CG	3.01	0.40
2:B:31:ASP:N	2:B:176:SER:HB2	2.36	0.40
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.54	0.40
3:C:326:GLU:HA	11:K:125:MET:SD	2.62	0.40
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.51	0.40
8:H:108:SER:OG	8:H:111:LEU:HD23	2.22	0.40
11:K:135:PHE:CE2	11:K:139:ILE:HD11	2.56	0.40
15:O:80:LEU:HA	15:O:81:PRO:HD3	1.86	0.40
15:O:125:TRP:C	15:O:127:GLU:N	2.78	0.40
15:O:150:TRP:O	15:O:154:VAL:HG23	2.21	0.40
16:P:198:ASP:OD1	16:P:205:TYR:O	2.39	0.40
16:P:302:VAL:HG11	16:P:362:ARG:NH1	2.30	0.40
16:P:421:ILE:HA	16:P:440:HIS:O	2.21	0.40
16:P:653:SER:H	16:P:749:LYS:HB3	1.87	0.40
17:Q:22:ILE:HD12	17:Q:26:ARG:HE	1.78	0.40
17:Q:100:ALA:HB3	17:Q:211:TYR:HE2	1.87	0.40
17:Q:118:TRP:O	17:Q:122:GLU:HB2	2.21	0.40
17:Q:129:PHE:HE1	17:Q:169:SER:N	2.19	0.40
17:Q:239:PHE:HB2	17:Q:245:SER:OG	2.21	0.40
17:Q:341:ARG:CZ	17:Q:369:TRP:CD1	3.04	0.40
1:A:475:ARG:C	2:B:1059:PRO:CG	2.93	0.40
1:A:597:LYS:CD	2:B:1082:HIS:CD2	3.05	0.40
1:A:854:GLY:HA3	1:A:974:THR:O	2.21	0.40
1:A:1268:ASP:OD1	9:I:61:ARG:NH2	2.52	0.40
1:A:1600:ARG:NH2	1:A:1621:PHE:CE2	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ILE:HD13	2:B:377:MET:CE	2.52	0.40
2:B:547:HIS:CB	2:B:697:LEU:O	2.69	0.40
2:B:1060:VAL:HG22	2:B:1065:ARG:NH2	2.35	0.40
2:B:1070:ARG:HH11	2:B:1070:ARG:HD2	1.75	0.40
3:C:326:GLU:HG3	11:K:125:MET:HE1	2.03	0.40
5:E:11:ARG:HH21	5:E:141:VAL:HG21	1.87	0.40
8:H:39:THR:O	8:H:123:MET:HA	2.22	0.40
13:M:11:GLU:O	13:M:87:SER:HA	2.21	0.40
14:N:87:TYR:HA	14:N:142:THR:N	2.37	0.40
16:P:290:GLU:HB3	16:P:342:GLN:CG	2.52	0.40
16:P:470:SER:O	16:P:504:THR:HG22	2.21	0.40
17:Q:178:THR:HG22	17:Q:303:GLU:OE1	2.22	0.40
17:Q:187:THR:C	17:Q:380:TRP:HE1	2.27	0.40
17:Q:204:ARG:NH2	17:Q:205:ILE:HD11	2.37	0.40
17:Q:474:GLU:HB3	17:Q:478:ARG:HH11	1.86	0.40
18:R:362:ALA:O	18:R:365:TRP:HB2	2.21	0.40
18:R:402:ASN:O	18:R:405:ILE:HB	2.20	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	1449/1664 (87%)	1375 (95%)	60 (4%)	14 (1%)	12	48
2	B	1164/1203 (97%)	1095 (94%)	51 (4%)	18 (2%)	8	40
3	C	303/335 (90%)	288 (95%)	12 (4%)	3 (1%)	12	48
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	20
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	12	48
6	F	98/155 (63%)	95 (97%)	2 (2%)	1 (1%)	12	48
7	G	187/326 (57%)	173 (92%)	12 (6%)	2 (1%)	11	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	91/125 (73%)	80 (88%)	8 (9%)	3 (3%)	3	21
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2	16
13	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	6	32
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	5	29
15	O	467/627 (74%)	426 (91%)	35 (8%)	6 (1%)	9	42
16	P	569/894 (64%)	474 (83%)	75 (13%)	20 (4%)	3	20
17	Q	398/514 (77%)	347 (87%)	41 (10%)	10 (2%)	4	26
18	R	291/507 (57%)	243 (84%)	42 (14%)	6 (2%)	5	30
All	All	5861/7778 (75%)	5374 (92%)	393 (7%)	94 (2%)	10	38

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	LYS
1	A	479	ALA
1	A	1651	THR
2	B	111	ASP
2	B	895	PHE
2	B	1097	ASP
3	C	224	THR
4	D	99	LEU
9	I	41	GLN
15	O	237	ILE
15	O	325	ILE
16	P	188	GLN
16	P	321	LYS
16	P	332	ASN
16	P	444	PRO
16	P	500	ILE
16	P	501	PRO
17	Q	8	PRO
17	Q	9	ILE
17	Q	15	CYS
1	A	415	ASP
1	A	448	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1500	GLN
1	A	1533	GLU
1	A	1606	SER
2	B	817	ARG
2	B	1049	THR
2	B	1140	LYS
4	D	98	GLY
5	E	50	MET
9	I	5	GLY
16	P	236	ILE
16	P	426	ALA
16	P	657	SER
16	P	745	ALA
16	P	752	LEU
17	Q	7	GLY
17	Q	196	SER
18	R	11	ARG
18	R	267	GLY
18	R	422	GLY
1	A	69	GLU
1	A	450	LYS
2	B	78	PRO
2	B	208	VAL
2	B	209	GLN
2	B	1070	ARG
2	B	1084	THR
7	G	99	ASP
9	I	21	ASN
12	L	46	VAL
13	M	85	LYS
15	O	82	SER
15	O	469	ARG
16	P	201	GLU
16	P	241	PRO
16	P	247	ILE
16	P	666	SER
16	P	777	MET
17	Q	197	GLU
1	A	1299	ASN
2	B	834	LYS
3	C	297	HIS
7	G	100	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	43	THR
13	M	36	THR
14	N	115	SER
15	O	130	PRO
15	O	187	MET
16	P	294	PHE
17	Q	13	ASP
1	A	451	VAL
1	A	564	PRO
2	B	80	ASN
2	B	117	VAL
2	B	1062	GLY
3	C	32	ASN
5	E	146	HIS
17	Q	16	PRO
17	Q	193	PHE
18	R	249	SER
1	A	1512	PRO
2	B	1063	ARG
16	P	568	ILE
17	Q	148	PRO
18	R	362	ALA
6	F	74	ILE
14	N	70	LEU
16	P	421	ILE
18	R	295	PRO
14	N	39	PRO
2	B	833	PRO
2	B	954	PHE
16	P	203	ILE

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	1297/1465 (88%)	1205 (93%)	92 (7%)	13 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1025/1053 (97%)	962 (94%)	63 (6%)	17	38
3	C	269/296 (91%)	254 (94%)	15 (6%)	19	40
4	D	55/116 (47%)	50 (91%)	5 (9%)	9	27
5	E	194/197 (98%)	180 (93%)	14 (7%)	13	35
6	F	90/137 (66%)	85 (94%)	5 (6%)	19	40
7	G	171/291 (59%)	158 (92%)	13 (8%)	12	33
8	H	115/128 (90%)	107 (93%)	8 (7%)	14	35
9	I	89/110 (81%)	84 (94%)	5 (6%)	19	40
10	J	64/65 (98%)	56 (88%)	8 (12%)	4	16
11	K	91/130 (70%)	82 (90%)	9 (10%)	7	24
12	L	39/57 (68%)	34 (87%)	5 (13%)	4	15
13	M	98/371 (26%)	85 (87%)	13 (13%)	4	14
14	N	135/220 (61%)	128 (95%)	7 (5%)	21	42
15	O	439/576 (76%)	383 (87%)	56 (13%)	4	15
16	P	539/828 (65%)	386 (72%)	153 (28%)	0	2
17	Q	383/476 (80%)	320 (84%)	63 (16%)	2	10
18	R	286/474 (60%)	223 (78%)	63 (22%)	1	6
All	All	5379/6990 (77%)	4782 (89%)	597 (11%)	8	19

All (597) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	40	ASN
1	A	61	LEU
1	A	83	VAL
1	A	136	LEU
1	A	174	SER
1	A	186	SER
1	A	202	THR
1	A	230	ARG
1	A	257	ASN
1	A	262	THR
1	A	266	VAL
1	A	271	ARG
1	A	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	312	SER
1	A	315	ILE
1	A	346	SER
1	A	373	LEU
1	A	379	GLU
1	A	393	SER
1	A	406	LEU
1	A	407	GLN
1	A	408	LYS
1	A	410	LYS
1	A	413	LEU
1	A	414	GLU
1	A	447	THR
1	A	451	VAL
1	A	472	MET
1	A	503	VAL
1	A	518	GLU
1	A	524	ILE
1	A	555	LYS
1	A	611	GLU
1	A	627	ASP
1	A	661	THR
1	A	666	VAL
1	A	670	ILE
1	A	684	ASP
1	A	700	ILE
1	A	708	THR
1	A	709	ARG
1	A	739	VAL
1	A	747	ILE
1	A	758	GLU
1	A	783	LYS
1	A	794	VAL
1	A	815	ARG
1	A	878	ARG
1	A	955	ARG
1	A	957	VAL
1	A	966	LEU
1	A	988	SER
1	A	1021	ARG
1	A	1026	GLN
1	A	1033	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1071	ASP
1	A	1085	LEU
1	A	1098	SER
1	A	1102	LEU
1	A	1118	VAL
1	A	1123	VAL
1	A	1131	LYS
1	A	1136	VAL
1	A	1150	LYS
1	A	1159	ASP
1	A	1162	ASN
1	A	1204	THR
1	A	1215	VAL
1	A	1226	VAL
1	A	1273	THR
1	A	1275	THR
1	A	1276	THR
1	A	1310	LYS
1	A	1314	GLN
1	A	1320	GLN
1	A	1441	LYS
1	A	1455	ARG
1	A	1508	VAL
1	A	1518	VAL
1	A	1531	ASP
1	A	1533	GLU
1	A	1536	ILE
1	A	1601	GLN
1	A	1604	GLU
1	A	1605	THR
1	A	1609	SER
1	A	1611	MET
1	A	1616	GLU
1	A	1633	GLN
1	A	1635	ASP
1	A	1649	VAL
2	B	17	ARG
2	B	22	GLU
2	B	37	LEU
2	B	53	THR
2	B	57	ASP
2	B	65	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	79	LEU
2	B	81	SER
2	B	87	ASN
2	B	97	VAL
2	B	117	VAL
2	B	187	SER
2	B	221	SER
2	B	228	SER
2	B	231	HIS
2	B	236	ILE
2	B	239	VAL
2	B	276	ILE
2	B	305	ARG
2	B	306	LEU
2	B	311	ARG
2	B	315	LYS
2	B	357	ILE
2	B	481	VAL
2	B	486	VAL
2	B	490	LYS
2	B	523	GLU
2	B	537	SER
2	B	583	LEU
2	B	622	ILE
2	B	658	LEU
2	B	720	GLN
2	B	725	THR
2	B	731	VAL
2	B	753	LYS
2	B	782	ASP
2	B	811	LEU
2	B	813	LEU
2	B	822	THR
2	B	829	ASN
2	B	833	PRO
2	B	835	GLU
2	B	858	ILE
2	B	871	ILE
2	B	883	GLU
2	B	897	GLU
2	B	977	ILE
2	B	998	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1026	ILE
2	B	1038	HIS
2	B	1047	ARG
2	B	1060	VAL
2	B	1064	LYS
2	B	1069	ILE
2	B	1075	GLU
2	B	1103	VAL
2	B	1125	THR
2	B	1136	GLU
2	B	1141	LEU
2	B	1153	ILE
2	B	1163	GLN
2	B	1165	ASN
2	B	1174	THR
3	C	38	LYS
3	C	43	ASN
3	C	61	THR
3	C	77	SER
3	C	91	VAL
3	C	97	LEU
3	C	118	SER
3	C	138	VAL
3	C	142	ARG
3	C	181	ASP
3	C	193	LEU
3	C	224	THR
3	C	243	SER
3	C	277	ARG
3	C	279	VAL
4	D	15	THR
4	D	29	GLN
4	D	38	GLN
4	D	80	THR
4	D	99	LEU
5	E	4	GLU
5	E	31	THR
5	E	33	GLU
5	E	74	ASP
5	E	90	VAL
5	E	92	THR
5	E	93	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	107	THR
5	E	131	THR
5	E	136	ASN
5	E	142	VAL
5	E	162	ARG
5	E	163	GLU
5	E	177	ARG
6	F	59	GLN
6	F	74	ILE
6	F	87	LYS
6	F	99	LEU
6	F	109	VAL
7	G	21	LYS
7	G	24	VAL
7	G	35	SER
7	G	39	VAL
7	G	139	ILE
7	G	147	LEU
7	G	167	THR
7	G	169	VAL
7	G	223	GLU
7	G	230	ARG
7	G	239	THR
7	G	241	ARG
7	G	243	VAL
8	H	3	ASN
8	H	9	ILE
8	H	39	THR
8	H	108	SER
8	H	111	LEU
8	H	112	ILE
8	H	114	VAL
8	H	121	LEU
9	I	2	SER
9	I	3	VAL
9	I	15	ASP
9	I	45	LEU
9	I	81	THR
10	J	3	VAL
10	J	9	SER
10	J	10	CYS
10	J	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	27	GLU
10	J	34	THR
10	J	45	CYS
10	J	48	ARG
11	K	44	ARG
11	K	45	GLU
11	K	51	THR
11	K	68	GLU
11	K	99	ASN
11	K	103	ILE
11	K	118	GLN
11	K	123	ASP
11	K	133	SER
12	L	38	LEU
12	L	41	SER
12	L	55	ILE
12	L	57	LEU
12	L	66	GLN
13	M	17	ASP
13	M	18	GLN
13	M	31	ARG
13	M	44	LYS
13	M	48	LYS
13	M	52	VAL
13	M	63	GLU
13	M	65	TYR
13	M	77	VAL
13	M	84	GLU
13	M	98	SER
13	M	104	SER
13	M	109	ARG
14	N	51	GLN
14	N	89	ILE
14	N	124	THR
14	N	135	LYS
14	N	153	VAL
14	N	167	LYS
14	N	178	GLU
15	O	66	ASN
15	O	67	ASP
15	O	69	THR
15	O	78	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	80	LEU
15	O	87	ARG
15	O	101	SER
15	O	110	SER
15	O	111	ARG
15	O	117	GLN
15	O	171	CYS
15	O	175	MET
15	O	180	LEU
15	O	181	ARG
15	O	190	ILE
15	O	192	THR
15	O	194	LEU
15	O	202	ASN
15	O	203	ASP
15	O	204	THR
15	O	205	ARG
15	O	212	THR
15	O	213	SER
15	O	215	LEU
15	O	225	LEU
15	O	228	GLN
15	O	232	LEU
15	O	234	ILE
15	O	237	ILE
15	O	239	SER
15	O	240	ILE
15	O	245	GLN
15	O	248	LEU
15	O	341	THR
15	O	350	GLU
15	O	354	SER
15	O	363	THR
15	O	376	TYR
15	O	381	ILE
15	O	395	LEU
15	O	407	SER
15	O	410	VAL
15	O	415	GLU
15	O	437	THR
15	O	454	VAL
15	O	489	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	494	THR
15	O	526	LEU
15	O	543	ILE
15	O	578	SER
15	O	579	LEU
15	O	581	THR
15	O	584	GLN
15	O	597	LEU
15	O	599	LEU
15	O	602	TYR
16	P	21	GLN
16	P	25	LEU
16	P	26	TYR
16	P	49	THR
16	P	55	LEU
16	P	64	LEU
16	P	187	ILE
16	P	195	ASN
16	P	201	GLU
16	P	207	SER
16	P	212	SER
16	P	214	LEU
16	P	220	THR
16	P	225	LEU
16	P	227	LEU
16	P	232	ASN
16	P	233	VAL
16	P	236	ILE
16	P	237	GLU
16	P	243	LYS
16	P	245	ILE
16	P	252	GLU
16	P	256	ARG
16	P	257	ARG
16	P	260	LEU
16	P	261	VAL
16	P	263	ILE
16	P	264	ILE
16	P	270	GLN
16	P	271	ILE
16	P	276	SER
16	P	282	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	286	VAL
16	P	290	GLU
16	P	292	LEU
16	P	297	ILE
16	P	300	LEU
16	P	314	GLN
16	P	321	LYS
16	P	323	ASN
16	P	326	ILE
16	P	329	ILE
16	P	331	LYS
16	P	333	PHE
16	P	343	LEU
16	P	345	ASP
16	P	347	LEU
16	P	359	SER
16	P	360	TRP
16	P	363	ILE
16	P	370	GLN
16	P	377	ARG
16	P	379	LYS
16	P	381	ILE
16	P	384	ASP
16	P	386	MET
16	P	390	GLN
16	P	397	LYS
16	P	402	ILE
16	P	403	ARG
16	P	407	ARG
16	P	408	ILE
16	P	412	ASN
16	P	415	LEU
16	P	417	THR
16	P	419	ARG
16	P	421	ILE
16	P	423	ILE
16	P	424	VAL
16	P	430	ASN
16	P	433	VAL
16	P	439	LYS
16	P	440	HIS
16	P	442	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	448	THR
16	P	453	VAL
16	P	455	LYS
16	P	456	VAL
16	P	460	ASP
16	P	463	LEU
16	P	464	LEU
16	P	465	VAL
16	P	468	VAL
16	P	473	HIS
16	P	474	LYS
16	P	480	VAL
16	P	492	LEU
16	P	494	CYS
16	P	496	THR
16	P	497	VAL
16	P	498	LEU
16	P	500	ILE
16	P	508	ILE
16	P	511	ILE
16	P	531	PHE
16	P	534	VAL
16	P	538	LEU
16	P	539	VAL
16	P	545	SER
16	P	546	GLU
16	P	555	THR
16	P	556	GLN
16	P	567	ILE
16	P	580	ASN
16	P	582	ASP
16	P	584	ARG
16	P	593	VAL
16	P	596	ILE
16	P	600	GLU
16	P	609	ASN
16	P	615	ASN
16	P	617	HIS
16	P	625	ASP
16	P	626	LEU
16	P	630	LEU
16	P	632	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	634	THR
16	P	635	ASN
16	P	637	LEU
16	P	638	LEU
16	P	646	ASP
16	P	647	GLU
16	P	649	ILE
16	P	654	LEU
16	P	656	HIS
16	P	659	LEU
16	P	660	LYS
16	P	662	LEU
16	P	664	GLU
16	P	665	ASN
16	P	667	ASP
16	P	671	SER
16	P	676	SER
16	P	679	LEU
16	P	693	PHE
16	P	694	ILE
16	P	700	LEU
16	P	706	GLU
16	P	711	LEU
16	P	712	ASP
16	P	726	SER
16	P	730	GLU
16	P	731	LEU
16	P	736	ILE
16	P	748	GLU
16	P	749	LYS
16	P	751	SER
16	P	753	PHE
16	P	757	GLN
16	P	762	ARG
16	P	768	TYR
16	P	772	ILE
16	P	777	MET
17	Q	17	SER
17	Q	26	ARG
17	Q	27	ARG
17	Q	94	LYS
17	Q	101	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	103	LEU
17	Q	111	ILE
17	Q	112	LEU
17	Q	138	LEU
17	Q	139	LYS
17	Q	143	THR
17	Q	144	ILE
17	Q	145	ASN
17	Q	147	GLN
17	Q	149	GLN
17	Q	150	GLU
17	Q	154	LEU
17	Q	159	THR
17	Q	164	ILE
17	Q	167	LEU
17	Q	169	SER
17	Q	173	SER
17	Q	176	VAL
17	Q	187	THR
17	Q	204	ARG
17	Q	207	LEU
17	Q	218	SER
17	Q	226	LEU
17	Q	232	LEU
17	Q	248	SER
17	Q	273	VAL
17	Q	278	GLU
17	Q	286	LEU
17	Q	288	GLU
17	Q	290	THR
17	Q	291	ASP
17	Q	297	ARG
17	Q	301	HIS
17	Q	312	LEU
17	Q	318	LEU
17	Q	328	LEU
17	Q	332	LEU
17	Q	337	SER
17	Q	348	ILE
17	Q	363	SER
17	Q	367	PHE
17	Q	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	378	LEU
17	Q	379	LYS
17	Q	384	GLN
17	Q	419	LEU
17	Q	435	GLN
17	Q	436	LEU
17	Q	439	ILE
17	Q	443	GLN
17	Q	444	GLU
17	Q	453	PHE
17	Q	494	SER
17	Q	495	LYS
17	Q	496	GLU
17	Q	498	LEU
17	Q	502	ILE
17	Q	513	MET
18	R	1	MET
18	R	4	VAL
18	R	8	LEU
18	R	10	ASN
18	R	11	ARG
18	R	28	SER
18	R	34	ILE
18	R	74	GLN
18	R	80	ARG
18	R	84	TRP
18	R	85	ARG
18	R	87	VAL
18	R	143	THR
18	R	150	GLN
18	R	155	GLN
18	R	156	LYS
18	R	165	ILE
18	R	167	LYS
18	R	168	ILE
18	R	175	ILE
18	R	178	LEU
18	R	181	THR
18	R	202	THR
18	R	206	ARG
18	R	209	ARG
18	R	210	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	211	ARG
18	R	212	HIS
18	R	216	LEU
18	R	218	ASP
18	R	231	LEU
18	R	235	ILE
18	R	238	THR
18	R	242	ILE
18	R	247	ILE
18	R	248	LYS
18	R	250	LEU
18	R	255	VAL
18	R	266	SER
18	R	269	ASP
18	R	272	GLN
18	R	276	GLN
18	R	294	VAL
18	R	298	GLN
18	R	299	THR
18	R	302	ARG
18	R	307	LYS
18	R	308	PHE
18	R	313	LEU
18	R	319	ASN
18	R	322	LYS
18	R	323	SER
18	R	345	LEU
18	R	359	MET
18	R	364	VAL
18	R	367	ILE
18	R	373	LEU
18	R	374	LEU
18	R	401	ILE
18	R	402	ASN
18	R	403	GLN
18	R	410	TYR
18	R	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	HIS
1	A	382	GLN
1	A	407	GLN
1	A	425	ASN
1	A	431	GLN
1	A	470	HIS
1	A	535	GLN
1	A	590	ASN
1	A	636	HIS
1	A	1026	GLN
1	A	1088	HIS
1	A	1162	ASN
1	A	1314	GLN
1	A	1320	GLN
2	B	87	ASN
2	B	146	ASN
2	B	182	GLN
2	B	321	GLN
2	B	422	GLN
2	B	462	GLN
2	B	473	GLN
2	B	554	GLN
2	B	702	ASN
2	B	893	ASN
2	B	1163	GLN
3	C	232	GLN
3	C	323	ASN
3	C	335	GLN
5	E	5	ASN
5	E	32	GLN
6	F	59	GLN
7	G	23	GLN
7	G	56	ASN
7	G	59	GLN
7	G	126	GLN
9	I	44	ASN
9	I	97	HIS
12	L	53	HIS
13	M	18	GLN
14	N	61	ASN
14	N	132	GLN
15	O	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	105	ASN
15	O	117	GLN
15	O	210	ASN
15	O	228	GLN
15	O	245	GLN
15	O	342	HIS
15	O	362	ASN
15	O	371	HIS
15	O	390	GLN
15	O	488	HIS
15	O	497	ASN
15	O	521	ASN
15	O	533	GLN
15	O	547	ASN
15	O	549	ASN
16	P	228	ASN
16	P	348	HIS
16	P	368	HIS
16	P	388	ASN
16	P	461	HIS
16	P	635	ASN
17	Q	325	GLN
17	Q	406	GLN
18	R	160	HIS
18	R	184	ASN
18	R	212	HIS
18	R	272	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	SO4	R	601	-	4,4,4	0.27	0	6,6,6	0.13	0
20	SO4	Q	1002	-	4,4,4	0.25	0	6,6,6	0.25	0
20	SO4	P	901	-	4,4,4	0.23	0	6,6,6	0.24	0
20	SO4	P	902	-	4,4,4	0.24	0	6,6,6	0.24	0
20	SO4	P	903	-	4,4,4	0.23	0	6,6,6	0.12	0

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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	601	SO4	4	0
20	Q	1002	SO4	1	0
20	P	902	SO4	1	0
20	P	903	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
7	G	1
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	24:VAL	C	25:THR	N	4.53
1	I	45:LEU	C	46:LYS	N	3.17
1	A	438:ILE	C	439:ASP	N	2.97
1	A	991:LYS	C	992:PRO	N	2.86

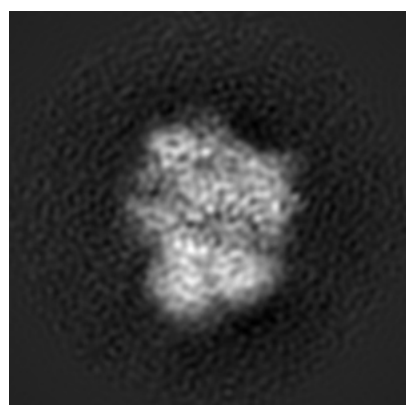
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3590. These allow visual inspection of the internal detail of the map and identification of artifacts.

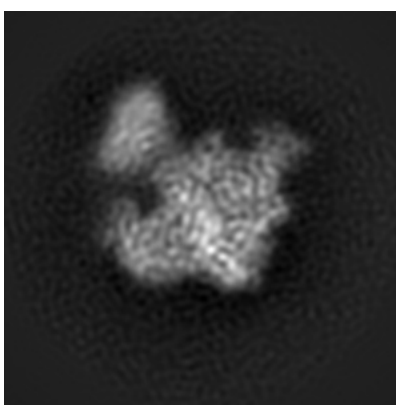
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

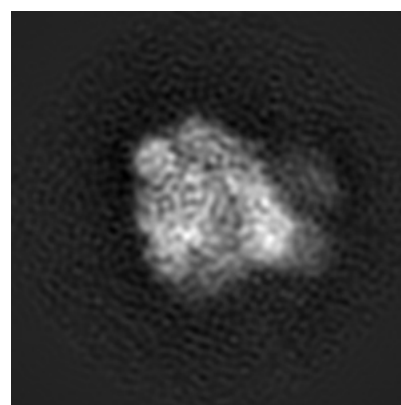
6.1.1 Primary map



X



Y

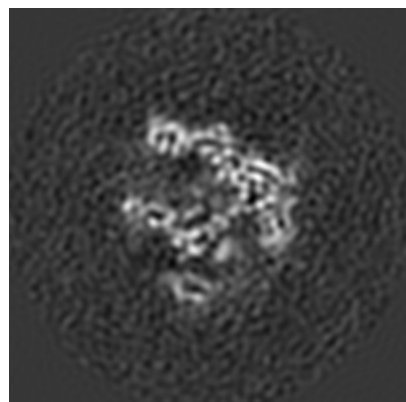


Z

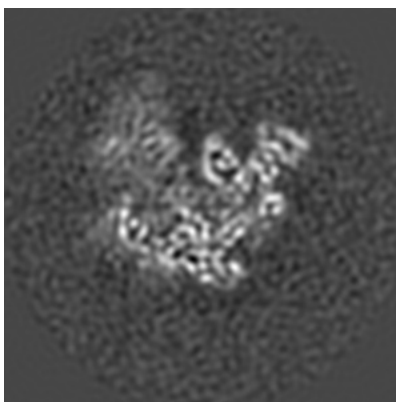
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

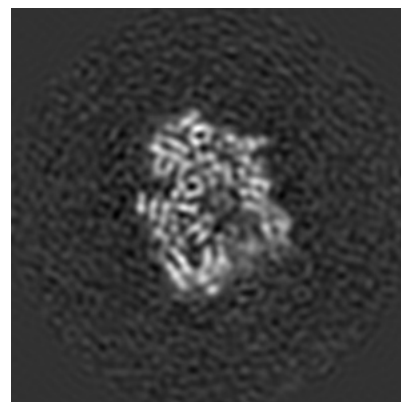
6.2.1 Primary map



X Index: 120



Y Index: 120

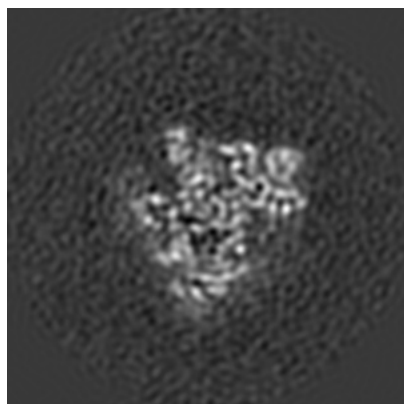


Z Index: 120

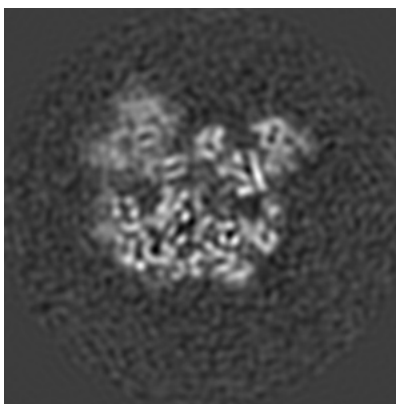
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

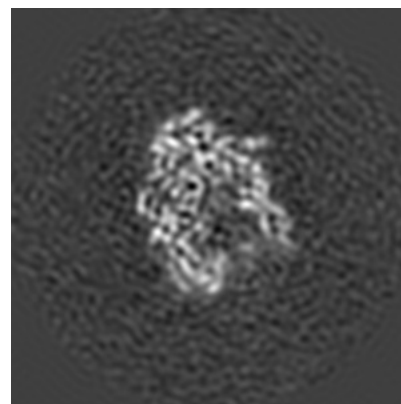
6.3.1 Primary map



X Index: 111



Y Index: 109

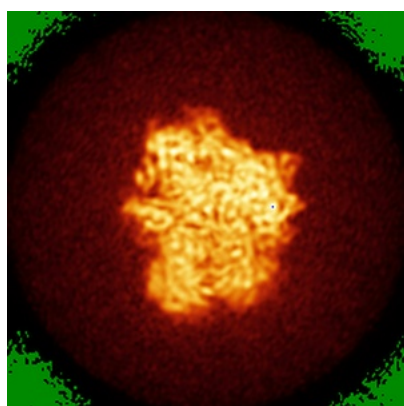


Z Index: 122

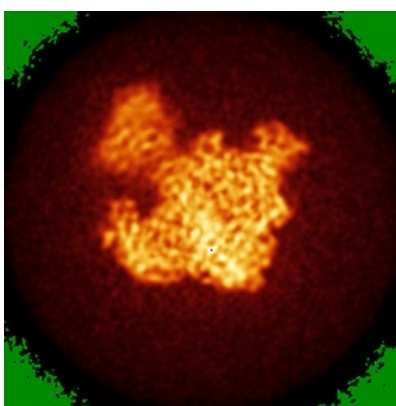
The images above show the largest variance slices of the map in three orthogonal directions.

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

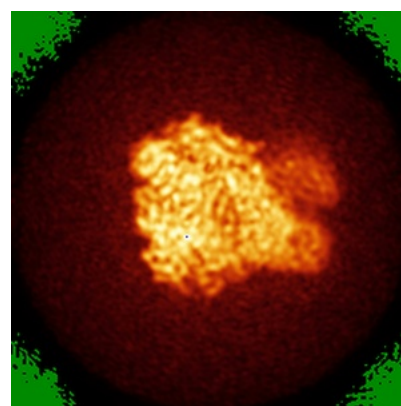
6.4.1 Primary map



X



Y

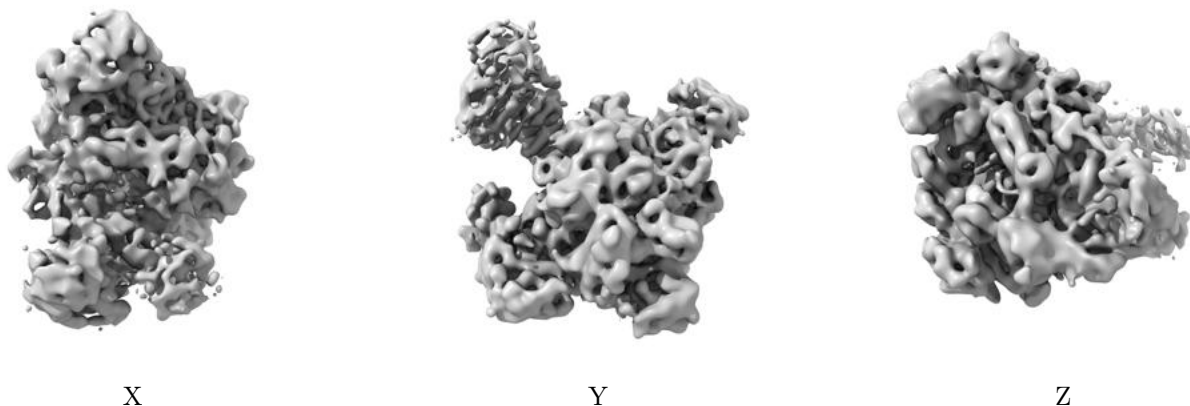


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0205. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

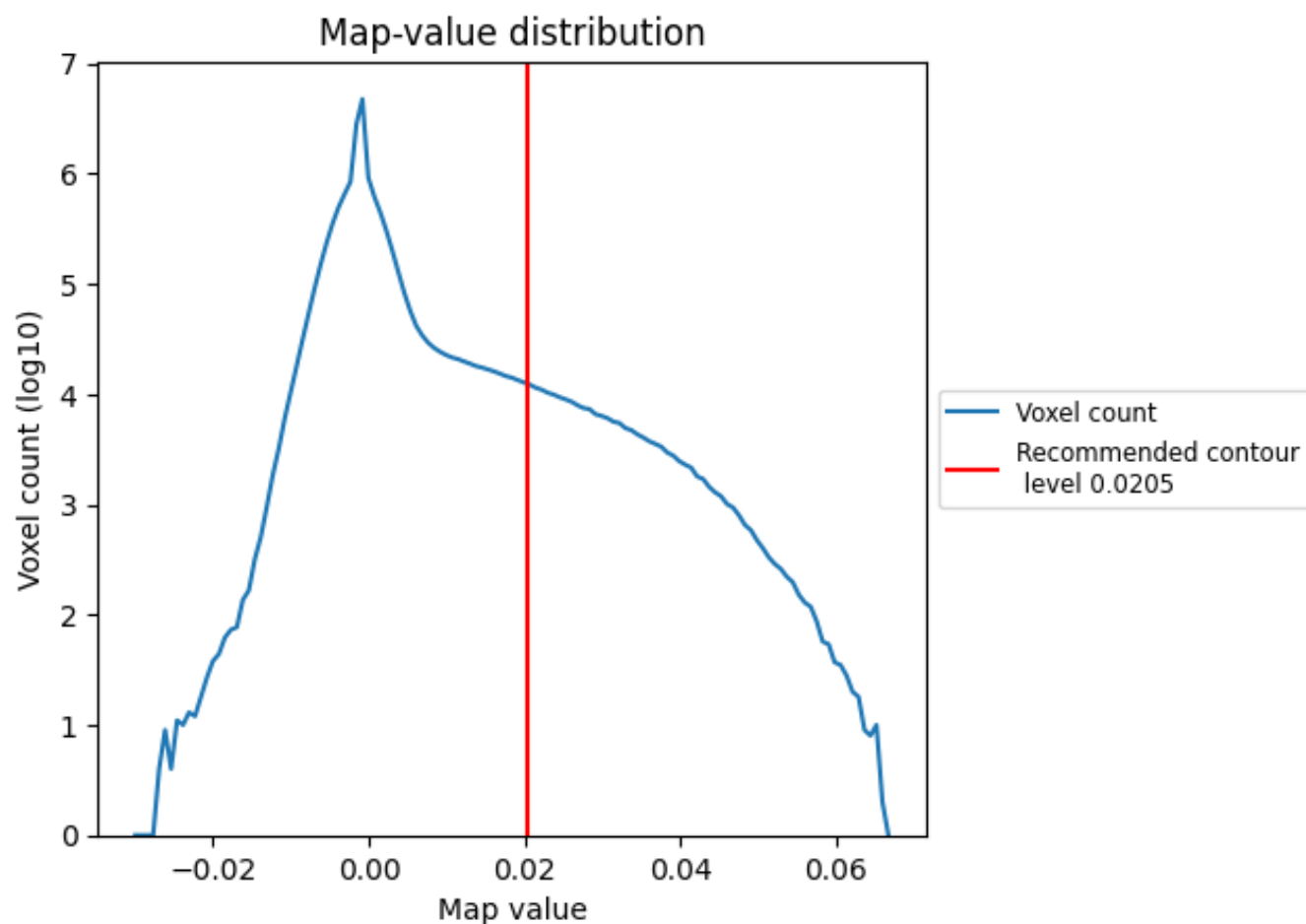
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

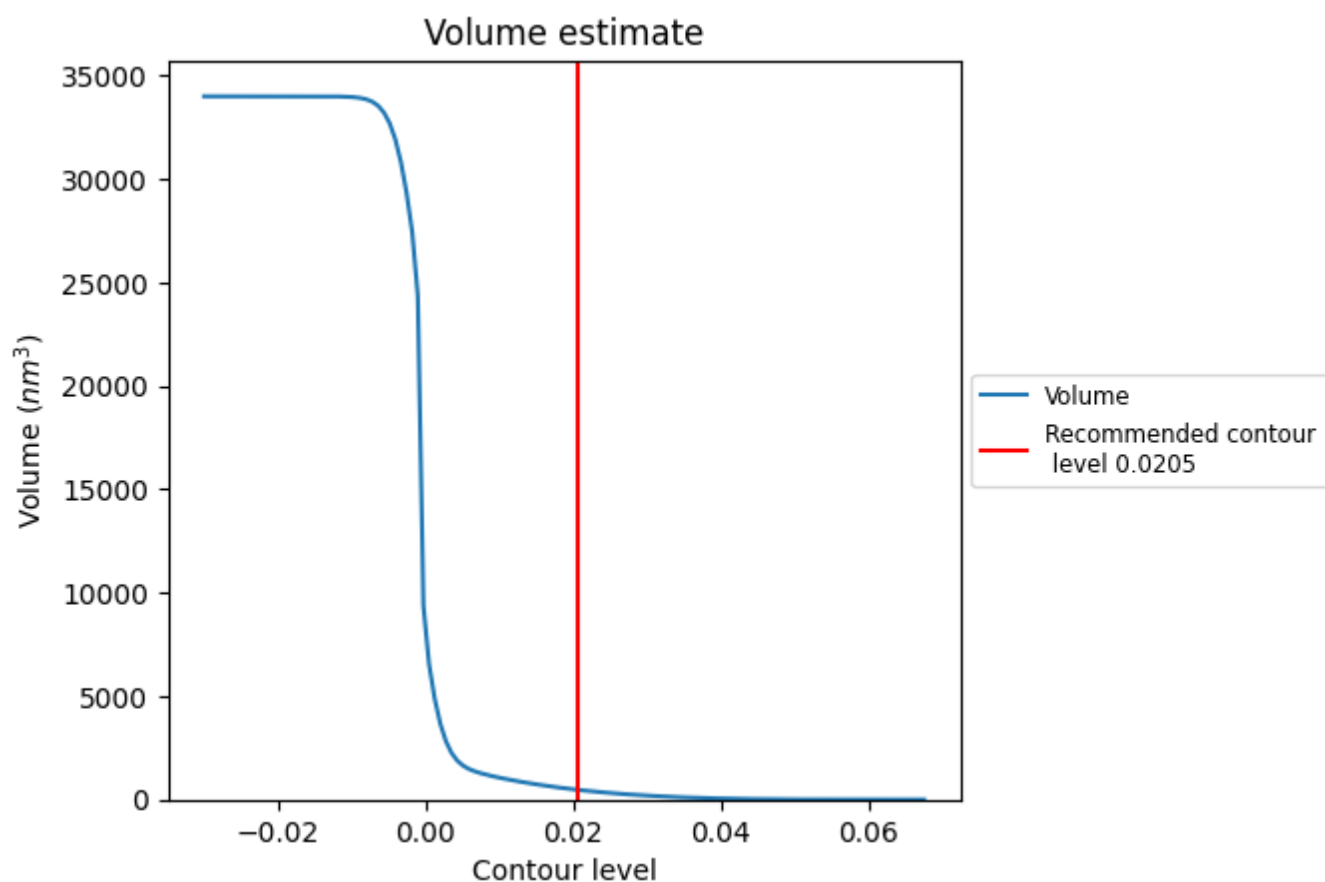
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

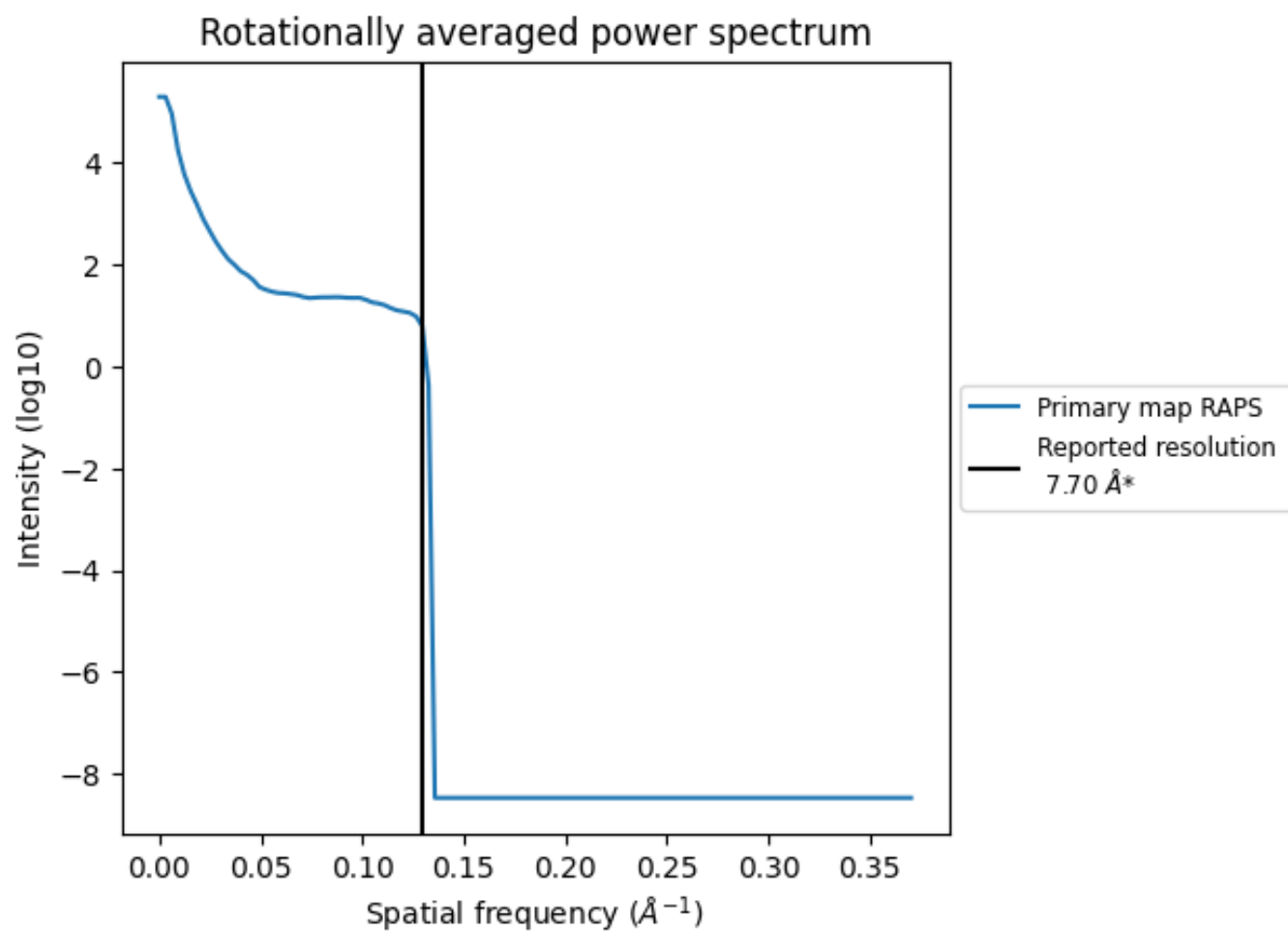
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 475 nm³; this corresponds to an approximate mass of 429 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 0.130 Å⁻¹

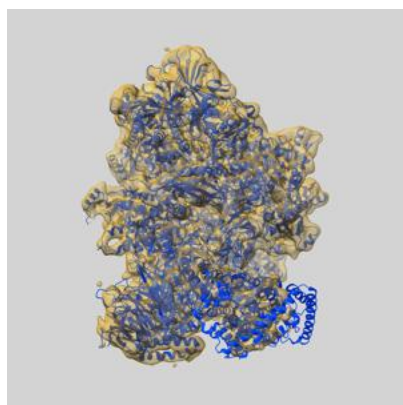
8 Fourier-Shell correlation

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

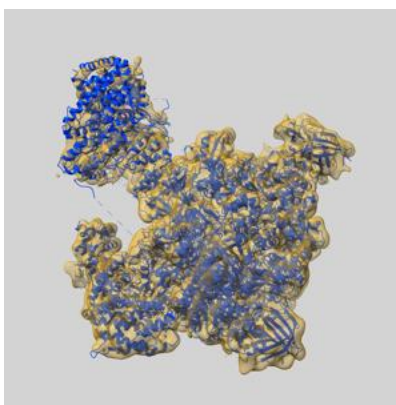
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3590 and PDB model 5N5Y. Per-residue inclusion information can be found in section [3](#) on page [8](#).

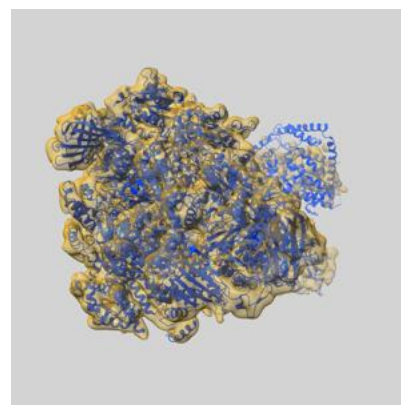
9.1 Map-model overlay [i](#)



X



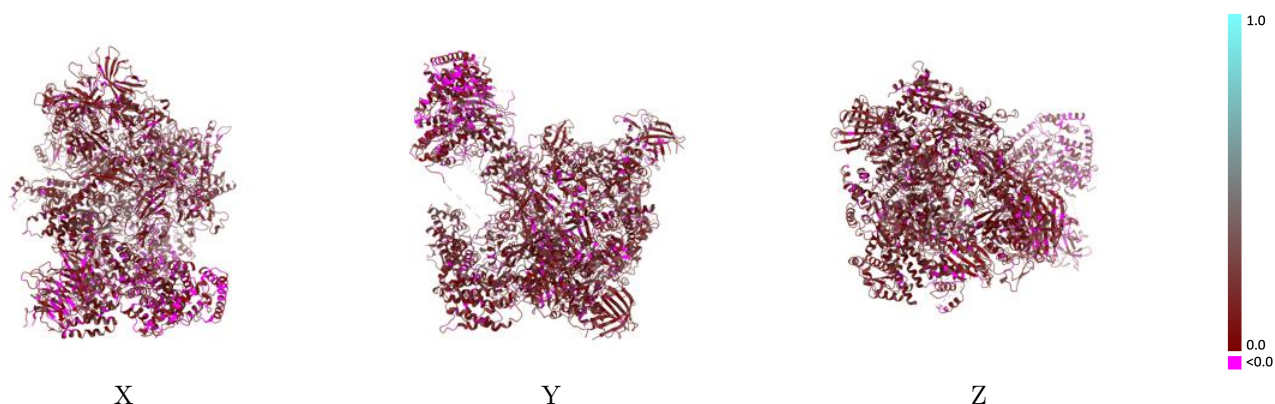
Y



Z

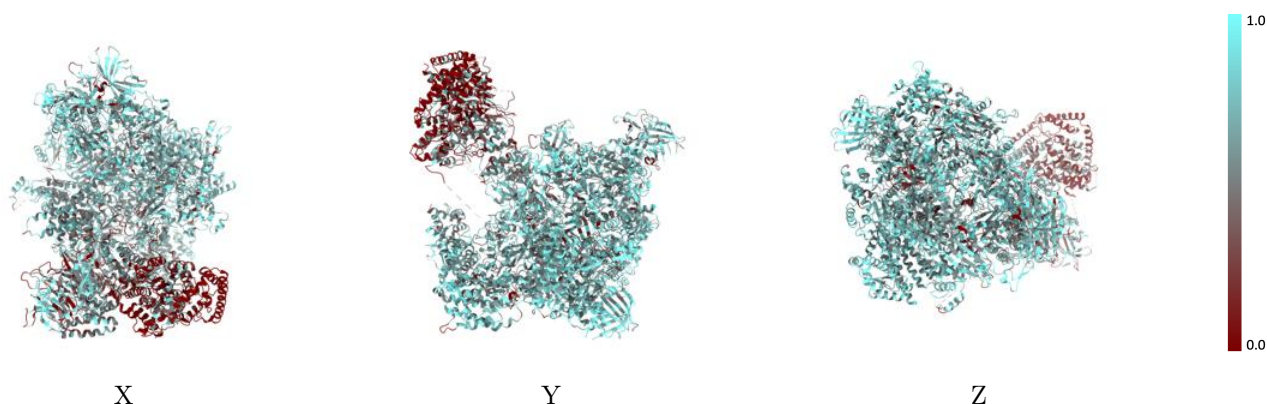
The images above show the 3D surface view of the map at the recommended contour level 0.0205 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



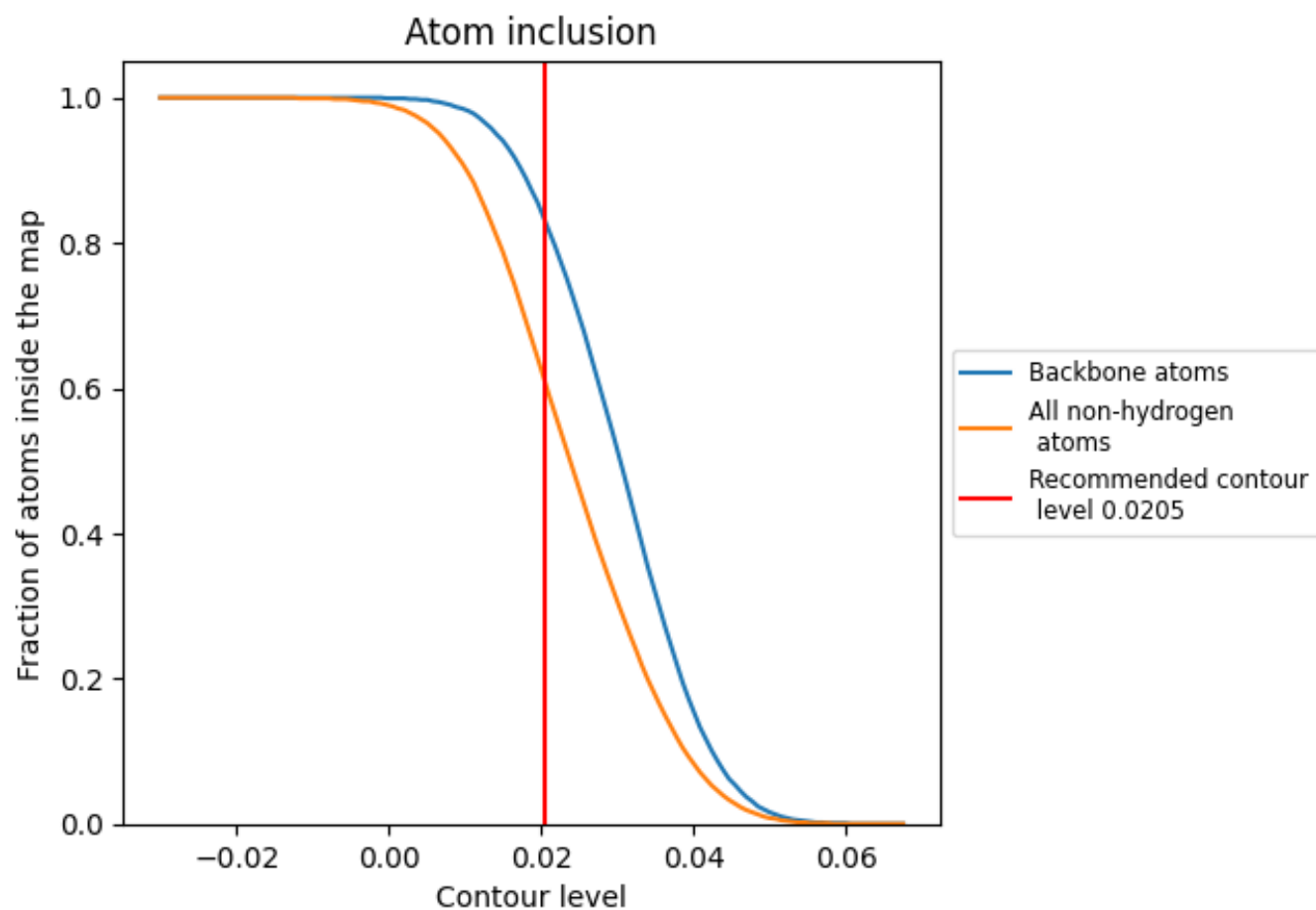
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0205).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 61% 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 (0.0205) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6090	 0.1360
A	 0.6710	 0.1450
B	 0.6630	 0.1390
C	 0.7390	 0.1510
D	 0.7010	 0.1650
E	 0.7490	 0.1640
F	 0.6800	 0.1590
G	 0.7360	 0.1430
H	 0.7800	 0.1650
I	 0.4990	 0.1470
J	 0.7050	 0.1390
K	 0.7080	 0.1590
L	 0.6560	 0.1360
M	 0.6540	 0.1420
N	 0.6120	 0.1470
O	 0.6660	 0.1450
P	 0.3550	 0.0870
Q	 0.2790	 0.0930
R	 0.5080	 0.1370

