



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 8A3T / pdb_00008a3t
EMDB ID : EMD-15123
Title : S. cerevisiae APC/C-Cdh1 complex
Authors : Barford, D.; Vazquez-Fernandez, E.; Zhang, Z.; Yang, J.
Deposited on : 2022-06-09
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

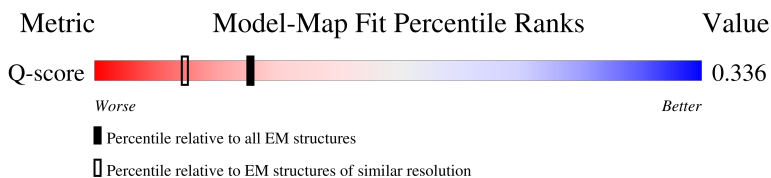
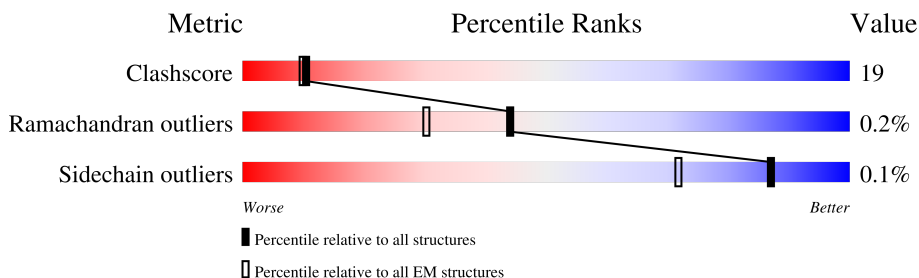
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

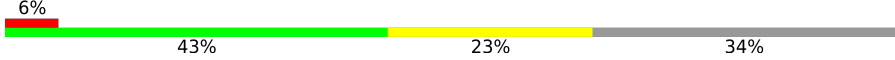
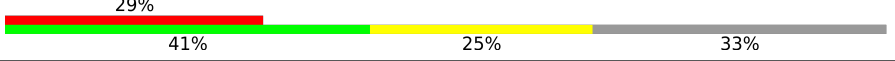
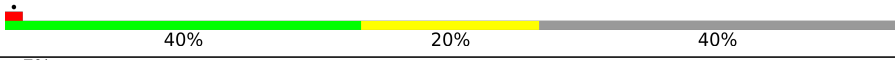
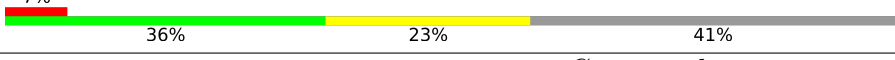
The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	F	758	
1	H	758	
2	J	850	
2	K	850	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	124	
3	W	124	
4	E	265	
5	A	250	
6	B	566	
7	S	1518	
8	C	1748	
9	O	685	
10	D	626	
10	P	626	
11	I	170	
12	N	368	
13	Q	652	
14	T	853	
15	U	165	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 61351 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 Anaphase-promoting complex subunit CDC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	502	Total	C	N	O	S	0	0
			3991	2569	656	739	27		
1	H	505	Total	C	N	O	S	0	0
			4031	2593	664	747	27		

- Molecule 2 is a protein called Anaphase-promoting complex subunit CDC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	509	Total	C	N	O	S	0	0
			4128	2661	675	769	23		
2	K	505	Total	C	N	O	S	0	0
			4102	2642	673	764	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	841	LYS	-	expression tag	UNP P09798
J	842	SER	-	expression tag	UNP P09798
J	843	SER	-	expression tag	UNP P09798
J	844	ILE	-	expression tag	UNP P09798
J	845	PRO	-	expression tag	UNP P09798
J	846	GLU	-	expression tag	UNP P09798
J	847	ASN	-	expression tag	UNP P09798
J	848	LEU	-	expression tag	UNP P09798
J	849	TYR	-	expression tag	UNP P09798
J	850	PHE	-	expression tag	UNP P09798
K	841	LYS	-	expression tag	UNP P09798
K	842	SER	-	expression tag	UNP P09798
K	843	SER	-	expression tag	UNP P09798
K	844	ILE	-	expression tag	UNP P09798
K	845	PRO	-	expression tag	UNP P09798
K	846	GLU	-	expression tag	UNP P09798
K	847	ASN	-	expression tag	UNP P09798

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	848	LEU	-	expression tag	UNP P09798
K	849	TYR	-	expression tag	UNP P09798
K	850	PHE	-	expression tag	UNP P09798

- Molecule 3 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	35	Total	C	N	O	S	0	0
			284	174	51	58	1		
3	W	37	Total	C	N	O	S	0	0
			300	184	54	61	1		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	130	Total	C	N	O	S	0	0
			1091	678	201	205	7		

- Molecule 5 is a protein called Anaphase-promoting complex subunit DOC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	219	Total	C	N	O	S	0	0
			1743	1118	304	311	10		

- Molecule 6 is a protein called CDH1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	440	Total	C	N	O	S	0	0
			3418	2143	602	660	13		

- Molecule 7 is a protein called HSL1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	6	Total	C	N	O	0	0
			45	27	7	11		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	1410	Total	C	N	O	S	0	0
			10863	7023	1756	2038	46		

- Molecule 9 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	658	Total	C	N	O	S	0	0
			5288	3402	869	990	27		

- Molecule 10 is a protein called Anaphase-promoting complex subunit CDC23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	560	Total	C	N	O	S	0	0
			4524	2925	729	844	26		
10	P	556	Total	C	N	O	S	0	0
			4518	2922	738	831	27		

- Molecule 11 is a protein called Anaphase-promoting complex subunit SWM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total	C	N	O	S	0	0
			906	568	158	176	4		

- Molecule 12 is a protein called Anaphase-promoting complex subunit MND2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	96	Total	C	N	O	S	0	0
			784	504	138	139	3		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	623	Total	C	N	O	S	0	0
			5083	3278	842	950	13		

- Molecule 14 is a protein called Anaphase-promoting complex subunit 2.

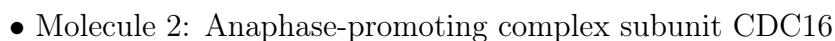
Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	645	Total	C	N	O	S	0	0
			5337	3466	871	976	24		

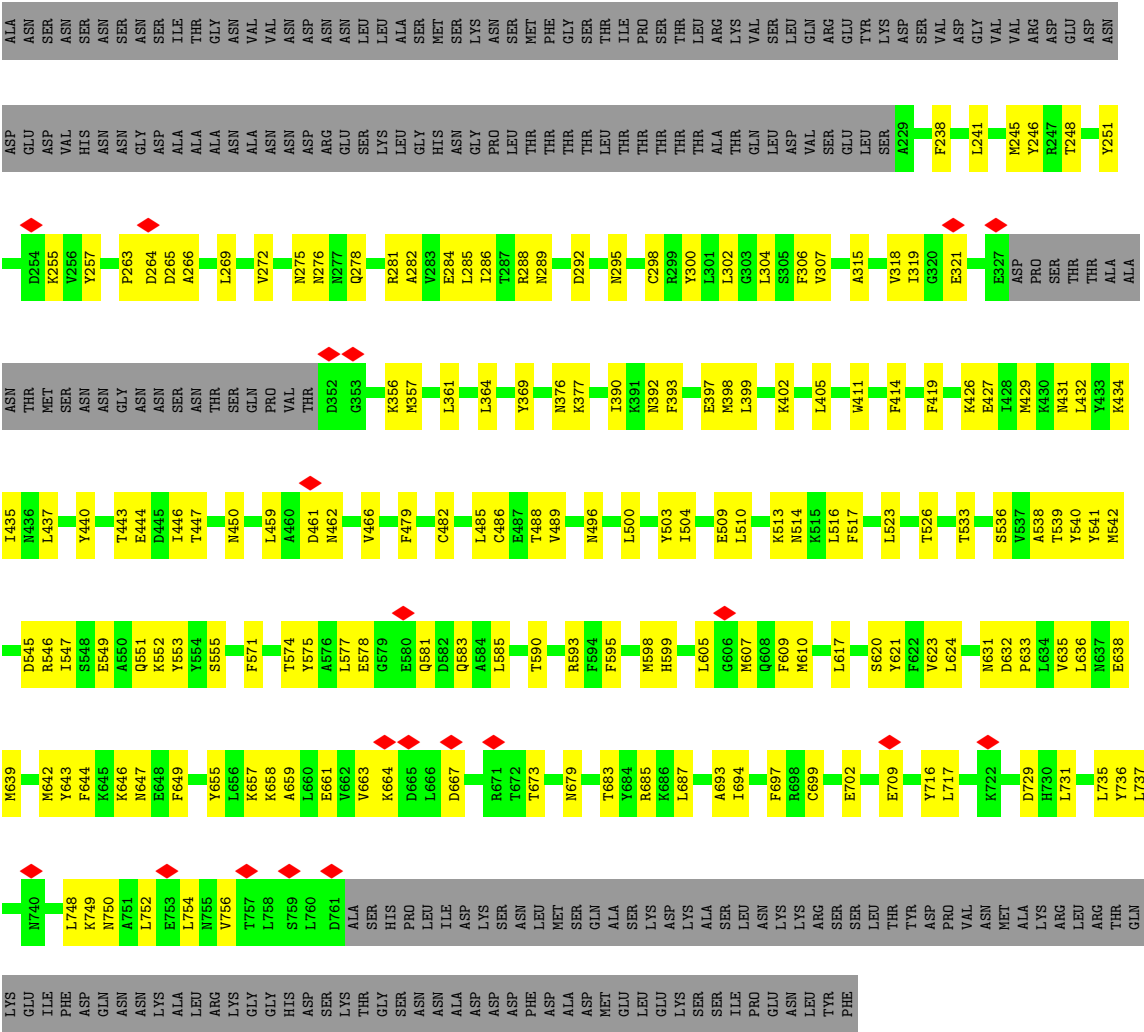
- Molecule 15 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	114	Total	C	N	O	S	0	0
			912	574	164	162	12		

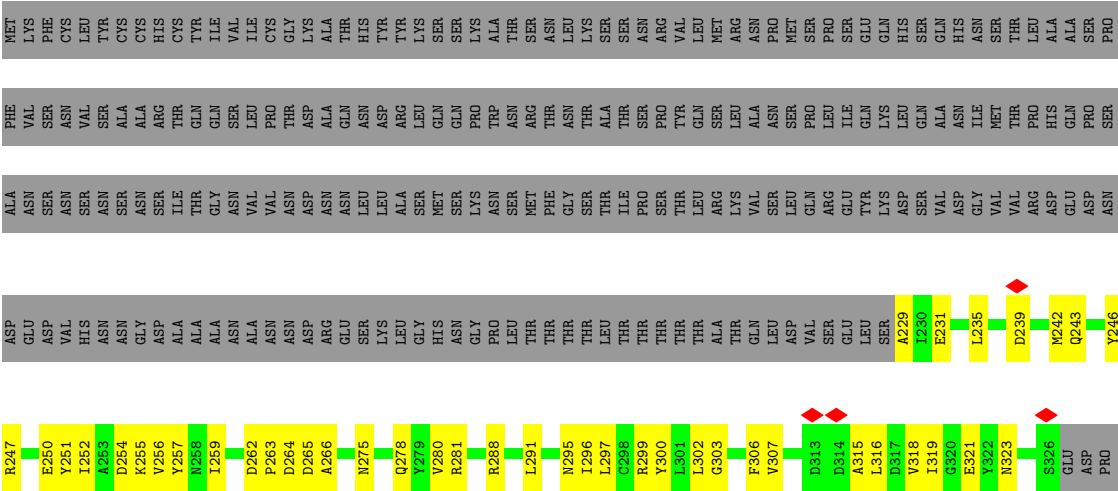
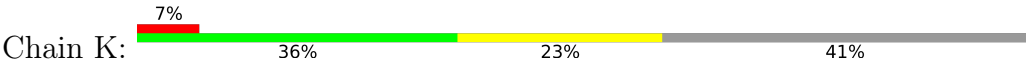
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

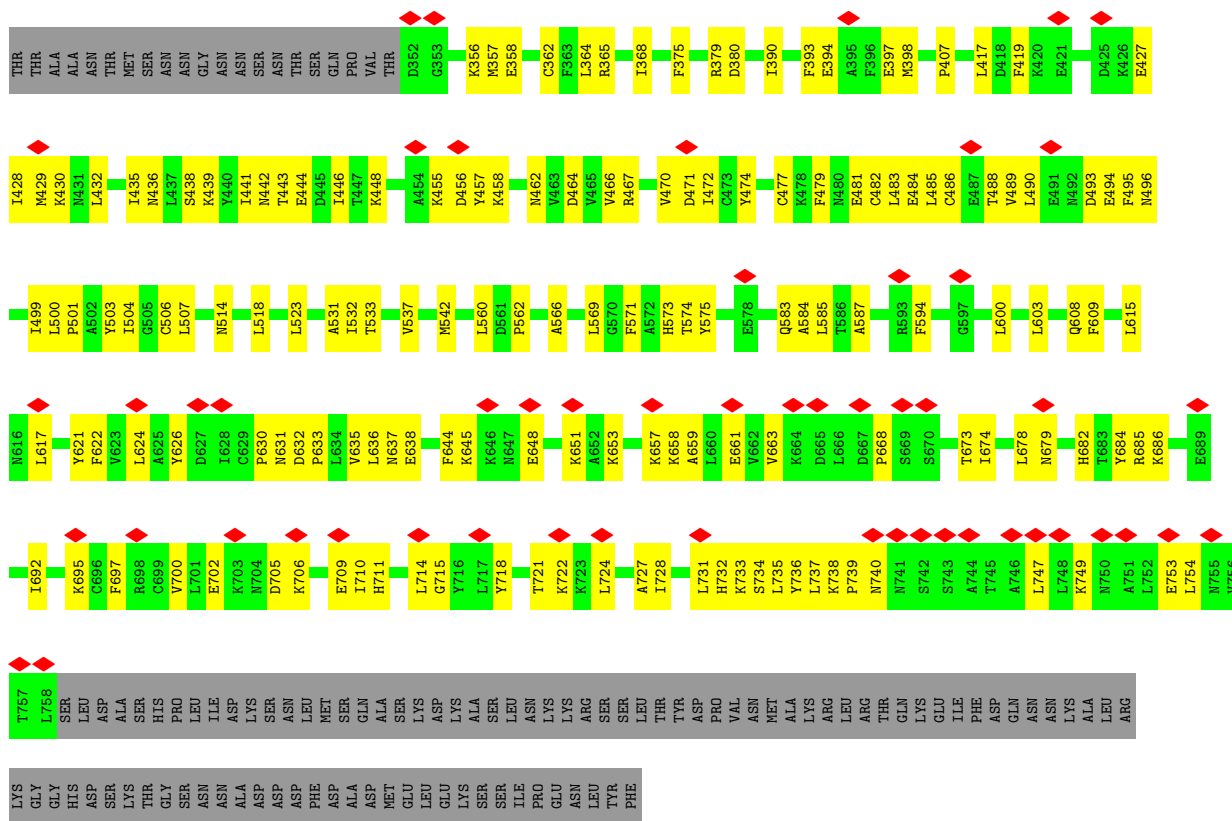
Mol	Chain	Residues	Atoms		AltConf
16	U	3	Total 3	Zn 3	0



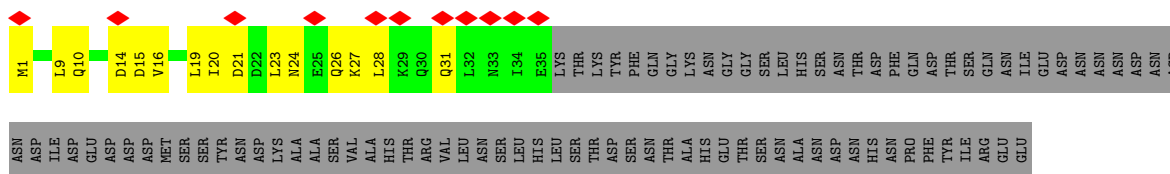


• Molecule 2: Anaphase-promoting complex subunit CDC16

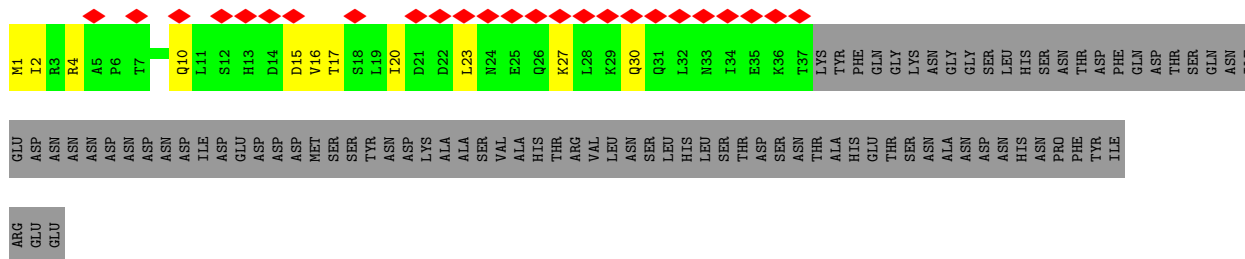




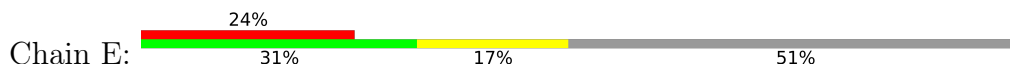
• Molecule 3: Anaphase-promoting complex subunit CDC26

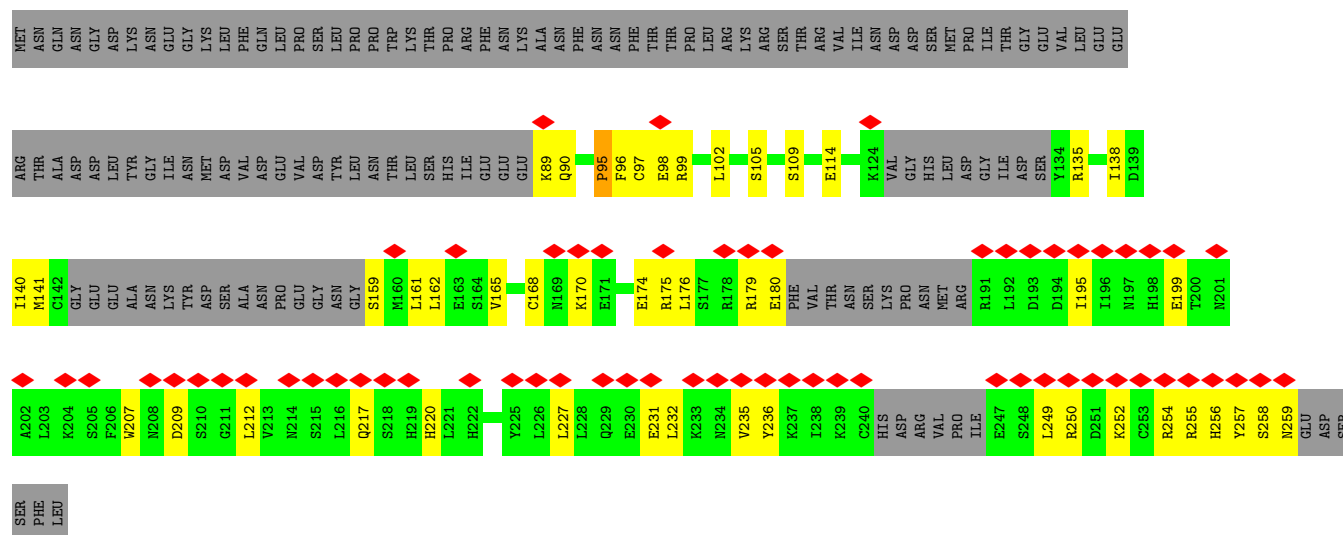


• Molecule 3: Anaphase-promoting complex subunit CDC26



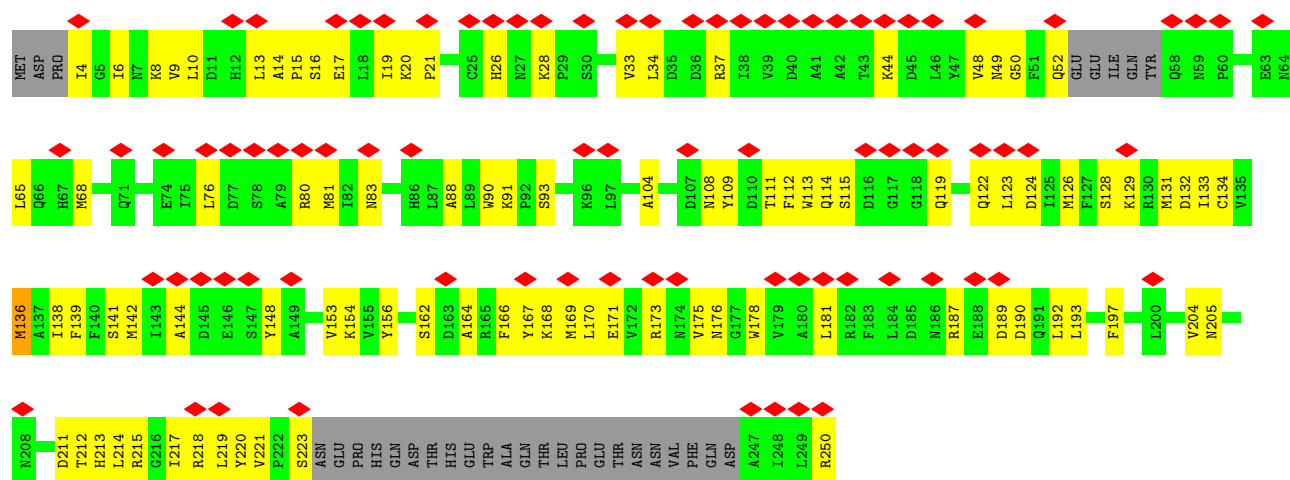
• Molecule 4: Anaphase-promoting complex subunit 9





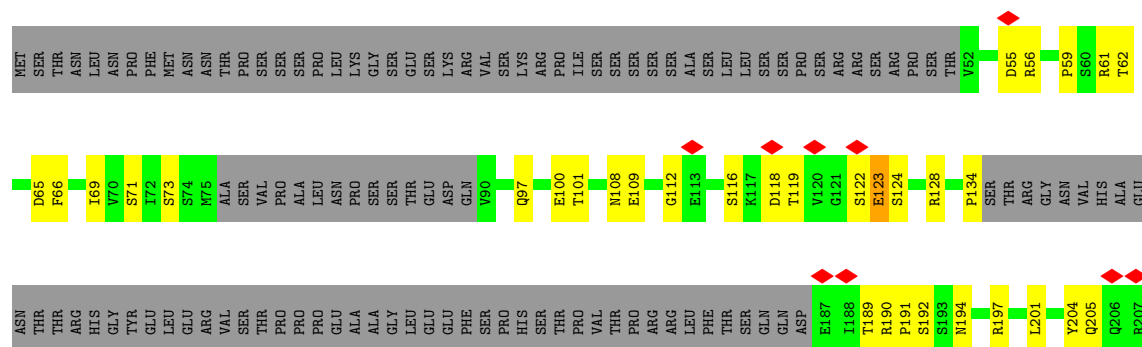
• Molecule 5: Anaphase-promoting complex subunit DOC1

Chain A: 33% 50% 38% 12%



• Molecule 6: CDH1 isoform 1

Chain B: 49% 46% 32% 22%

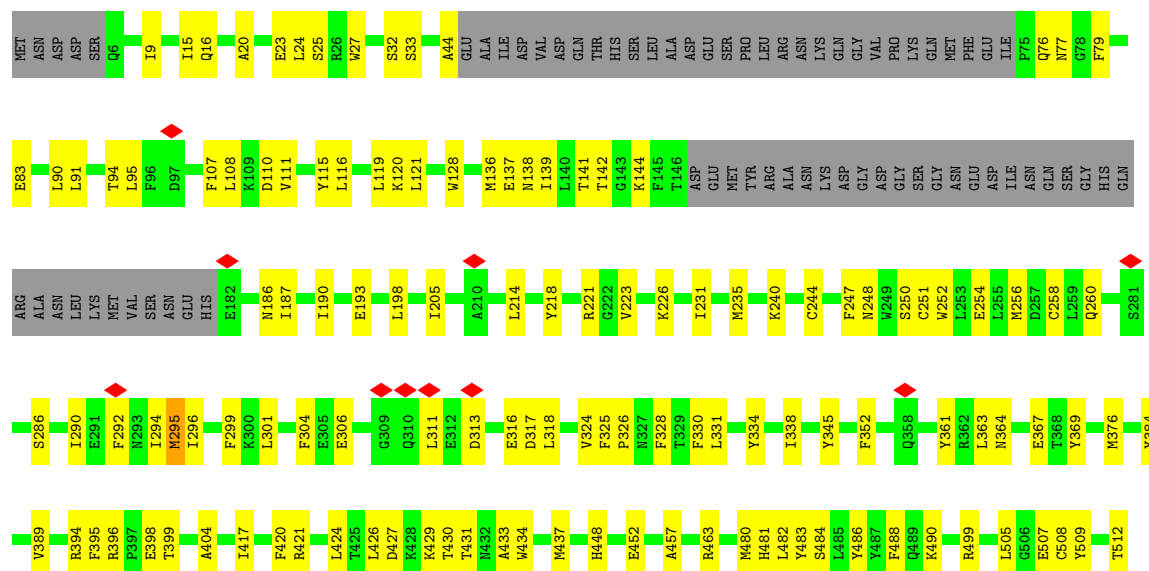


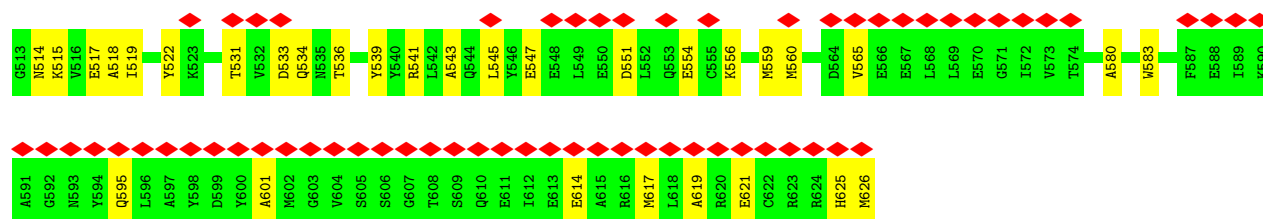
- Molecule 8: Anaphase-promoting complex subunit 1

Category	Value	Color
NET	132	Green
THR	133	Green
SER	134	Green
LYS	135	Green
PRO	136	Green
SER	137	Green
THR	138	Green
ARG	139	Green
ASN	140	Green
ASP	141	Green
TYR	142	Green
LEU	143	Green
PRO	144	Green
GLU	145	Green
THR	146	Green
HIS	147	Green
ASN	148	Green
GLY	149	Green
GLU	150	Green
TYR	151	Green
THR	152	Green
GLY	153	Green
ASP	154	Green
SER	155	Green
PRO	156	Green
E27	157	Green
I32	158	Yellow
N33	159	Yellow
I34	160	Yellow
I35	161	Yellow
N36	162	Yellow
K37	163	Yellow
I38	164	Yellow
G39	165	Yellow
S48	166	Yellow
E49	167	Yellow
D50	168	Yellow
V54	169	Yellow
I58	170	Yellow
E59	171	Yellow
R64	172	Yellow
Y68	173	Yellow
I72	174	Yellow
A75	175	Yellow
G76	176	Yellow
Y77	177	Yellow
I78	178	Yellow
D79	179	Yellow
F80	180	Yellow
E81	181	Yellow
E82	182	Yellow

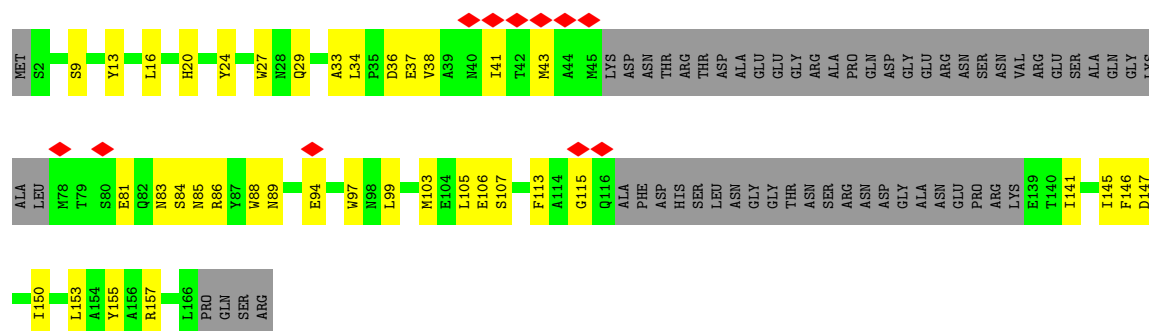




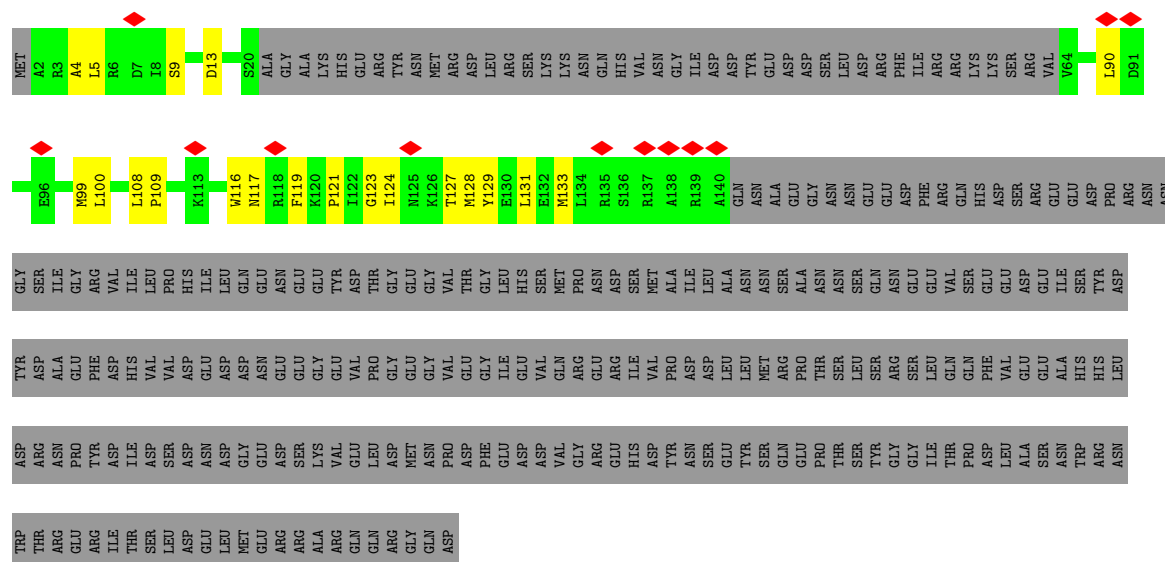




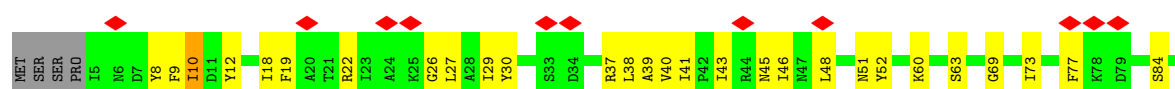
• Molecule 11: Anaphase-promoting complex subunit SWM1

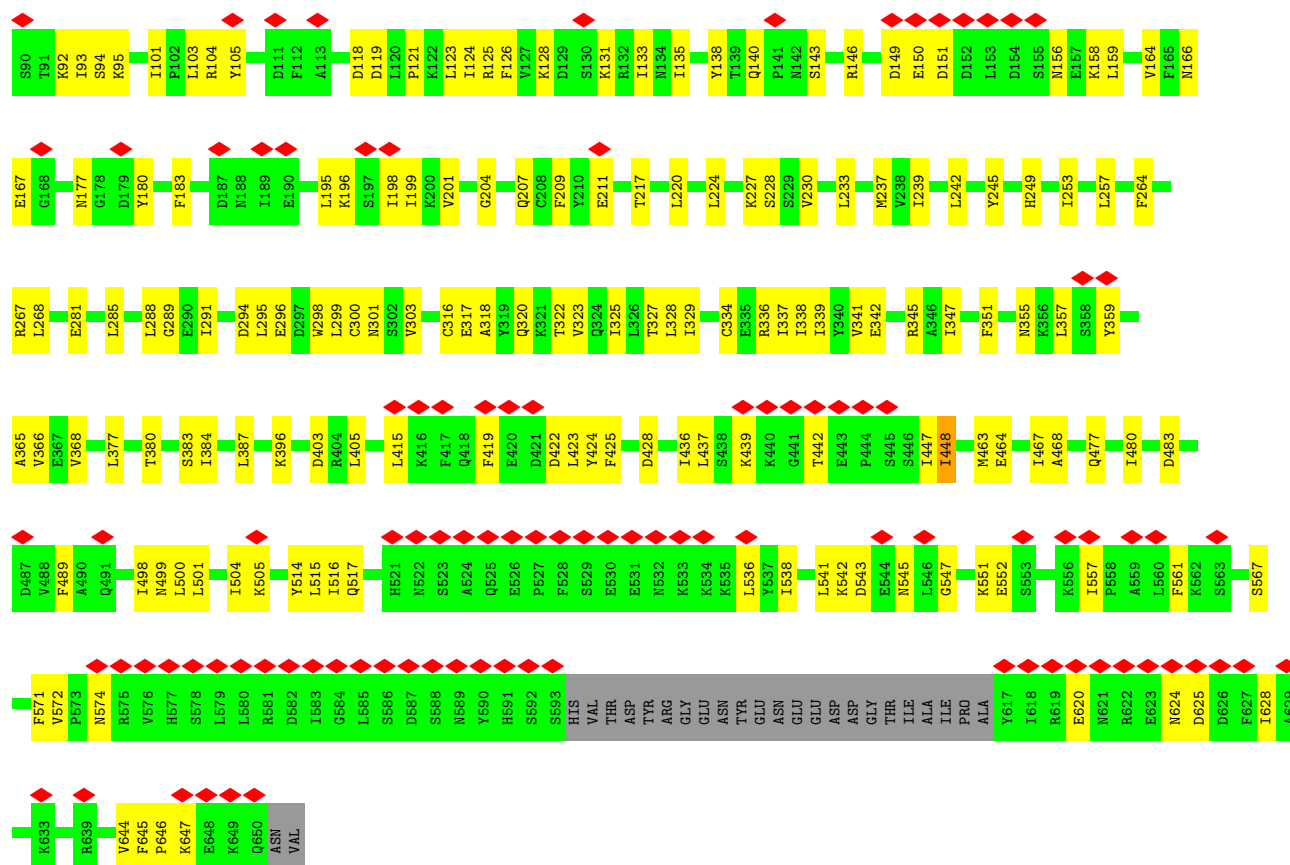


• Molecule 12: Anaphase-promoting complex subunit MND2

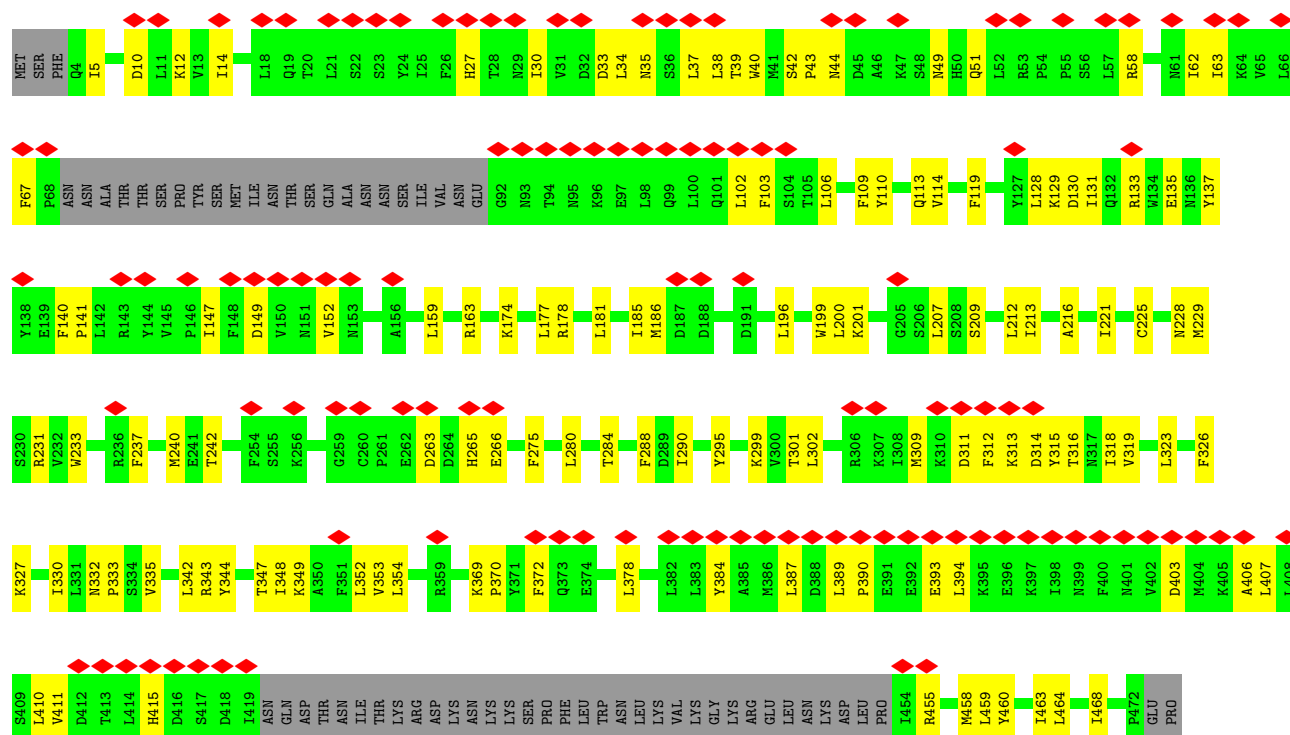
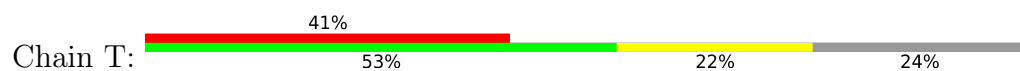


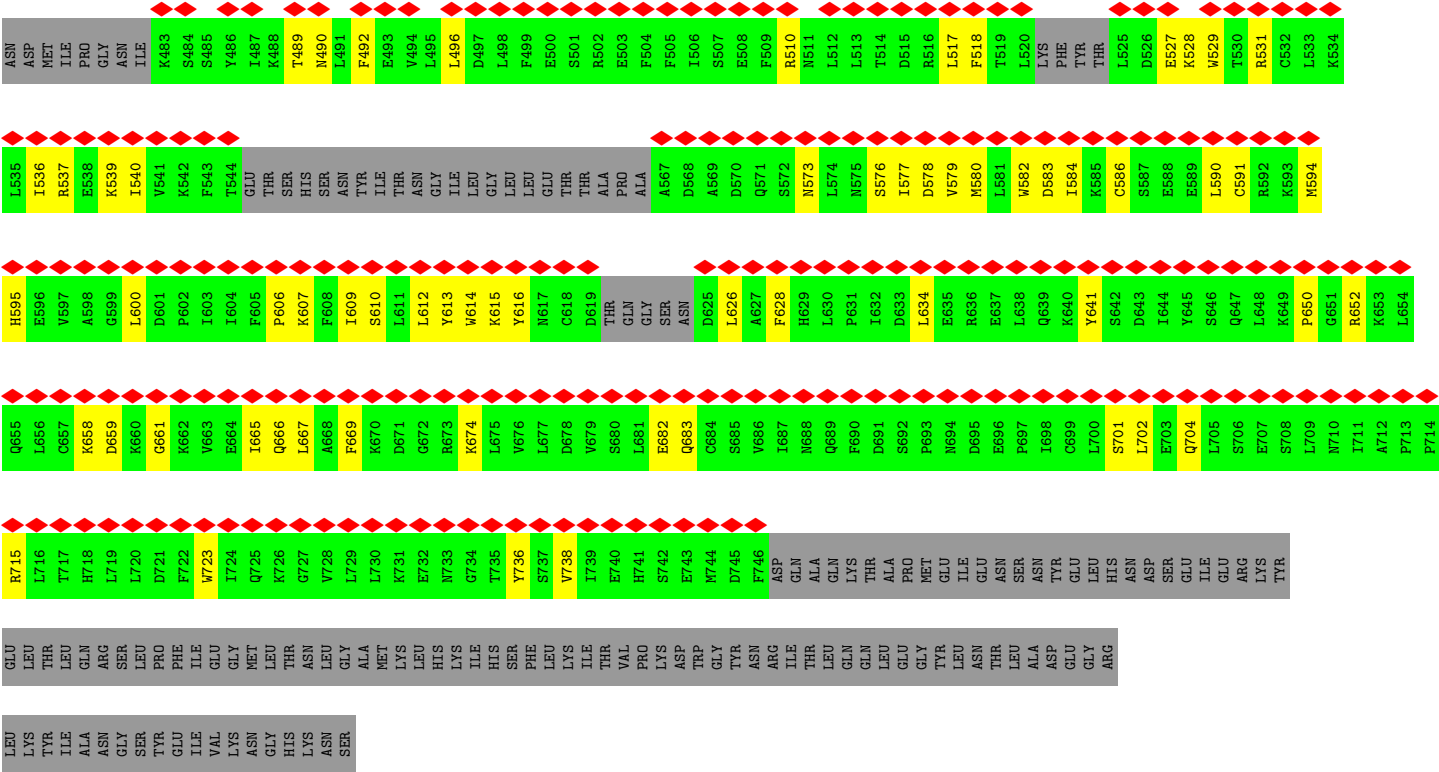
• Molecule 13: Anaphase-promoting complex subunit 4



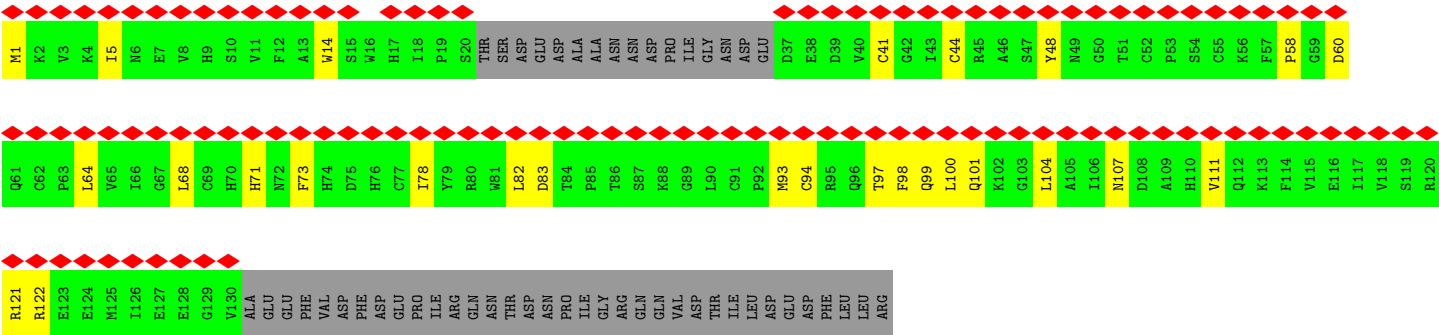


• Molecule 14: Anaphase-promoting complex subunit 2





● Molecule 15: Anaphase-promoting complex subunit 11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	F	0.15	0/4079	0.41	0/5525
1	H	0.16	0/4118	0.39	0/5574
2	J	0.16	0/4214	0.41	0/5692
2	K	0.18	0/4188	0.40	0/5657
3	G	0.22	0/285	0.58	0/384
3	W	0.15	0/301	0.41	0/405
4	E	0.72	1/1108 (0.1%)	0.63	2/1481 (0.1%)
5	A	0.13	0/1785	0.38	1/2418 (0.0%)
6	B	0.14	0/3487	0.34	0/4730
7	S	0.13	0/44	0.47	0/59
8	C	0.13	0/11088	0.35	1/15080 (0.0%)
9	O	0.13	0/5387	0.34	0/7291
10	D	0.10	0/4621	0.27	0/6243
10	P	0.14	0/4616	0.35	1/6228 (0.0%)
11	I	0.20	0/930	0.55	0/1263
12	N	0.13	0/800	0.35	0/1076
13	Q	0.11	0/5190	0.31	0/7020
14	T	0.24	2/5455 (0.0%)	0.53	4/7387 (0.1%)
15	U	0.13	0/936	0.30	0/1265
All	All	0.18	3/62632 (0.0%)	0.39	9/84778 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	95	PRO	N-CD	23.42	1.80	1.47
14	T	650	PRO	CB-CG	-11.42	0.92	1.49
14	T	650	PRO	CG-CD	-6.38	1.29	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	650	PRO	CB-CG-CD	23.07	179.94	106.10
14	T	650	PRO	N-CD-CG	-18.80	75.00	103.20
4	E	95	PRO	CA-N-CD	-16.71	88.61	112.00
14	T	650	PRO	CA-CB-CG	-16.21	73.70	104.50
14	T	650	PRO	CA-N-CD	-9.39	98.85	112.00
4	E	95	PRO	N-CD-CG	-7.50	91.95	103.20
8	C	845	PRO	N-CA-CB	6.62	110.20	103.25
10	P	295	MET	CG-SD-CE	-6.17	87.32	100.90
5	A	136	MET	CB-CG-SD	5.73	129.88	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	635	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3991	0	3947	177	0
1	H	4031	0	4003	206	0
2	J	4128	0	4096	184	0
2	K	4102	0	4065	231	0
3	G	284	0	293	21	0
3	W	300	0	313	18	0
4	E	1091	0	1058	69	0
5	A	1743	0	1714	84	0
6	B	3418	0	3307	192	0
7	S	45	0	43	1	0
8	C	10863	0	10672	389	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	O	5288	0	5299	179	0
10	D	4524	0	4391	136	0
10	P	4518	0	4410	193	0
11	I	906	0	813	62	0
12	N	784	0	784	25	0
13	Q	5083	0	5093	157	0
14	T	5337	0	5314	229	0
15	U	912	0	873	28	0
16	U	3	0	0	0	0
All	All	61351	0	60488	2298	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 19.

All (2298) 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)
9:O:431:LEU:HD13	9:O:472:TYR:CZ	1.16	1.65
6:B:190:ARG:HB2	11:I:97:TRP:CZ3	1.32	1.62
10:P:27:TRP:CH2	10:P:115:TYR:CE1	1.85	1.61
9:O:170:TRP:CZ3	9:O:174:GLN:HG3	1.32	1.61
10:P:301:LEU:HD22	10:P:334:TYR:CE2	1.33	1.57
10:P:301:LEU:HD22	10:P:334:TYR:CZ	1.35	1.57
2:K:242:MET:CE	2:K:243:GLN:HE22	1.23	1.50
14:T:309:MET:HE2	14:T:315:TYR:CD1	1.47	1.48
14:T:237:PHE:CB	14:T:240:MET:HE2	1.42	1.45
10:P:27:TRP:CZ2	10:P:115:TYR:CE1	2.07	1.41
4:E:95:PRO:CD	4:E:95:PRO:N	1.80	1.39
14:T:309:MET:SD	14:T:314:ASP:HB3	1.62	1.39
14:T:103:PHE:HE2	14:T:147:ILE:O	1.04	1.37
14:T:309:MET:SD	14:T:314:ASP:CB	2.11	1.38
14:T:237:PHE:HB2	14:T:240:MET:CE	1.52	1.37
2:K:575:TYR:CE2	6:B:222:PHE:CZ	2.12	1.37
10:P:27:TRP:CZ2	10:P:115:TYR:HE1	1.43	1.36
2:K:242:MET:CE	2:K:243:GLN:NE2	1.85	1.35
6:B:190:ARG:N	11:I:97:TRP:CH2	1.94	1.35
6:B:190:ARG:HB2	11:I:97:TRP:CE3	1.61	1.35
10:P:301:LEU:CD2	10:P:334:TYR:CE2	2.11	1.33
9:O:431:LEU:CD1	9:O:472:TYR:CZ	2.11	1.33
10:P:9:ILE:HD12	10:P:292:PHE:CE1	1.64	1.31
14:T:309:MET:CE	14:T:315:TYR:CE1	2.16	1.29

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:309:MET:CE	14:T:315:TYR:CD1	2.15	1.28
10:D:536:THR:C	10:D:576:GLU:OE2	1.78	1.27
6:B:504:SER:C	6:B:505:MET:HE2	1.57	1.27
6:B:190:ARG:CB	11:I:97:TRP:CZ3	2.19	1.25
2:K:242:MET:HE3	2:K:243:GLN:NE2	1.45	1.24
10:P:301:LEU:CD2	10:P:334:TYR:OH	1.85	1.24
4:E:95:PRO:HD2	4:E:96:PHE:N	1.54	1.22
9:O:170:TRP:CZ3	9:O:174:GLN:CG	2.22	1.21
8:C:463:GLN:OE1	8:C:479:SER:C	1.83	1.21
9:O:431:LEU:HD13	9:O:472:TYR:OH	1.39	1.20
10:D:536:THR:O	10:D:576:GLU:OE2	1.54	1.20
14:T:384:TYR:CE2	14:T:394:LEU:HD22	1.77	1.20
8:C:463:GLN:NE2	8:C:480:GLU:HA	1.53	1.20
14:T:103:PHE:CE2	14:T:147:ILE:O	1.95	1.19
2:K:575:TYR:CE2	6:B:222:PHE:CE1	2.30	1.18
4:E:255:ARG:NH2	4:E:256:HIS:HB2	1.57	1.18
9:O:170:TRP:CH2	9:O:174:GLN:HG3	1.79	1.17
2:K:736:TYR:CD1	1:H:599:LYS:HG2	1.79	1.17
2:J:748:LEU:O	2:J:752:LEU:HD22	1.45	1.16
14:T:181:LEU:HD13	14:T:196:LEU:HD23	1.20	1.16
2:K:575:TYR:CZ	6:B:222:PHE:CE1	2.35	1.15
14:T:577:ILE:HA	14:T:580:MET:HE1	1.18	1.15
13:Q:403:ASP:OD1	13:Q:415:LEU:HD13	1.47	1.14
10:P:139:ILE:HD13	12:N:119:PHE:HE1	1.08	1.14
10:P:27:TRP:CZ3	10:P:115:TYR:CE1	2.37	1.13
10:D:201:TYR:CE1	10:D:203:ILE:HB	1.83	1.13
10:P:286:SER:OG	10:P:292:PHE:CD1	2.03	1.11
2:K:736:TYR:O	1:H:599:LYS:HE2	1.47	1.11
14:T:309:MET:SD	14:T:314:ASP:HB2	1.82	1.11
14:T:309:MET:CE	14:T:314:ASP:HB2	1.79	1.11
8:C:463:GLN:HE22	8:C:480:GLU:CA	1.63	1.11
10:P:301:LEU:HD22	10:P:334:TYR:OH	1.40	1.11
10:P:27:TRP:CZ2	10:P:115:TYR:OH	2.04	1.10
10:P:27:TRP:CZ2	10:P:115:TYR:CZ	2.39	1.10
10:P:301:LEU:CD2	10:P:334:TYR:HE2	1.55	1.10
1:F:165:MET:HE3	1:F:173:GLY:HA3	1.32	1.09
1:F:51:GLU:HG3	1:H:471:MET:HE2	1.30	1.09
2:K:242:MET:HE2	2:K:243:GLN:NE2	1.60	1.09
8:C:463:GLN:NE2	8:C:481:GLY:N	2.00	1.08
10:D:247:PHE:HD1	10:D:295:MET:HE2	1.14	1.08
2:K:739:PRO:HG3	1:H:599:LYS:NZ	1.69	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:201:TYR:HE1	10:D:203:ILE:HB	0.94	1.07
10:P:559:MET:HE2	10:P:580:ALA:HA	1.26	1.07
8:C:463:GLN:OE1	8:C:479:SER:O	1.71	1.07
10:P:139:ILE:HD13	12:N:119:PHE:CE1	1.89	1.07
14:T:384:TYR:CE2	14:T:389:LEU:HB3	1.90	1.06
8:C:463:GLN:HE22	8:C:480:GLU:HA	1.02	1.06
4:E:95:PRO:HD2	4:E:96:PHE:H	1.10	1.06
10:P:27:TRP:CH2	10:P:115:TYR:CZ	2.43	1.06
10:P:301:LEU:CD2	10:P:334:TYR:CZ	2.28	1.06
2:J:748:LEU:HD23	2:J:752:LEU:HD21	1.38	1.05
14:T:309:MET:HE3	14:T:315:TYR:CE1	1.87	1.05
14:T:309:MET:HE1	14:T:314:ASP:HB2	1.37	1.05
10:P:9:ILE:HD12	10:P:292:PHE:HE1	0.90	1.04
10:D:201:TYR:HE1	10:D:203:ILE:CB	1.70	1.04
9:O:431:LEU:HD13	9:O:472:TYR:CE1	1.93	1.03
8:C:463:GLN:NE2	8:C:481:GLY:H	1.57	1.03
2:J:749:LYS:HA	2:J:752:LEU:HD23	1.38	1.03
10:P:139:ILE:CD1	12:N:119:PHE:HE1	1.70	1.03
2:K:736:TYR:HD1	1:H:599:LYS:HG2	1.16	1.02
1:F:51:GLU:HG3	1:H:471:MET:CE	1.89	1.02
13:Q:334:CYS:SG	13:Q:377:LEU:HB2	2.00	1.02
1:F:471:MET:HE1	1:H:52:LEU:HA	1.38	1.01
1:H:459:PHE:CD1	1:H:478:LEU:HD12	1.95	1.01
8:C:454:LEU:HD21	8:C:459:PRO:HB3	1.43	1.01
14:T:309:MET:HE2	14:T:315:TYR:CE1	1.86	1.00
2:J:756:VAL:HG22	10:P:512:THR:HG22	1.00	0.99
14:T:384:TYR:CE2	14:T:389:LEU:CB	2.45	0.99
14:T:455:ARG:HA	14:T:458:MET:SD	2.01	0.99
2:J:756:VAL:HG22	10:P:512:THR:CG2	1.91	0.99
6:B:190:ARG:HB2	11:I:97:TRP:CH2	1.96	0.99
8:C:463:GLN:CD	8:C:480:GLU:HA	1.87	0.99
10:P:9:ILE:CD1	10:P:292:PHE:CE1	2.46	0.98
9:O:170:TRP:CZ2	9:O:174:GLN:NE2	2.30	0.98
10:P:27:TRP:CE2	10:P:115:TYR:HE1	1.81	0.98
10:D:537:SER:HA	10:D:576:GLU:OE1	1.64	0.98
13:Q:150:GLU:CB	14:T:327:LYS:HE3	1.94	0.98
2:K:739:PRO:HG3	1:H:599:LYS:HZ1	1.22	0.97
1:F:51:GLU:CG	1:H:471:MET:HE2	1.94	0.97
1:H:662:LEU:HD11	1:H:689:MET:HE1	1.45	0.96
14:T:181:LEU:HD13	14:T:196:LEU:CD2	1.95	0.96
2:J:756:VAL:CG2	10:P:512:THR:HG22	1.95	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:27:TRP:HZ2	10:P:115:TYR:OH	1.41	0.96
10:P:136:MET:O	10:P:139:ILE:HG22	1.66	0.96
13:Q:351:PHE:HD1	13:Q:355:ASN:OD1	1.46	0.96
14:T:384:TYR:CZ	14:T:389:LEU:HG	2.01	0.95
1:H:60:LEU:HD21	1:H:64:SER:HB3	1.47	0.95
13:Q:403:ASP:OD1	13:Q:415:LEU:CD1	2.15	0.95
14:T:181:LEU:HB2	14:T:196:LEU:HD21	1.45	0.95
14:T:309:MET:HE2	14:T:315:TYR:HD1	1.16	0.95
10:P:301:LEU:HD23	10:P:334:TYR:OH	1.67	0.95
2:J:284:GLU:OE2	2:K:493:ASP:HA	1.67	0.94
10:P:559:MET:CE	10:P:580:ALA:HA	1.97	0.94
4:E:95:PRO:CD	4:E:96:PHE:N	2.32	0.93
9:O:431:LEU:HD13	9:O:472:TYR:CE2	2.01	0.93
4:E:95:PRO:CD	4:E:96:PHE:H	1.81	0.93
10:P:27:TRP:CH2	10:P:115:TYR:HE1	1.46	0.92
14:T:384:TYR:CE2	14:T:394:LEU:CD2	2.53	0.92
6:B:504:SER:C	6:B:505:MET:CE	2.41	0.92
1:H:117:ASN:O	1:H:121:LEU:HD22	1.68	0.92
8:C:463:GLN:OE1	8:C:480:GLU:N	2.02	0.92
14:T:103:PHE:CZ	14:T:147:ILE:HA	2.05	0.91
6:B:190:ARG:N	11:I:97:TRP:HH2	1.53	0.91
8:C:463:GLN:NE2	8:C:480:GLU:CA	2.24	0.91
9:O:431:LEU:CD1	9:O:472:TYR:OH	2.10	0.91
11:I:37:GLU:HB3	11:I:84:SER:HB3	1.52	0.91
2:J:750:ASN:HD22	3:G:20:ILE:HD12	1.36	0.91
4:E:255:ARG:CZ	4:E:256:HIS:HB2	2.01	0.91
13:Q:151:ASP:CG	14:T:327:LYS:HZ2	1.77	0.90
10:D:247:PHE:HA	10:D:295:MET:HE3	1.53	0.90
14:T:577:ILE:HA	14:T:580:MET:CE	2.02	0.90
1:H:459:PHE:CE1	1:H:478:LEU:HD12	2.08	0.89
2:K:242:MET:HE2	2:K:243:GLN:HE21	1.35	0.89
2:K:736:TYR:O	1:H:599:LYS:CE	2.20	0.89
10:P:301:LEU:CD1	10:P:334:TYR:HE2	1.85	0.89
5:A:81:MET:SD	5:A:220:TYR:HB3	2.12	0.89
9:O:170:TRP:CH2	9:O:174:GLN:NE2	2.40	0.89
10:D:247:PHE:CD1	10:D:295:MET:HE2	2.05	0.88
14:T:384:TYR:HE2	14:T:394:LEU:HD22	1.31	0.88
10:P:509:TYR:O	10:P:512:THR:OG1	1.92	0.88
8:C:463:GLN:OE1	8:C:480:GLU:CA	2.21	0.88
13:Q:351:PHE:CD1	13:Q:355:ASN:OD1	2.27	0.87
8:C:475:LEU:HD11	8:C:491:LEU:HB3	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:736:TYR:HD1	1:H:599:LYS:CG	1.86	0.87
6:B:190:ARG:CB	11:I:97:TRP:CE3	2.50	0.87
6:B:190:ARG:CA	11:I:97:TRP:CH2	2.57	0.86
8:C:1165:GLU:HG3	8:C:1242:ASN:ND2	1.90	0.86
10:P:301:LEU:HD13	10:P:334:TYR:CE2	2.10	0.86
2:J:748:LEU:O	2:J:752:LEU:CD2	2.23	0.86
10:P:345:TYR:HB3	10:P:376:MET:HE2	1.58	0.86
14:T:384:TYR:CD2	14:T:394:LEU:CD2	2.58	0.86
2:K:467:ARG:NH1	2:K:471:ASP:OD1	2.07	0.86
10:P:519:ILE:HD11	10:P:545:LEU:HD22	1.58	0.86
1:F:51:GLU:CD	1:H:472:PRO:HD2	2.01	0.86
2:K:575:TYR:CD2	6:B:222:PHE:CZ	2.63	0.85
1:H:47:GLU:HA	1:H:47:GLU:OE2	1.75	0.85
14:T:738:VAL:HG11	15:U:1:MET:CG	2.05	0.85
1:F:535:THR:HG23	1:F:536:MET:SD	2.16	0.85
2:K:496:ASN:HB3	2:K:499:ILE:HG22	1.59	0.85
2:K:736:TYR:CD1	1:H:599:LYS:CG	2.59	0.85
13:Q:150:GLU:HB2	14:T:327:LYS:HE3	1.59	0.85
14:T:181:LEU:CD1	14:T:196:LEU:HD23	2.05	0.85
2:K:736:TYR:HA	1:H:599:LYS:CE	2.07	0.84
10:D:247:PHE:HA	10:D:295:MET:CE	2.07	0.84
14:T:237:PHE:CB	14:T:240:MET:CE	2.30	0.84
2:K:736:TYR:HA	1:H:599:LYS:HG3	1.58	0.84
1:F:51:GLU:OE2	1:H:471:MET:HA	1.77	0.84
2:J:246:TYR:OH	2:J:275:ASN:HB3	1.76	0.84
4:E:255:ARG:HH22	4:E:256:HIS:HB2	1.43	0.84
6:B:532:SER:HB3	6:B:542:TRP:HH2	1.43	0.84
8:C:463:GLN:NE2	8:C:480:GLU:C	2.37	0.83
8:C:454:LEU:HD21	8:C:459:PRO:CB	2.09	0.83
2:K:242:MET:HE3	2:K:243:GLN:HE22	0.66	0.82
2:K:736:TYR:HA	1:H:599:LYS:HE3	1.60	0.82
8:C:491:LEU:HB2	8:C:500:SER:HB3	1.61	0.82
6:B:504:SER:O	6:B:505:MET:HE2	1.77	0.82
14:T:384:TYR:CE1	14:T:389:LEU:HG	2.14	0.82
1:F:103:TYR:CD1	1:F:151:PRO:HG3	2.14	0.82
4:E:249:LEU:HA	4:E:252:LYS:HE2	1.62	0.82
14:T:384:TYR:HD2	14:T:394:LEU:HD21	1.45	0.82
9:O:170:TRP:CH2	9:O:174:GLN:CG	2.53	0.81
10:P:139:ILE:CD1	12:N:119:PHE:CE1	2.58	0.81
6:B:205:GLN:HE22	10:D:377:GLN:HE21	1.28	0.81
2:K:575:TYR:HE2	6:B:222:PHE:CZ	1.97	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:384:TYR:CD2	14:T:394:LEU:HD21	2.15	0.81
1:F:595:THR:O	1:F:599:LYS:HG3	1.81	0.81
10:P:345:TYR:CB	10:P:376:MET:HE2	2.11	0.81
14:T:43:PRO:HD2	14:T:113:GLN:HG3	1.61	0.81
2:K:739:PRO:CG	1:H:599:LYS:HZ1	1.92	0.81
2:J:255:LYS:HD3	2:K:432:LEU:HD11	1.62	0.80
5:A:44:LYS:HZ2	5:A:50:GLY:HA2	1.46	0.80
2:K:566:ALA:HB2	3:W:1:MET:CE	2.12	0.80
10:P:301:LEU:CG	10:P:334:TYR:HE2	1.95	0.80
2:J:466:VAL:HG21	2:J:489:VAL:HG21	1.61	0.80
2:J:731:LEU:HB3	2:J:748:LEU:HD12	1.61	0.80
2:K:575:TYR:OH	6:B:222:PHE:CE1	2.33	0.80
1:F:479:GLY:HA3	1:F:495:PHE:HD2	1.46	0.79
2:K:435:ILE:O	2:K:439:LYS:NZ	2.15	0.79
8:C:929:PHE:HE2	8:C:989:PRO:HD2	1.46	0.79
6:B:112:GLY:HA3	6:B:230:ARG:HH12	1.47	0.79
10:P:256:MET:HE2	10:P:256:MET:HA	1.64	0.79
6:B:386:GLN:HB2	6:B:406:ASP:HB3	1.63	0.79
13:Q:383:SER:O	13:Q:387:LEU:HD22	1.83	0.79
10:P:301:LEU:CD1	10:P:334:TYR:CE2	2.66	0.79
8:C:463:GLN:CD	8:C:480:GLU:CA	2.52	0.79
13:Q:151:ASP:CG	14:T:327:LYS:NZ	2.39	0.79
10:D:537:SER:HA	10:D:576:GLU:CD	2.06	0.79
10:P:534:GLN:OE1	10:P:534:GLN:N	2.17	0.78
14:T:387:LEU:HD21	14:T:529:TRP:CH2	2.19	0.78
8:C:1523:PHE:HA	8:C:1526:MET:HE3	1.65	0.78
9:O:431:LEU:CG	9:O:472:TYR:OH	2.32	0.78
14:T:196:LEU:HD12	14:T:200:LEU:HD23	1.63	0.78
14:T:237:PHE:O	14:T:240:MET:CG	2.31	0.78
2:J:509:GLU:OE1	2:J:509:GLU:C	2.27	0.78
1:H:159:LEU:HD11	1:H:163:LEU:HD21	1.64	0.78
1:F:165:MET:HE3	1:F:173:GLY:CA	2.13	0.78
2:J:393:PHE:CE1	2:J:397:GLU:HB2	2.18	0.77
9:O:419:ALA:HB2	12:N:4:ALA:H	1.50	0.77
8:C:1541:LEU:HD12	8:C:1544:PHE:CD2	2.19	0.77
14:T:237:PHE:O	14:T:240:MET:HG2	1.84	0.77
10:P:595:GLN:HA	10:P:626:MET:HE2	1.66	0.77
8:C:463:GLN:OE1	8:C:480:GLU:HA	1.84	0.77
10:P:27:TRP:CZ3	10:P:115:TYR:HE1	1.90	0.77
2:J:748:LEU:CD2	2:J:752:LEU:HD21	2.15	0.77
1:H:471:MET:HG2	1:H:474:CYS:H	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:44:LYS:NZ	5:A:50:GLY:HA2	2.00	0.77
8:C:1308:ILE:HG22	8:C:1309:MET:HE3	1.67	0.77
10:P:119:LEU:HD23	10:P:119:LEU:O	1.85	0.76
14:T:387:LEU:HD21	14:T:529:TRP:CZ2	2.21	0.76
1:H:697:GLN:HA	1:H:700:GLU:HG2	1.66	0.76
9:O:170:TRP:HZ3	9:O:174:GLN:HG3	1.41	0.76
13:Q:150:GLU:HB3	14:T:327:LYS:HE3	1.66	0.76
14:T:384:TYR:OH	14:T:393:GLU:HB2	1.85	0.76
6:B:190:ARG:HD3	11:I:97:TRP:CE3	2.21	0.75
8:C:1355:LEU:HD12	8:C:1390:ILE:HG13	1.66	0.75
14:T:384:TYR:CD2	14:T:394:LEU:HD22	2.21	0.75
2:J:610:MET:HE1	2:J:642:MET:HB2	1.68	0.75
2:K:585:LEU:HD11	2:K:609:PHE:HE1	1.51	0.75
1:H:169:HIS:ND1	1:H:172:GLU:OE2	2.19	0.75
6:B:65:ASP:OD1	6:B:66:PHE:N	2.19	0.75
2:J:393:PHE:O	2:J:393:PHE:CD1	2.40	0.75
1:H:635:ARG:HH22	1:H:648:CYS:HB2	1.51	0.75
2:K:467:ARG:CZ	2:K:471:ASP:OD1	2.35	0.75
2:K:575:TYR:CZ	6:B:222:PHE:HE1	1.99	0.75
15:U:104:LEU:O	15:U:107:ASN:ND2	2.20	0.75
1:F:165:MET:CE	1:F:173:GLY:HA3	2.13	0.75
10:P:27:TRP:CZ3	10:P:115:TYR:CD1	2.74	0.74
11:I:115:GLY:HA3	11:I:157:ARG:HH12	1.50	0.74
14:T:576:SER:O	14:T:580:MET:SD	2.44	0.74
2:J:607:MET:HE2	2:J:638:GLU:OE2	1.88	0.74
2:J:748:LEU:HD23	2:J:752:LEU:CD2	2.17	0.74
10:P:235:MET:SD	10:P:258:CYS:HB3	2.27	0.74
8:C:950:MET:SD	8:C:953:ARG:NH1	2.60	0.74
2:K:288:ARG:C	2:K:288:ARG:HD3	2.11	0.74
2:K:397:GLU:OE2	2:K:397:GLU:C	2.31	0.74
2:K:297:LEU:HA	2:K:357:MET:HE2	1.68	0.74
4:E:255:ARG:HH12	4:E:256:HIS:CG	2.05	0.74
1:H:469:ASP:O	1:H:497:ARG:NH2	2.21	0.73
1:H:526:SER:O	1:H:530:ASN:ND2	2.21	0.73
10:P:621:GLU:HG2	10:P:625:HIS:CE1	2.23	0.73
2:J:251:TYR:OH	2:K:436:ASN:OD1	2.06	0.73
4:E:135:ARG:HD3	4:E:138:ILE:HD11	1.70	0.73
1:F:54:TYR:HE1	1:F:71:VAL:HG22	1.53	0.73
2:K:288:ARG:HD3	2:K:288:ARG:O	1.89	0.73
9:O:431:LEU:CD1	9:O:472:TYR:CE2	2.67	0.73
3:G:14:ASP:OD1	3:G:15:ASP:N	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:50:PRO:HA	9:O:245:GLN:HG2	1.71	0.73
9:O:96:LEU:HD23	9:O:194:HIS:HB3	1.70	0.73
2:K:496:ASN:HB3	2:K:499:ILE:CG2	2.19	0.73
1:H:723:VAL:HG12	1:H:725:ARG:HH12	1.53	0.73
1:F:51:GLU:OE1	1:H:472:PRO:HD2	1.89	0.73
10:D:77:ASN:HD21	10:P:77:ASN:HD22	1.37	0.73
10:P:9:ILE:CD1	10:P:292:PHE:CZ	2.71	0.73
2:K:455:LYS:HG3	2:K:456:ASP:OD1	1.89	0.72
8:C:1155:LEU:HD11	8:C:1167:TYR:HE1	1.53	0.72
1:F:543:TRP:CZ3	1:F:562:ALA:HA	2.25	0.72
6:B:190:ARG:CB	11:I:97:TRP:CH2	2.62	0.72
1:F:35:GLN:HE22	1:F:148:VAL:H	1.35	0.72
13:Q:125:ARG:HG3	13:Q:138:TYR:HA	1.70	0.72
15:U:83:ASP:O	15:U:121:ARG:NH2	2.21	0.72
8:C:662:MET:CE	8:C:664:TRP:NE1	2.53	0.72
10:D:398:GLU:N	10:D:398:GLU:OE2	2.22	0.72
13:Q:26:GLY:HA2	13:Q:43:ILE:HG22	1.71	0.72
1:H:194:ILE:HG23	1:H:199:ALA:HB3	1.71	0.72
13:Q:365:ALA:HA	13:Q:463:MET:CE	2.20	0.72
2:K:566:ALA:HB2	3:W:1:MET:HE3	1.69	0.72
1:H:497:ARG:HH12	1:H:501:LEU:HG	1.55	0.71
6:B:189:THR:C	11:I:97:TRP:CH2	2.68	0.71
10:P:136:MET:O	10:P:139:ILE:CG2	2.38	0.71
1:H:505:ARG:HE	1:H:507:LYS:HB2	1.56	0.71
14:T:384:TYR:CE2	14:T:389:LEU:HB2	2.24	0.71
14:T:666:GLN:NE2	14:T:674:LYS:HB3	2.06	0.71
1:H:165:MET:HE2	1:H:193:ALA:HB1	1.73	0.71
8:C:1356:LEU:HD11	8:C:1405:GLU:HG3	1.73	0.71
13:Q:542:LYS:HE2	13:Q:545:ASN:HB3	1.73	0.71
2:K:390:ILE:HD12	2:K:417:LEU:HD13	1.73	0.71
4:E:255:ARG:NH1	4:E:256:HIS:HA	2.05	0.71
9:O:170:TRP:CE3	9:O:170:TRP:O	2.43	0.71
10:P:556:LYS:HA	10:P:583:TRP:HH2	1.56	0.71
6:B:254:VAL:O	7:S:831:LEU:N	2.24	0.71
8:C:404:ARG:NH2	8:C:409:GLU:OE1	2.24	0.71
8:C:1051:LEU:HD12	8:C:1081:GLY:HA2	1.73	0.71
4:E:255:ARG:CZ	4:E:256:HIS:CB	2.68	0.71
1:F:457:ARG:HH21	4:E:96:PHE:HE2	1.38	0.70
9:O:386:ILE:HD11	9:O:406:ILE:HG21	1.73	0.70
14:T:384:TYR:CD2	14:T:389:LEU:HB2	2.26	0.70
1:H:159:LEU:HD12	1:H:159:LEU:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:665:TYR:HB3	1:H:682:MET:SD	2.31	0.70
8:C:662:MET:HE2	8:C:664:TRP:CE2	2.26	0.70
2:K:739:PRO:HG3	1:H:599:LYS:HZ2	1.56	0.70
14:T:666:GLN:HE22	14:T:674:LYS:HB3	1.56	0.70
8:C:929:PHE:CE2	8:C:989:PRO:HD2	2.25	0.70
13:Q:268:LEU:HD21	13:Q:303:VAL:HG22	1.74	0.70
1:F:206:VAL:HG22	4:E:161:LEU:HD22	1.74	0.70
2:J:546:ARG:HH22	11:I:37:GLU:HG3	1.57	0.70
2:K:307:VAL:HG22	2:K:368:ILE:HD11	1.73	0.70
8:C:1082:LEU:HD11	8:C:1086:MET:HE3	1.73	0.70
14:T:129:LYS:HB2	14:T:133:ARG:HH21	1.54	0.70
1:F:187:LEU:HD13	1:H:42:ASN:HD21	1.56	0.70
1:F:479:GLY:HA3	1:F:495:PHE:CD2	2.27	0.70
1:H:530:ASN:OD1	4:E:252:LYS:NZ	2.19	0.70
2:J:633:PRO:HB3	2:J:663:VAL:HG21	1.74	0.69
8:C:811:ALA:N	8:C:1635:GLN:OE1	2.25	0.69
10:P:9:ILE:HG13	10:P:292:PHE:HZ	1.58	0.69
14:T:384:TYR:CZ	14:T:389:LEU:CB	2.76	0.69
14:T:384:TYR:CZ	14:T:389:LEU:CG	2.75	0.69
3:G:23:LEU:HD12	3:G:26:GLN:HE21	1.58	0.69
8:C:454:LEU:HD12	8:C:456:LEU:HD23	1.74	0.69
13:Q:220:LEU:HD23	13:Q:480:ILE:HD11	1.75	0.69
14:T:178:ARG:HE	14:T:207:LEU:HD21	1.57	0.69
15:U:48:TYR:HB3	15:U:64:LEU:HD11	1.75	0.69
9:O:431:LEU:HD22	9:O:472:TYR:OH	1.92	0.69
13:Q:104:ARG:HA	13:Q:104:ARG:NH1	2.07	0.69
2:J:661:GLU:HA	2:J:664:LYS:HG2	1.75	0.69
1:H:652:LEU:HA	1:H:655:LEU:HD12	1.75	0.69
10:D:537:SER:N	10:D:576:GLU:OE2	2.26	0.69
8:C:1224:LEU:HA	8:C:1227:ILE:HD12	1.75	0.69
8:C:1490:HIS:HA	8:C:1493:LYS:HE3	1.75	0.68
2:K:585:LEU:HD11	2:K:609:PHE:CE1	2.29	0.68
8:C:213:LEU:HD13	8:C:380:LEU:HD21	1.75	0.68
8:C:463:GLN:HE22	8:C:480:GLU:C	2.01	0.68
13:Q:403:ASP:CG	13:Q:415:LEU:CD1	2.66	0.68
8:C:475:LEU:HD21	8:C:491:LEU:HD13	1.75	0.68
14:T:613:TYR:HE2	15:U:58:PRO:HG3	1.57	0.68
1:F:498:LEU:HD21	1:F:505:ARG:HD3	1.74	0.68
10:D:79:PHE:HB3	10:D:81:LEU:HD23	1.76	0.68
14:T:43:PRO:HD2	14:T:113:GLN:HE21	1.58	0.68
8:C:722:ILE:HG13	8:C:722:ILE:O	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:181:LEU:HB2	14:T:196:LEU:CD2	2.23	0.68
8:C:465:MET:HB2	8:C:477:LEU:O	1.93	0.68
8:C:1291:TRP:O	8:C:1295:MET:HG2	1.94	0.68
1:F:128:ASN:HD22	4:E:179:ARG:HH21	1.41	0.68
1:H:30:LEU:O	1:H:34:ILE:HG13	1.94	0.68
8:C:798:LEU:O	8:C:810:ARG:NH1	2.27	0.68
14:T:652:ARG:NH2	15:U:60:ASP:OD1	2.27	0.68
10:P:252:TRP:HZ3	10:P:295:MET:HE2	1.57	0.67
1:F:706:VAL:HG21	6:B:557:LEU:HD11	1.75	0.67
6:B:324:GLY:HA3	6:B:343:HIS:HB2	1.76	0.67
2:J:245:MET:HG3	2:K:394:GLU:OE1	1.94	0.67
2:K:296:ILE:HD12	2:K:299:ARG:HD3	1.77	0.67
2:K:496:ASN:O	2:K:499:ILE:HG22	1.93	0.67
8:C:662:MET:CE	8:C:664:TRP:CE2	2.76	0.67
9:O:659:GLU:HA	13:Q:342:GLU:OE2	1.95	0.67
2:K:356:LYS:HD2	2:K:358:GLU:H	1.60	0.67
14:T:387:LEU:HD12	14:T:387:LEU:O	1.95	0.67
1:H:130:PHE:CE2	1:H:153:LEU:HD21	2.29	0.67
1:H:161:GLY:O	1:H:165:MET:HG2	1.95	0.67
4:E:97:CYS:HB3	4:E:102:LEU:HD21	1.77	0.67
9:O:376:GLU:OE1	9:O:376:GLU:N	2.26	0.67
2:K:733:LYS:O	2:K:737:LEU:HD12	1.94	0.67
3:G:10:GLN:OE1	3:G:10:GLN:N	2.28	0.67
1:H:159:LEU:CD1	1:H:163:LEU:HD21	2.24	0.67
9:O:61:ASN:HB2	9:O:65:ARG:HG2	1.77	0.66
10:P:286:SER:OG	10:P:292:PHE:CE1	2.43	0.66
2:J:269:LEU:HD22	2:J:285:LEU:HD22	1.76	0.66
2:K:621:TYR:HA	2:K:624:LEU:HG	1.77	0.66
14:T:369:LYS:HG2	14:T:370:PRO:HD3	1.75	0.66
1:F:713:HIS:ND1	1:F:732:GLU:OE2	2.28	0.66
2:K:390:ILE:CD1	2:K:417:LEU:HD13	2.24	0.66
9:O:100:GLY:HA2	9:O:195:ILE:HG23	1.76	0.66
2:K:736:TYR:C	1:H:599:LYS:HE2	2.20	0.66
14:T:332:ASN:HB3	14:T:335:VAL:HG23	1.78	0.66
1:F:738:ASN:OD1	2:J:593:ARG:NH2	2.29	0.66
2:J:393:PHE:O	2:J:393:PHE:HD1	1.77	0.66
14:T:237:PHE:HB3	14:T:240:MET:HE2	1.70	0.66
1:F:165:MET:HE1	1:F:170:SER:O	1.95	0.66
1:F:471:MET:HE1	1:H:52:LEU:CA	2.22	0.66
9:O:440:THR:OG1	13:Q:119:ASP:OD2	2.05	0.66
1:F:730:ILE:HD11	2:J:621:TYR:CE1	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:429:MET:HA	2:K:429:MET:HE2	1.78	0.66
10:P:306:GLU:OE2	10:P:463:ARG:NH1	2.28	0.66
1:H:200:THR:HA	1:H:445:ARG:HH22	1.61	0.66
1:H:703:VAL:HG12	1:H:712:ALA:HB1	1.78	0.66
8:C:1082:LEU:CD1	8:C:1086:MET:HE3	2.25	0.66
1:F:495:PHE:CE1	1:F:512:PHE:HD1	2.14	0.65
15:U:97:THR:HG21	15:U:122:ARG:HH21	1.60	0.65
1:H:607:HIS:O	1:H:611:TYR:HE2	1.78	0.65
9:O:441:ALA:HA	13:Q:119:ASP:OD1	1.96	0.65
10:P:621:GLU:O	10:P:625:HIS:ND1	2.29	0.65
8:C:54:VAL:HG23	8:C:72:ILE:HD13	1.77	0.65
10:P:301:LEU:CG	10:P:334:TYR:CE2	2.75	0.65
11:I:29:GLN:OE1	11:I:29:GLN:N	2.30	0.65
6:B:432:ALA:C	6:B:477:MET:HE1	2.21	0.65
8:C:1167:TYR:O	8:C:1167:TYR:HD2	1.80	0.65
14:T:34:LEU:HD12	14:T:37:LEU:HD12	1.79	0.65
8:C:1164:ASP:OD1	8:C:1166:GLU:N	2.29	0.65
1:H:117:ASN:O	1:H:121:LEU:CD2	2.42	0.65
8:C:586:LEU:HD23	8:C:624:LEU:HD21	1.78	0.65
1:H:537:PRO:O	1:H:543:TRP:NE1	2.28	0.65
10:P:515:LYS:HB3	10:P:545:LEU:HD21	1.78	0.65
13:Q:365:ALA:HA	13:Q:463:MET:HE1	1.78	0.65
1:F:735:VAL:HG22	2:J:593:ARG:HG3	1.79	0.64
6:B:189:THR:C	11:I:97:TRP:HH2	2.04	0.64
6:B:340:LEU:HD21	6:B:376:PRO:HD2	1.79	0.64
8:C:1150:GLN:NE2	8:C:1167:TYR:OH	2.29	0.64
13:Q:8:TYR:CD2	13:Q:646:PRO:HB3	2.32	0.64
13:Q:253:ILE:HG22	13:Q:257:LEU:HD12	1.78	0.64
1:F:506:VAL:HB	1:F:536:MET:HE2	1.79	0.64
2:K:617:LEU:HB3	2:K:621:TYR:CE2	2.32	0.64
6:B:381:ILE:HG12	6:B:417:LYS:HG3	1.78	0.64
8:C:205:PHE:HB2	8:C:216:TYR:HE1	1.62	0.64
3:G:23:LEU:O	3:G:27:LYS:HG2	1.98	0.64
8:C:703:ILE:HG23	8:C:707:LEU:HD23	1.78	0.64
13:Q:357:LEU:HD23	13:Q:359:TYR:H	1.63	0.64
14:T:387:LEU:CG	14:T:529:TRP:CZ2	2.79	0.64
10:P:556:LYS:HA	10:P:583:TRP:CH2	2.33	0.64
9:O:170:TRP:CH2	9:O:174:GLN:CD	2.75	0.64
14:T:577:ILE:CA	14:T:580:MET:HE1	2.12	0.64
2:J:393:PHE:HE2	2:K:251:TYR:CG	2.15	0.64
5:A:81:MET:HE1	5:A:134:CYS:SG	2.38	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:384:TYR:CZ	14:T:389:LEU:HB3	2.33	0.64
2:J:393:PHE:HE1	2:J:397:GLU:HB2	1.61	0.64
10:D:422:ARG:HD3	11:I:27:TRP:CZ2	2.33	0.64
9:O:431:LEU:CD2	9:O:472:TYR:OH	2.46	0.64
5:A:112:PHE:HE2	5:A:213:HIS:CE1	2.16	0.64
6:B:505:MET:HE2	6:B:505:MET:N	2.11	0.64
13:Q:150:GLU:HB2	14:T:327:LYS:CE	2.27	0.64
8:C:1384:ASN:O	8:C:1388:ASN:ND2	2.30	0.64
14:T:49:ASN:OD1	14:T:51:GLN:NE2	2.31	0.64
2:J:434:LYS:HA	2:J:437:LEU:HD13	1.79	0.63
2:J:731:LEU:O	2:J:735:LEU:HD12	1.98	0.63
10:D:187:ILE:HG23	10:D:224:ILE:HD11	1.80	0.63
13:Q:40:VAL:C	13:Q:41:ILE:HD13	2.24	0.63
14:T:407:LEU:O	14:T:411:VAL:HG23	1.98	0.63
8:C:1102:ILE:H	8:C:1102:ILE:HD12	1.63	0.63
8:C:1164:ASP:OD1	8:C:1167:TYR:N	2.28	0.63
8:C:81:GLU:HB2	8:C:122:ASN:HB2	1.80	0.63
8:C:127:GLU:HG3	8:C:152:TYR:CE1	2.34	0.63
8:C:480:GLU:O	8:C:488:LYS:N	2.32	0.63
8:C:662:MET:HE1	8:C:664:TRP:CZ2	2.34	0.63
10:P:483:TYR:HE2	12:N:123:GLY:HA3	1.63	0.63
14:T:309:MET:HE3	14:T:315:TYR:HE1	1.59	0.63
6:B:245:ARG:NH1	6:B:247:ILE:HD11	2.14	0.63
8:C:1271:LEU:HD13	8:C:1274:ILE:HD11	1.81	0.63
8:C:1576:GLU:HG2	8:C:1583:VAL:HG12	1.81	0.63
14:T:103:PHE:HZ	14:T:147:ILE:HA	1.64	0.63
8:C:1609:TYR:HD1	8:C:1636:ARG:HA	1.62	0.63
2:K:569:LEU:O	2:K:573:HIS:ND1	2.16	0.63
8:C:1166:GLU:HG2	8:C:1537:PRO:HB3	1.80	0.63
2:J:263:PRO:HB2	2:J:295:ASN:HD21	1.64	0.63
2:J:679:ASN:O	2:J:683:THR:HG23	1.98	0.63
2:K:583:GLN:HE22	6:B:226:MET:HB3	1.64	0.63
8:C:213:LEU:CD1	8:C:380:LEU:HD21	2.29	0.63
8:C:636:GLU:OE2	8:C:703:ILE:HB	1.99	0.63
14:T:30:ILE:O	14:T:34:LEU:N	2.22	0.63
1:F:714:TYR:HE1	1:F:747:ILE:HG12	1.64	0.63
6:B:287:LEU:N	6:B:296:VAL:O	2.30	0.63
9:O:336:ASN:HB3	9:O:372:ASN:HD21	1.63	0.63
2:K:721:THR:HG22	2:K:722:LYS:H	1.63	0.62
2:K:739:PRO:CG	1:H:599:LYS:NZ	2.54	0.62
9:O:56:PRO:HB2	9:O:57:LEU:HD12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:424:LEU:HD21	10:P:434:TRP:CE2	2.33	0.62
4:E:255:ARG:NH1	4:E:256:HIS:CB	2.62	0.62
8:C:1155:LEU:HD11	8:C:1167:TYR:CE1	2.33	0.62
10:P:79:PHE:CD1	10:P:115:TYR:OH	2.52	0.62
10:P:128:TRP:CH2	10:P:187:ILE:HD13	2.34	0.62
10:P:286:SER:OG	10:P:292:PHE:HD1	1.80	0.62
2:J:278:GLN:OE1	2:J:281:ARG:NH1	2.31	0.62
2:J:255:LYS:HG2	2:K:462:ASN:HD21	1.65	0.62
5:A:133:ILE:HA	5:A:221:VAL:HG12	1.81	0.62
8:C:1495:ILE:HD11	8:C:1542:LYS:HG3	1.82	0.62
10:P:27:TRP:CE2	10:P:115:TYR:CE1	2.68	0.62
10:P:248:ASN:ND2	10:P:251:CYS:SG	2.72	0.62
10:P:252:TRP:CZ3	10:P:295:MET:HE2	2.34	0.62
14:T:595:HIS:HD2	14:T:600:LEU:HB2	1.64	0.62
1:F:443:ILE:HD11	1:F:458:LEU:HB2	1.81	0.62
1:H:751:LEU:HD22	1:H:755:HIS:HE1	1.65	0.62
10:D:452:GLU:OE1	10:D:456:ARG:NH2	2.32	0.62
14:T:103:PHE:CE2	14:T:147:ILE:C	2.77	0.62
1:F:457:ARG:HB3	4:E:140:ILE:HD13	1.80	0.62
2:K:736:TYR:CA	1:H:599:LYS:HE3	2.29	0.62
1:H:692:TYR:HA	1:H:695:ALA:HB3	1.81	0.62
9:O:85:LEU:H	9:O:85:LEU:HD12	1.65	0.62
10:P:509:TYR:HE2	10:P:514:ASN:O	1.83	0.62
13:Q:29:ILE:HG22	13:Q:38:LEU:HB3	1.82	0.62
8:C:553:TRP:HZ2	8:C:575:GLU:HG2	1.64	0.62
8:C:626:ARG:HH21	8:C:727:LEU:HB2	1.65	0.62
13:Q:140:GLN:HB2	13:Q:143:SER:HB3	1.81	0.62
14:T:384:TYR:OH	14:T:393:GLU:CB	2.47	0.62
2:J:610:MET:HE2	2:J:642:MET:HA	1.80	0.62
6:B:429:ALA:O	6:B:473:GLN:NE2	2.31	0.62
14:T:149:ASP:HB3	14:T:152:VAL:HG22	1.82	0.62
14:T:387:LEU:CD2	14:T:529:TRP:CZ2	2.83	0.62
2:J:466:VAL:CG2	2:J:489:VAL:HG21	2.30	0.62
8:C:795:GLU:O	8:C:810:ARG:NH2	2.31	0.62
14:T:579:VAL:O	14:T:583:ASP:N	2.30	0.62
2:K:250:GLU:OE2	2:K:250:GLU:C	2.43	0.62
4:E:255:ARG:NH1	4:E:256:HIS:CA	2.63	0.62
6:B:191:PRO:HG3	11:I:86:ARG:HG3	1.81	0.62
1:H:187:LEU:HD22	1:H:190:SER:H	1.64	0.61
8:C:1082:LEU:HD11	8:C:1086:MET:CE	2.29	0.61
9:O:170:TRP:CE3	9:O:174:GLN:CG	2.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:280:PHE:HE1	10:D:285:GLY:HA2	1.65	0.61
13:Q:489:PHE:HE2	13:Q:516:ILE:HG21	1.65	0.61
2:J:466:VAL:HG21	2:J:489:VAL:CG2	2.29	0.61
2:K:566:ALA:HB2	3:W:1:MET:HE1	1.82	0.61
1:H:459:PHE:HD1	1:H:478:LEU:HD12	1.58	0.61
6:B:252:TYR:HE1	6:B:542:TRP:C	2.08	0.61
10:P:187:ILE:HA	10:P:190:ILE:HB	1.81	0.61
13:Q:515:LEU:HD11	13:Q:536:LEU:HB2	1.81	0.61
2:J:411:TRP:HZ2	2:J:446:ILE:HD11	1.65	0.61
5:A:119:GLN:NE2	5:A:204:VAL:HA	2.16	0.61
13:Q:45:ASN:HB2	13:Q:48:LEU:HG	1.81	0.61
9:O:52:LEU:HD13	13:Q:423:LEU:HD22	1.81	0.61
1:F:51:GLU:OE2	1:H:472:PRO:HD2	2.00	0.61
2:K:753:GLU:HA	1:H:629:LEU:HD11	1.81	0.61
10:P:621:GLU:HG2	10:P:625:HIS:HE1	1.61	0.61
11:I:33:ALA:HB1	11:I:38:VAL:HG11	1.82	0.61
14:T:221:ILE:HB	14:T:275:PHE:HE1	1.66	0.61
14:T:309:MET:HE1	14:T:315:TYR:CD1	2.26	0.61
4:E:95:PRO:HD2	4:E:95:PRO:C	2.22	0.61
6:B:190:ARG:HB2	11:I:97:TRP:CD2	2.32	0.61
10:P:119:LEU:HD23	10:P:119:LEU:C	2.26	0.61
14:T:738:VAL:HG11	15:U:1:MET:HG3	1.80	0.61
1:F:88:PHE:CE1	1:F:105:PHE:HE1	2.19	0.61
2:K:323:ASN:HA	2:K:365:ARG:HH12	1.66	0.61
4:E:89:LYS:HD3	4:E:90:GLN:N	2.15	0.61
4:E:105:SER:O	4:E:109:SER:OG	2.17	0.61
2:J:516:LEU:HD21	2:J:539:THR:HG23	1.83	0.61
10:P:223:VAL:HG21	11:I:9:SER:HB2	1.82	0.61
1:H:607:HIS:O	1:H:611:TYR:CE2	2.53	0.61
5:A:114:GLN:NE2	5:A:211:ASP:HB3	2.16	0.61
6:B:356:VAL:HG22	6:B:370:ASP:HA	1.83	0.61
10:P:301:LEU:HD21	10:P:318:LEU:HD12	1.83	0.60
5:A:104:ALA:HB2	5:A:113:TRP:HB3	1.83	0.60
9:O:251:VAL:HG21	9:O:298:PHE:CZ	2.37	0.60
11:I:38:VAL:O	11:I:41:ILE:HG22	2.00	0.60
13:Q:121:PRO:O	13:Q:336:ARG:NH2	2.34	0.60
14:T:33:ASP:OD2	14:T:62:ILE:HD11	2.01	0.60
15:U:1:MET:HA	15:U:1:MET:HE3	1.82	0.60
2:J:636:LEU:HB2	2:J:659:ALA:HB2	1.82	0.60
14:T:518:PHE:HE1	14:T:661:GLY:H	1.49	0.60
1:F:30:LEU:HD12	1:H:433:LEU:HD13	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:278:PHE:HZ	10:D:296:ILE:HD11	1.65	0.60
11:I:94:GLU:CD	11:I:94:GLU:H	2.08	0.60
13:Q:104:ARG:HA	13:Q:104:ARG:HH11	1.66	0.60
2:K:566:ALA:CB	3:W:1:MET:HE3	2.30	0.60
6:B:432:ALA:HB1	6:B:477:MET:CE	2.31	0.60
6:B:520:HIS:O	6:B:533:GLY:N	2.35	0.60
2:K:575:TYR:CD2	6:B:222:PHE:HZ	2.17	0.60
6:B:448:GLY:H	6:B:452:ARG:H	1.50	0.60
10:D:300:LYS:O	10:D:304:PHE:HB2	2.02	0.60
1:H:31:GLN:O	1:H:35:GLN:NE2	2.34	0.60
5:A:15:PRO:HB2	5:A:19:ILE:HG12	1.84	0.60
6:B:544:LEU:HD23	6:B:545:PHE:N	2.17	0.60
1:F:120:ILE:HG12	1:F:163:LEU:HD13	1.82	0.60
8:C:610:PHE:HE1	8:C:614:LYS:HD2	1.65	0.60
9:O:193:VAL:HA	9:O:196:GLN:HG2	1.84	0.60
13:Q:22:ARG:HH11	13:Q:46:ILE:HG23	1.67	0.60
14:T:237:PHE:HB3	14:T:240:MET:SD	2.41	0.60
9:O:46:SER:HA	9:O:49:ARG:HG3	1.84	0.60
9:O:164:GLU:OE2	10:P:394:ARG:NE	2.28	0.60
13:Q:105:TYR:OH	13:Q:227:LYS:HA	2.02	0.60
1:F:34:ILE:O	1:F:38:ILE:HG22	2.02	0.59
5:A:6:ILE:HG23	8:C:1309:MET:HG3	1.84	0.59
5:A:205:ASN:OD1	5:A:212:THR:OG1	2.19	0.59
11:I:103:MET:SD	11:I:103:MET:C	2.84	0.59
2:J:446:ILE:O	2:J:450:ASN:ND2	2.34	0.59
6:B:118:ASP:OD2	6:B:128:ARG:NH2	2.35	0.59
6:B:190:ARG:H	11:I:97:TRP:HH2	1.24	0.59
8:C:211:LYS:O	8:C:380:LEU:HG	2.02	0.59
10:P:480:MET:SD	10:P:480:MET:N	2.65	0.59
1:F:492:LEU:O	1:F:496:ASN:HB2	2.01	0.59
1:F:495:PHE:HE1	1:F:512:PHE:HD1	1.49	0.59
2:J:302:LEU:HD22	2:J:318:VAL:HG21	1.83	0.59
1:H:634:ALA:HA	1:H:637:ILE:HD12	1.84	0.59
10:D:74:ILE:N	10:P:83:GLU:OE2	2.35	0.59
10:P:205:ILE:HG21	10:P:240:LYS:HD2	1.83	0.59
2:K:736:TYR:CA	1:H:599:LYS:CE	2.80	0.59
1:H:580:GLN:O	1:H:584:HIS:ND1	2.32	0.59
6:B:269:ILE:HG22	6:B:279:VAL:HG12	1.83	0.59
8:C:1510:GLN:HG3	8:C:1553:CYS:HB3	1.84	0.59
14:T:510:ARG:HH21	14:T:577:ILE:HG23	1.68	0.59
1:F:59:ILE:HG13	1:H:466:HIS:HB2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:635:ARG:CZ	1:H:635:ARG:HB2	2.32	0.59
14:T:237:PHE:O	14:T:240:MET:HG3	2.01	0.59
2:J:729:ASP:OD1	2:J:729:ASP:N	2.34	0.59
9:O:331:THR:HG21	10:D:452:GLU:OE2	2.02	0.59
6:B:261:ALA:HB3	6:B:268:LEU:HD11	1.85	0.59
6:B:370:ASP:N	6:B:376:PRO:O	2.34	0.59
10:D:134:GLU:HG3	11:I:20:HIS:HB3	1.85	0.59
10:D:187:ILE:HD12	10:D:224:ILE:HD11	1.84	0.59
10:P:121:LEU:CD1	10:P:190:ILE:HG23	2.33	0.59
13:Q:93:ILE:HG23	13:Q:164:VAL:HG13	1.83	0.59
14:T:387:LEU:HG	14:T:529:TRP:CZ2	2.38	0.59
1:F:646:CYS:SG	1:F:681:LYS:HG3	2.43	0.59
2:J:709:GLU:HG2	3:G:10:GLN:HG2	1.84	0.59
6:B:303:ASN:ND2	6:B:321:GLN:OE1	2.34	0.59
10:D:537:SER:HA	10:D:576:GLU:OE2	2.03	0.59
2:K:702:GLU:OE2	1:H:169:HIS:NE2	2.36	0.58
1:F:78:LEU:HB2	1:F:87:ALA:HB2	1.85	0.58
1:F:625:GLU:N	1:F:625:GLU:OE1	2.35	0.58
1:F:730:ILE:HD11	2:J:621:TYR:CZ	2.37	0.58
8:C:1326:LEU:HD21	8:C:1379:THR:HA	1.84	0.58
9:O:382:MET:HA	9:O:385:ILE:HD12	1.85	0.58
10:P:27:TRP:CD2	10:P:115:TYR:HE1	2.21	0.58
10:P:138:ASN:OD1	11:I:29:GLN:NE2	2.36	0.58
8:C:598:TYR:HA	8:C:605:TYR:HE2	1.67	0.58
2:J:255:LYS:HG2	2:K:462:ASN:ND2	2.18	0.58
4:E:254:ARG:NH2	4:E:258:SER:OG	2.36	0.58
9:O:251:VAL:HG21	9:O:298:PHE:HZ	1.68	0.58
13:Q:498:ILE:HD11	13:Q:516:ILE:HB	1.85	0.58
6:B:411:VAL:HB	6:B:421:LEU:HB2	1.85	0.58
8:C:741:ARG:NH2	8:C:778:THR:OG1	2.32	0.58
8:C:1735:GLN:HE22	14:T:5:ILE:HG13	1.67	0.58
10:D:205:ILE:HG13	10:D:206:ASP:H	1.68	0.58
13:Q:322:THR:HG21	13:Q:448:ILE:HD11	1.86	0.58
1:F:504:ALA:O	1:F:536:MET:HE1	2.04	0.58
2:K:674:ILE:HD12	2:K:700:VAL:HG23	1.84	0.58
8:C:1274:ILE:HB	8:C:1279:ILE:HD13	1.84	0.58
10:P:483:TYR:CE2	12:N:123:GLY:HA3	2.38	0.58
11:I:94:GLU:OE2	11:I:94:GLU:N	2.31	0.58
14:T:527:GLU:OE2	14:T:531:ARG:NH1	2.37	0.58
8:C:58:ILE:HG23	8:C:59:GLU:H	1.67	0.58
8:C:918:LEU:O	8:C:953:ARG:NH2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1314:ILE:HG12	8:C:1316:VAL:HG12	1.85	0.58
8:C:1617:THR:HG23	8:C:1619:ASP:H	1.68	0.58
1:F:533:MET:O	1:F:537:PRO:HD3	2.04	0.58
1:H:159:LEU:HD12	1:H:159:LEU:C	2.28	0.58
8:C:749:TYR:HA	8:C:752:VAL:HG12	1.85	0.58
8:C:1588:SER:OG	8:C:1591:CYS:SG	2.60	0.58
10:P:448:HIS:O	10:P:452:GLU:HG3	2.04	0.58
11:I:36:ASP:OD2	11:I:37:GLU:N	2.35	0.58
2:J:541:TYR:OH	11:I:84:SER:HB2	2.04	0.58
2:J:756:VAL:HG23	10:P:482:LEU:HD13	1.86	0.58
13:Q:294:ASP:OD1	13:Q:295:LEU:N	2.37	0.58
2:K:302:LEU:HD22	2:K:318:VAL:HG11	1.85	0.58
6:B:505:MET:N	6:B:505:MET:SD	2.76	0.58
8:C:1366:TYR:CD1	8:C:1387:THR:HG21	2.39	0.58
10:D:332:LYS:HB2	10:D:355:ILE:HD11	1.86	0.58
1:H:171:LYS:H	1:H:171:LYS:HD3	1.68	0.57
5:A:166:PHE:HZ	5:A:169:MET:HG2	1.67	0.57
6:B:500:TRP:CD1	6:B:502:CYS:HG	2.22	0.57
9:O:60:ASP:OD1	9:O:60:ASP:N	2.37	0.57
9:O:417:GLU:H	12:N:4:ALA:HB1	1.68	0.57
1:F:50:ALA:HB1	1:F:74:TYR:HA	1.85	0.57
2:J:547:ILE:HG13	2:J:577:LEU:HD22	1.85	0.57
8:C:1514:ASN:HD22	8:C:1550:GLU:HG2	1.70	0.57
2:K:653:LYS:HE2	2:K:657:LYS:HD2	1.85	0.57
5:A:37:ARG:NH2	5:A:52:GLN:O	2.35	0.57
13:Q:365:ALA:O	13:Q:463:MET:HE3	2.04	0.57
14:T:237:PHE:HB3	14:T:240:MET:CE	2.32	0.57
2:J:479:PHE:HB3	2:J:510:LEU:HD11	1.86	0.57
2:K:316:LEU:HD11	2:K:321:GLU:HA	1.86	0.57
6:B:378:PHE:CD2	6:B:379:GLU:HG3	2.40	0.57
6:B:399:LYS:HD3	6:B:413:GLU:HA	1.87	0.57
8:C:500:SER:HB2	8:C:551:PHE:CG	2.38	0.57
8:C:1309:MET:HA	8:C:1309:MET:HE2	1.85	0.57
9:O:81:ILE:O	9:O:85:LEU:HD12	2.04	0.57
5:A:128:SER:HB3	8:C:1235:GLU:HG3	1.86	0.57
14:T:280:LEU:O	14:T:284:THR:HG23	2.05	0.57
8:C:1547:MET:HA	8:C:1547:MET:HE3	1.86	0.57
10:P:345:TYR:HB2	10:P:376:MET:HE2	1.87	0.57
1:H:206:VAL:HG13	1:H:207:PHE:HD1	1.70	0.57
1:H:455:ALA:HB3	1:H:481:LEU:HD21	1.86	0.57
1:H:694:VAL:O	1:H:697:GLN:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:432:ALA:O	6:B:446:GLY:N	2.35	0.57
13:Q:27:LEU:HB2	13:Q:41:ILE:HB	1.87	0.57
13:Q:365:ALA:HA	13:Q:463:MET:HE3	1.86	0.57
14:T:43:PRO:CD	14:T:113:GLN:HE21	2.18	0.57
6:B:529:THR:HA	6:B:542:TRP:O	2.04	0.56
13:Q:217:THR:HB	13:Q:483:ASP:HB3	1.86	0.56
4:E:141:MET:N	4:E:141:MET:SD	2.78	0.56
4:E:175:ARG:HG3	4:E:180:GLU:HB2	1.87	0.56
8:C:1244:GLN:HB3	8:C:1285:LEU:HD22	1.87	0.56
1:F:532:LEU:HD12	1:F:542:THR:HG22	1.86	0.56
2:J:246:TYR:CD2	2:J:276:ASN:HB3	2.40	0.56
2:J:575:TYR:CE1	2:J:583:GLN:NE2	2.63	0.56
2:K:653:LYS:HG3	2:K:684:TYR:HE1	1.70	0.56
4:E:255:ARG:NH1	4:E:256:HIS:CG	2.72	0.56
8:C:501:PRO:HG2	8:C:607:ARG:HD3	1.87	0.56
8:C:568:VAL:HG12	8:C:569:VAL:HG23	1.88	0.56
8:C:1406:VAL:O	8:C:1410:VAL:HG23	2.04	0.56
9:O:390:GLU:HB2	9:O:428:PHE:HE1	1.70	0.56
10:P:301:LEU:HD13	10:P:334:TYR:CD2	2.40	0.56
13:Q:625:ASP:OD1	13:Q:647:LYS:NZ	2.28	0.56
14:T:196:LEU:CD1	14:T:200:LEU:HD23	2.32	0.56
2:J:750:ASN:ND2	3:G:23:LEU:HD23	2.20	0.56
2:K:636:LEU:HB2	2:K:659:ALA:HB2	1.87	0.56
2:K:731:LEU:HD21	2:K:747:LEU:HB3	1.87	0.56
6:B:55:ASP:OD1	6:B:56:ARG:N	2.38	0.56
8:C:1586:GLU:HA	8:C:1586:GLU:OE2	2.06	0.56
5:A:17:GLU:CD	5:A:17:GLU:H	2.13	0.56
10:P:9:ILE:HG13	10:P:292:PHE:CZ	2.37	0.56
10:P:509:TYR:O	10:P:509:TYR:CD2	2.58	0.56
1:F:461:SER:OG	1:F:462:GLN:OE1	2.23	0.56
2:J:245:MET:HG3	2:K:394:GLU:CD	2.30	0.56
2:K:250:GLU:OE2	2:K:251:TYR:N	2.39	0.56
1:H:177:HIS:O	1:H:190:SER:OG	2.20	0.56
6:B:482:ASN:HB2	6:B:545:PHE:HE2	1.71	0.56
11:I:141:ILE:HD12	11:I:153:LEU:CD2	2.35	0.56
1:H:123:LEU:HA	1:H:126:ILE:HG22	1.88	0.56
8:C:428:LEU:HB3	8:C:433:LEU:HD11	1.86	0.56
10:P:256:MET:HE2	10:P:256:MET:CA	2.35	0.56
2:J:393:PHE:CD1	2:J:393:PHE:C	2.83	0.56
2:K:622:PHE:CE2	2:K:638:GLU:HB3	2.40	0.56
14:T:228:ASN:ND2	14:T:242:THR:HG22	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:691:ARG:HD2	1:H:694:VAL:HB	1.88	0.56
5:A:112:PHE:CE2	5:A:213:HIS:CE1	2.94	0.56
5:A:126:MET:SD	5:A:197:PHE:HD1	2.29	0.56
8:C:588:LEU:O	8:C:614:LYS:NZ	2.25	0.56
8:C:927:THR:HG21	8:C:986:SER:HB2	1.87	0.56
13:Q:366:VAL:HG23	13:Q:467:ILE:HD12	1.88	0.56
1:F:116:VAL:HG11	1:F:167:LEU:HD13	1.88	0.56
2:K:644:PHE:HE2	2:K:686:LYS:HG3	1.71	0.56
8:C:766:LEU:HD12	8:C:771:VAL:HG11	1.87	0.56
10:D:269:ASN:ND2	10:D:312:GLU:OE2	2.39	0.56
10:D:531:THR:OG1	10:D:534:GLN:NE2	2.40	0.56
2:K:617:LEU:HB3	2:K:621:TYR:HE2	1.70	0.55
2:K:736:TYR:HA	1:H:599:LYS:CG	2.34	0.55
8:C:115:GLY:N	8:C:127:GLU:O	2.37	0.55
8:C:860:ILE:HG23	9:O:448:LEU:HD21	1.89	0.55
9:O:76:PRO:HG3	9:O:242:ILE:HG12	1.88	0.55
10:P:363:LEU:HD11	10:P:389:VAL:HG13	1.87	0.55
13:Q:151:ASP:OD1	14:T:327:LYS:HG2	2.07	0.55
1:F:41:LEU:HD21	1:H:79:PHE:HE2	1.71	0.55
2:K:393:PHE:CE1	2:K:397:GLU:HB2	2.41	0.55
2:K:753:GLU:OE2	3:W:27:LYS:NZ	2.37	0.55
3:W:27:LYS:HA	3:W:30:GLN:HE22	1.71	0.55
5:A:34:LEU:H	5:A:173:ARG:HH12	1.55	0.55
8:C:1609:TYR:CD1	8:C:1636:ARG:HA	2.40	0.55
10:D:498:ASP:HB3	10:D:501:ILE:HG22	1.89	0.55
1:F:490:MET:HE2	4:E:98:GLU:H	1.70	0.55
1:F:560:ILE:HG22	1:F:564:GLU:OE2	2.07	0.55
2:J:443:THR:O	2:J:447:THR:HG23	2.07	0.55
5:A:136:MET:HE3	5:A:181:LEU:HB3	1.87	0.55
6:B:504:SER:CA	6:B:505:MET:CE	2.84	0.55
8:C:426:ILE:HD11	8:C:448:MET:SD	2.46	0.55
9:O:431:LEU:HB2	9:O:472:TYR:OH	2.07	0.55
1:F:74:TYR:O	1:F:78:LEU:HD12	2.06	0.55
1:H:506:VAL:HG13	1:H:507:LYS:N	2.22	0.55
4:E:255:ARG:CZ	4:E:256:HIS:CA	2.84	0.55
1:H:635:ARG:NH2	1:H:648:CYS:HB2	2.21	0.55
6:B:122:SER:OG	6:B:192:SER:OG	2.24	0.55
8:C:1642:PHE:HD2	8:C:1694:LEU:HD21	1.72	0.55
2:K:736:TYR:C	1:H:599:LYS:CE	2.78	0.55
2:K:739:PRO:CD	1:H:599:LYS:HZ1	2.19	0.55
9:O:436:LYS:O	9:O:437:GLU:HG3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:551:LYS:NZ	13:Q:552:GLU:O	2.36	0.55
14:T:613:TYR:CE2	15:U:58:PRO:HG3	2.41	0.55
2:K:427:GLU:HA	2:K:430:LYS:HE3	1.89	0.55
2:K:587:ALA:HB2	6:B:222:PHE:HE2	1.70	0.55
1:H:608:TYR:HA	1:H:611:TYR:HD2	1.70	0.55
8:C:1139:ARG:NH2	8:C:1181:GLY:O	2.40	0.55
10:D:201:TYR:CE1	10:D:203:ILE:N	2.74	0.55
4:E:195:ILE:O	4:E:199:GLU:N	2.38	0.55
8:C:463:GLN:HE21	8:C:481:GLY:H	1.49	0.55
8:C:475:LEU:HD12	8:C:476:ILE:H	1.72	0.55
8:C:1292:ALA:O	8:C:1296:ILE:HG12	2.07	0.55
9:O:45:ILE:HD12	9:O:45:ILE:H	1.70	0.55
14:T:295:TYR:HE2	14:T:349:LYS:HE2	1.72	0.55
14:T:517:LEU:HD22	14:T:584:ILE:HG13	1.88	0.55
2:J:599:HIS:NE2	2:J:632:ASP:OD2	2.38	0.55
1:H:485:ILE:C	1:H:486:ILE:HD12	2.31	0.55
5:A:114:GLN:HE22	5:A:212:THR:H	1.53	0.55
8:C:48:SER:OG	8:C:50:ASP:O	2.24	0.55
8:C:1308:ILE:HG22	8:C:1309:MET:CE	2.35	0.55
10:D:396:ARG:HB2	10:D:399:THR:HG22	1.88	0.55
12:N:9:SER:OG	13:Q:320:GLN:OE1	2.25	0.55
1:F:98:HIS:HB3	1:F:101:ILE:HG13	1.89	0.55
2:J:241:LEU:HD13	2:J:272:VAL:HG22	1.88	0.55
2:K:686:LYS:NZ	3:W:15:ASP:OD2	2.40	0.55
14:T:537:ARG:NH1	14:T:578:ASP:OD2	2.40	0.55
15:U:100:LEU:HD13	15:U:107:ASN:OD1	2.07	0.55
8:C:64:ARG:NH2	9:O:539:GLU:OE2	2.40	0.54
13:Q:299:LEU:HD12	13:Q:405:LEU:HD13	1.88	0.54
2:J:376:ASN:OD1	2:J:377:LYS:N	2.41	0.54
2:K:594:PHE:CE2	6:B:218:LEU:HD23	2.42	0.54
8:C:403:LEU:HD13	8:C:494:PRO:HG3	1.89	0.54
10:P:226:LYS:NZ	10:P:254:GLU:OE1	2.32	0.54
13:Q:9:PHE:O	13:Q:10:ILE:HB	2.07	0.54
1:H:47:GLU:OE1	1:H:78:LEU:HD22	2.08	0.54
6:B:325:LEU:HD11	6:B:339:THR:HG23	1.89	0.54
14:T:233:TRP:HB3	14:T:301:THR:HG21	1.89	0.54
6:B:222:PHE:CD1	6:B:222:PHE:C	2.85	0.54
6:B:389:CYS:O	6:B:431:LYS:NZ	2.37	0.54
6:B:432:ALA:HB2	6:B:475:CYS:C	2.33	0.54
11:I:113:PHE:HB2	11:I:141:ILE:HB	1.89	0.54
1:F:721:ARG:HH12	1:F:753:LYS:HB3	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:187:ARG:HH12	8:C:1322:ASN:HB3	1.73	0.54
6:B:276:VAL:HG13	6:B:287:LEU:CD1	2.38	0.54
8:C:745:ILE:HD12	8:C:783:ILE:HG21	1.88	0.54
10:P:364:ASN:OD1	10:P:396:ARG:NH2	2.40	0.54
10:P:595:GLN:CA	10:P:626:MET:HE2	2.37	0.54
13:Q:18:ILE:HD11	13:Q:29:ILE:HG23	1.90	0.54
2:K:319:ILE:HD11	2:K:364:LEU:HD13	1.90	0.54
8:C:972:ILE:HB	8:C:975:GLN:HB3	1.90	0.54
10:P:531:THR:OG1	10:P:534:GLN:NE2	2.40	0.54
13:Q:499:ASN:HB3	13:Q:517:GLN:HB3	1.89	0.54
1:F:513:SER:OG	1:F:548:ASN:ND2	2.33	0.54
2:J:610:MET:CE	2:J:642:MET:HB2	2.36	0.54
1:H:516:LEU:HD21	1:H:524:LYS:HB3	1.90	0.54
6:B:514:HIS:ND1	6:B:536:ASP:OD2	2.38	0.54
8:C:662:MET:HE2	8:C:664:TRP:NE1	2.22	0.54
10:D:201:TYR:CE1	10:D:203:ILE:CB	2.62	0.54
13:Q:209:PHE:HB3	13:Q:500:LEU:HD21	1.89	0.54
13:Q:561:PHE:HD2	13:Q:628:ILE:HD13	1.73	0.54
2:K:446:ILE:HG21	2:K:472:ILE:HD11	1.89	0.54
1:H:577:TYR:CE2	1:H:599:LYS:HB3	2.43	0.54
6:B:365:ARG:HB3	6:B:367:LEU:HD13	1.90	0.54
8:C:608:ASP:OD1	8:C:609:LEU:N	2.41	0.54
1:F:748:ILE:O	1:F:752:GLN:HG2	2.07	0.54
8:C:59:GLU:HB2	9:O:534:LYS:HE2	1.90	0.54
8:C:1252:MET:HE2	8:C:1256:LEU:HD12	1.90	0.54
10:P:507:GLU:OE2	10:P:541:ARG:NH1	2.40	0.54
13:Q:366:VAL:CG2	13:Q:467:ILE:HD12	2.38	0.54
13:Q:423:LEU:HD23	13:Q:424:TYR:H	1.72	0.54
2:J:246:TYR:CE2	2:J:276:ASN:HB3	2.42	0.54
4:E:217:GLN:HB2	4:E:220:HIS:ND1	2.23	0.54
8:C:605:TYR:HA	8:C:610:PHE:CD2	2.43	0.54
10:P:27:TRP:N	10:P:27:TRP:CD1	2.75	0.54
2:K:573:HIS:NE2	3:W:4:ARG:HB2	2.23	0.53
9:O:123:LEU:HD11	9:O:143:ARG:HD2	1.90	0.53
10:P:324:VAL:HG22	10:P:325:PHE:CD1	2.43	0.53
1:F:123:LEU:HA	1:F:126:ILE:HG22	1.89	0.53
2:J:427:GLU:O	2:J:431:ASN:ND2	2.41	0.53
2:K:575:TYR:HB3	2:K:584:ALA:HB2	1.90	0.53
3:G:23:LEU:CD1	3:G:26:GLN:HE21	2.20	0.53
6:B:213:SER:HA	6:B:217:LEU:HD22	1.89	0.53
6:B:520:HIS:HB2	6:B:533:GLY:HA3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:979:ILE:HD11	8:C:1049:PHE:HB2	1.90	0.53
9:O:512:ASP:HB3	9:O:531:TYR:HE2	1.73	0.53
13:Q:41:ILE:HD13	13:Q:41:ILE:N	2.22	0.53
14:T:128:LEU:HD13	14:T:177:LEU:HD21	1.90	0.53
1:F:187:LEU:CD1	1:H:42:ASN:HD21	2.22	0.53
2:K:583:GLN:HE21	8:C:1142:ARG:HH22	1.56	0.53
1:H:127:ILE:HD11	1:H:153:LEU:CD1	2.39	0.53
9:O:15:PRO:HD2	9:O:241:LEU:HB2	1.90	0.53
14:T:14:ILE:HD12	14:T:109:PHE:HA	1.90	0.53
14:T:536:ILE:O	14:T:540:ILE:HG12	2.07	0.53
2:K:486:CYS:HA	2:K:489:VAL:HG12	1.89	0.53
1:H:614:LEU:HD13	1:H:630:TYR:CZ	2.43	0.53
6:B:350:LEU:HD22	6:B:357:LEU:HD21	1.91	0.53
6:B:391:LEU:HD11	6:B:400:LEU:HD21	1.89	0.53
11:I:145:ILE:HG23	11:I:146:PHE:CD2	2.43	0.53
13:Q:10:ILE:HG23	13:Q:19:PHE:HB2	1.90	0.53
13:Q:253:ILE:HG21	13:Q:325:ILE:HG21	1.90	0.53
14:T:343:ARG:O	14:T:347:THR:HG23	2.09	0.53
2:K:542:MET:HE1	3:W:2:ILE:HG21	1.89	0.53
2:K:668:PRO:O	2:K:673:THR:OG1	2.22	0.53
10:D:537:SER:CA	10:D:576:GLU:OE2	2.56	0.53
10:P:27:TRP:CE3	10:P:115:TYR:HE1	2.25	0.53
2:K:306:PHE:HB3	2:K:315:ALA:HB2	1.90	0.53
4:E:135:ARG:HB2	4:E:138:ILE:HG13	1.90	0.53
6:B:108:ASN:O	6:B:230:ARG:NH2	2.42	0.53
8:C:1285:LEU:HD12	8:C:1285:LEU:O	2.09	0.53
9:O:77:ILE:HG22	9:O:79:ASP:H	1.72	0.53
2:J:321:GLU:OE1	2:J:369:TYR:OH	2.25	0.53
2:J:694:ILE:HD13	2:J:717:LEU:HD13	1.91	0.53
5:A:93:SER:HB3	5:A:122:GLN:H	1.73	0.53
8:C:1154:LEU:HD11	8:C:1163:ALA:HB2	1.91	0.53
10:P:417:ILE:HG23	10:P:437:MET:HE3	1.90	0.53
13:Q:22:ARG:HD3	13:Q:46:ILE:HD12	1.90	0.53
14:T:37:LEU:HD11	14:T:62:ILE:HG21	1.91	0.53
14:T:528:LYS:HG3	14:T:529:TRP:CD1	2.44	0.53
1:F:506:VAL:HB	1:F:536:MET:CE	2.38	0.53
2:J:432:LEU:HD11	2:K:255:LYS:HE2	1.90	0.53
2:K:474:TYR:OH	3:W:1:MET:O	2.27	0.53
1:H:651:SER:O	1:H:655:LEU:HD12	2.09	0.53
5:A:148:TYR:HD2	5:A:213:HIS:NE2	2.07	0.53
8:C:381:PRO:HD2	8:C:384:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:756:ASN:OD1	8:C:756:ASN:N	2.39	0.53
8:C:956:THR:HG21	8:C:1494:PHE:HB3	1.90	0.53
10:P:363:LEU:HD23	10:P:396:ARG:HE	1.73	0.53
2:J:607:MET:HG3	2:J:638:GLU:OE2	2.09	0.53
1:H:69:ASP:HB3	1:H:147:LEU:HD11	1.91	0.53
8:C:120:TYR:HA	8:C:196:SER:HA	1.91	0.53
8:C:662:MET:CE	8:C:664:TRP:CZ2	2.92	0.53
9:O:623:PRO:HB2	9:O:660:PHE:HZ	1.73	0.53
10:P:396:ARG:NH1	11:I:13:TYR:OH	2.40	0.53
13:Q:201:VAL:HG13	13:Q:543:ASP:HB2	1.89	0.53
13:Q:628:ILE:HB	13:Q:645:PHE:HB2	1.91	0.53
1:H:506:VAL:HG13	1:H:507:LYS:H	1.73	0.52
6:B:437:PRO:HD2	6:B:479:TRP:CD1	2.44	0.52
9:O:208:ILE:HG12	9:O:212:ASP:OD1	2.09	0.52
9:O:329:LYS:HE2	9:O:337:TYR:CE2	2.44	0.52
10:P:481:HIS:O	10:P:484:SER:OG	2.27	0.52
13:Q:366:VAL:HG22	13:Q:467:ILE:CD1	2.39	0.52
14:T:387:LEU:HD21	14:T:529:TRP:CE2	2.44	0.52
14:T:387:LEU:HD21	14:T:529:TRP:CZ3	2.44	0.52
2:K:648:GLU:HB3	2:K:651:LYS:HZ1	1.74	0.52
1:H:645:ILE:HG21	1:H:668:ALA:HB2	1.90	0.52
8:C:1321:LEU:HD13	8:C:1376:PHE:HE1	1.74	0.52
9:O:10:THR:HG22	9:O:12:PHE:H	1.74	0.52
11:I:85:ASN:O	11:I:89:ASN:HB2	2.09	0.52
13:Q:95:LYS:NZ	13:Q:195:LEU:O	2.42	0.52
14:T:384:TYR:HE2	14:T:394:LEU:CD2	2.05	0.52
1:F:453:PHE:CE2	4:E:114:GLU:HA	2.43	0.52
2:J:459:LEU:HD21	2:K:259:ILE:HG13	1.91	0.52
1:H:157:ASN:HB2	1:H:180:ALA:HB2	1.90	0.52
13:Q:22:ARG:NH2	13:Q:52:TYR:OH	2.40	0.52
2:J:514:ASN:ND2	10:D:384:TYR:CE1	2.73	0.52
8:C:401:LEU:HD12	8:C:412:LEU:HD23	1.92	0.52
8:C:1702:LEU:HD23	8:C:1702:LEU:C	2.35	0.52
10:D:35:TRP:CZ3	10:D:295:MET:HE1	2.45	0.52
10:D:562:CYS:O	10:D:565:VAL:HG12	2.09	0.52
13:Q:149:ASP:OD1	13:Q:158:LYS:NZ	2.37	0.52
2:K:256:VAL:HG12	2:K:265:ASP:OD2	2.10	0.52
2:K:263:PRO:HB2	2:K:295:ASN:ND2	2.24	0.52
8:C:1213:GLN:HA	8:C:1216:MET:HG2	1.92	0.52
8:C:1483:ASP:O	8:C:1487:ILE:HG13	2.10	0.52
10:P:247:PHE:HA	10:P:295:MET:SD	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:323:VAL:HG23	13:Q:384:ILE:HG23	1.91	0.52
1:F:30:LEU:HD13	1:F:52:LEU:HD22	1.91	0.52
6:B:328:ILE:O	6:B:337:ILE:N	2.41	0.52
8:C:1133:MET:HA	8:C:1177:LEU:HD22	1.90	0.52
8:C:1626:PHE:HD2	8:C:1630:THR:HA	1.73	0.52
9:O:541:ASP:OD1	9:O:542:TYR:N	2.43	0.52
2:K:479:PHE:CD1	2:K:506:CYS:SG	3.03	0.52
1:H:192:GLU:O	1:H:196:LYS:HG2	2.09	0.52
8:C:1167:TYR:C	8:C:1167:TYR:CD2	2.84	0.52
8:C:1732:LEU:H	8:C:1732:LEU:HD23	1.74	0.52
9:O:247:LEU:O	9:O:251:VAL:HG23	2.10	0.52
10:P:27:TRP:CE3	10:P:115:TYR:CE1	2.96	0.52
10:P:119:LEU:C	10:P:119:LEU:CD2	2.83	0.52
13:Q:128:LYS:HG3	13:Q:133:ILE:HG12	1.91	0.52
14:T:35:ASN:O	14:T:38:LEU:HD12	2.10	0.52
14:T:319:VAL:O	14:T:323:LEU:HG	2.09	0.52
1:F:626:GLU:HB3	4:E:227:LEU:HD13	1.92	0.52
2:J:429:MET:HE1	2:J:432:LEU:HD23	1.92	0.52
6:B:189:THR:CA	11:I:97:TRP:HH2	2.22	0.52
8:C:959:VAL:HA	8:C:1543:HIS:NE2	2.25	0.52
9:O:251:VAL:HG13	9:O:304:LEU:HD12	1.90	0.52
8:C:166:SER:HB2	8:C:371:VAL:HG12	1.92	0.52
8:C:463:GLN:CD	8:C:480:GLU:C	2.78	0.52
8:C:1341:ILE:HD11	8:C:1528:VAL:HG21	1.91	0.52
9:O:435:VAL:HG13	9:O:582:ASP:HA	1.92	0.52
11:I:24:TYR:HB3	11:I:27:TRP:HE1	1.74	0.52
11:I:83:ASN:C	11:I:83:ASN:HD22	2.13	0.52
1:F:725:ARG:NH1	1:F:728:ASP:OD2	2.43	0.52
6:B:109:GLU:OE1	8:C:1100:LYS:HB3	2.10	0.52
8:C:630:GLY:O	8:C:634:ILE:HG23	2.10	0.52
8:C:863:ILE:O	8:C:867:ILE:HG23	2.10	0.52
8:C:1561:THR:OG1	8:C:1563:ASP:OD1	2.20	0.52
8:C:1587:ILE:HD12	8:C:1591:CYS:HB2	1.92	0.52
9:O:29:SER:O	9:O:30:GLN:HG3	2.10	0.52
9:O:331:THR:HG21	10:D:452:GLU:HB2	1.91	0.52
14:T:113:GLN:OE1	14:T:113:GLN:HA	2.08	0.52
1:F:453:PHE:HE1	4:E:96:PHE:CE1	2.27	0.51
2:J:514:ASN:HD21	10:D:384:TYR:HE1	1.53	0.51
2:J:643:TYR:HE2	2:J:655:TYR:CE2	2.28	0.51
2:J:754:LEU:HD23	3:G:27:LYS:HD3	1.92	0.51
8:C:605:TYR:HA	8:C:610:PHE:CE2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:382:MET:SD	9:O:406:ILE:HD12	2.50	0.51
9:O:442:GLU:C	9:O:442:GLU:OE1	2.53	0.51
13:Q:63:SER:HA	13:Q:73:ILE:HG22	1.92	0.51
2:J:281:ARG:HG2	2:K:495:PHE:HB2	1.92	0.51
2:J:509:GLU:OE1	2:J:509:GLU:O	2.28	0.51
4:E:232:LEU:O	4:E:236:TYR:CE1	2.64	0.51
8:C:585:LEU:O	8:C:614:LYS:NZ	2.41	0.51
8:C:1558:ASP:OD1	8:C:1559:ILE:N	2.43	0.51
9:O:107:GLY:HA3	10:P:384:TYR:HE1	1.74	0.51
14:T:683:GLN:OE1	14:T:723:TRP:NE1	2.44	0.51
2:K:407:PRO:HB3	2:K:438:SER:HB3	1.93	0.51
5:A:138:ILE:HD13	5:A:217:ILE:HD13	1.92	0.51
6:B:271:TRP:HZ2	6:B:525:ASN:HB3	1.75	0.51
6:B:544:LEU:HD23	6:B:545:PHE:H	1.73	0.51
13:Q:195:LEU:HD21	13:Q:198:ILE:HD11	1.91	0.51
15:U:104:LEU:HB2	15:U:107:ASN:HD22	1.75	0.51
2:K:278:GLN:OE1	2:K:281:ARG:NH1	2.43	0.51
2:K:428:ILE:HD13	2:K:457:TYR:CE1	2.46	0.51
5:A:9:VAL:O	5:A:13:LEU:HG	2.09	0.51
8:C:806:GLU:H	8:C:806:GLU:CD	2.18	0.51
10:P:352:PHE:HD2	10:P:369:TYR:CD1	2.28	0.51
1:F:196:LYS:HD2	1:F:196:LYS:C	2.35	0.51
1:F:730:ILE:HG21	2:J:624:LEU:HD11	1.91	0.51
2:K:239:ASP:OD1	2:K:242:MET:HE2	2.10	0.51
8:C:810:ARG:O	8:C:814:GLN:NE2	2.42	0.51
8:C:1580:LYS:HD3	8:C:1580:LYS:N	2.25	0.51
9:O:306:TYR:HB2	9:O:321:SER:OG	2.10	0.51
10:D:376:MET:HB3	10:D:378:LYS:HG3	1.91	0.51
14:T:33:ASP:OD1	14:T:58:ARG:HD3	2.10	0.51
14:T:312:PHE:HA	14:T:315:TYR:CD2	2.45	0.51
2:J:357:MET:HA	2:J:357:MET:HE2	1.93	0.51
2:K:566:ALA:CA	3:W:1:MET:HE3	2.40	0.51
1:H:737:MET:HG2	1:H:744:ASN:OD1	2.10	0.51
4:E:209:ASP:C	4:E:209:ASP:OD2	2.53	0.51
5:A:133:ILE:HG23	5:A:193:LEU:HB3	1.93	0.51
6:B:252:TYR:CE1	6:B:543:LYS:HB2	2.45	0.51
10:P:484:SER:OG	10:P:508:CYS:SG	2.69	0.51
11:I:106:GLU:CD	11:I:107:SER:H	2.18	0.51
8:C:422:LYS:HB3	8:C:451:LEU:HD11	1.92	0.51
10:P:90:LEU:O	10:P:94:THR:HG22	2.11	0.51
10:P:121:LEU:HD12	10:P:190:ILE:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:426:LEU:HD22	11:I:13:TYR:HB2	1.93	0.51
11:I:141:ILE:HG22	11:I:141:ILE:O	2.11	0.51
13:Q:199:ILE:HD11	13:Q:505:LYS:HB2	1.93	0.51
14:T:299:LYS:HE2	14:T:353:VAL:HG11	1.92	0.51
14:T:313:LYS:HA	14:T:316:THR:HG22	1.91	0.51
1:F:196:LYS:HD2	1:F:196:LYS:O	2.10	0.51
2:K:501:PRO:HG3	2:K:532:ILE:HD11	1.93	0.51
6:B:503:ASN:O	6:B:505:MET:HE1	2.11	0.51
9:O:258:TRP:HZ2	9:O:311:LYS:HB2	1.74	0.51
9:O:431:LEU:CB	9:O:472:TYR:OH	2.58	0.51
2:J:447:THR:HA	2:J:450:ASN:HD21	1.76	0.51
5:A:49:ASN:OD1	5:A:178:TRP:N	2.43	0.51
5:A:91:LYS:O	5:A:124:ASP:HB3	2.11	0.51
8:C:1032:SER:OG	9:O:370:ARG:NH1	2.44	0.51
10:D:297:LYS:O	10:D:301:LEU:HD12	2.11	0.51
14:T:103:PHE:CE2	14:T:147:ILE:HA	2.46	0.51
14:T:185:ILE:HG21	14:T:216:ALA:HB1	1.93	0.51
14:T:455:ARG:CA	14:T:458:MET:SD	2.90	0.51
8:C:463:GLN:HE22	8:C:481:GLY:H	1.47	0.51
14:T:738:VAL:HG11	15:U:1:MET:HG2	1.88	0.51
1:F:28:ILE:O	1:F:31:GLN:HG3	2.11	0.50
1:F:51:GLU:HG2	1:H:471:MET:HE2	1.86	0.50
2:J:754:LEU:HD11	3:G:23:LEU:HD21	1.93	0.50
5:A:48:VAL:HG21	5:A:76:LEU:HD21	1.92	0.50
5:A:167:TYR:CD2	5:A:168:LYS:HB2	2.46	0.50
6:B:118:ASP:OD1	6:B:119:THR:N	2.38	0.50
9:O:160:ILE:HD11	12:N:100:LEU:HD23	1.92	0.50
9:O:356:ASP:OD1	9:O:357:ALA:N	2.45	0.50
14:T:372:PHE:HD1	14:T:378:LEU:HD13	1.75	0.50
2:J:647:ASN:HA	2:J:649:PHE:CE2	2.47	0.50
1:H:78:LEU:HB3	1:H:87:ALA:HB2	1.92	0.50
1:H:703:VAL:HG21	1:H:716:LEU:HD22	1.92	0.50
8:C:1350:LYS:HG3	8:C:1351:ILE:HD12	1.93	0.50
9:O:431:LEU:CD1	9:O:472:TYR:CE1	2.73	0.50
10:P:427:ASP:HB2	10:P:430:THR:HG22	1.93	0.50
13:Q:126:PHE:H	13:Q:249:HIS:HE2	1.58	0.50
13:Q:342:GLU:OE1	13:Q:342:GLU:HA	2.12	0.50
1:F:188:TRP:CZ3	1:F:437:MET:HE1	2.46	0.50
2:J:431:ASN:O	2:J:435:ILE:HG12	2.11	0.50
1:H:159:LEU:O	1:H:163:LEU:HG	2.11	0.50
1:H:601:LEU:HD11	1:H:611:TYR:CZ	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:635:ARG:HH22	1:H:648:CYS:CB	2.21	0.50
5:A:6:ILE:H	5:A:6:ILE:HD12	1.76	0.50
8:C:95:ALA:HB2	8:C:110:PHE:HZ	1.75	0.50
10:D:469:PHE:HE1	10:D:473:GLN:HE21	1.57	0.50
10:P:509:TYR:CD2	10:P:509:TYR:C	2.89	0.50
15:U:68:LEU:HD12	15:U:99:GLN:HB2	1.93	0.50
1:F:117:ASN:O	1:F:121:LEU:HG	2.12	0.50
2:J:419:PHE:HB2	2:J:426:LYS:HE3	1.94	0.50
6:B:222:PHE:C	6:B:222:PHE:HD1	2.20	0.50
8:C:524:TYR:CG	8:C:525:PRO:HD2	2.46	0.50
8:C:734:VAL:HA	8:C:737:ARG:HH11	1.76	0.50
8:C:1615:ASN:O	8:C:1620:TYR:OH	2.20	0.50
13:Q:228:SER:HB3	13:Q:347:ILE:HD12	1.93	0.50
1:F:706:VAL:HG21	6:B:557:LEU:CD1	2.41	0.50
2:K:633:PRO:HB3	2:K:663:VAL:HG21	1.92	0.50
3:W:23:LEU:O	3:W:27:LYS:HG2	2.10	0.50
1:H:533:MET:HE1	4:E:252:LYS:HD2	1.93	0.50
5:A:132:ASP:HB3	5:A:192:LEU:HD13	1.92	0.50
6:B:349:CYS:SG	6:B:391:LEU:N	2.85	0.50
8:C:1385:VAL:O	8:C:1389:VAL:HG23	2.11	0.50
11:I:141:ILE:HD12	11:I:153:LEU:HD21	1.93	0.50
14:T:199:TRP:HE3	14:T:200:LEU:HD22	1.75	0.50
14:T:702:LEU:H	14:T:702:LEU:HD12	1.76	0.50
1:H:574:ALA:HB2	1:H:603:CYS:HB3	1.92	0.50
10:D:321:LEU:HB3	10:D:331:LEU:HD21	1.92	0.50
14:T:43:PRO:HB3	14:T:137:TYR:HE1	1.77	0.50
2:J:440:TYR:O	2:J:631:ASN:ND2	2.44	0.50
2:J:644:PHE:CE1	3:G:9:LEU:HD11	2.47	0.50
2:K:715:GLY:HA3	2:K:731:LEU:CD1	2.41	0.50
4:E:99:ARG:NH1	4:E:99:ARG:HA	2.27	0.50
6:B:526:ASP:OD1	6:B:526:ASP:N	2.45	0.50
8:C:779:TYR:O	9:O:605:ARG:NH2	2.44	0.50
8:C:1136:LEU:HD12	8:C:1177:LEU:HD21	1.93	0.50
9:O:192:ASN:O	9:O:193:VAL:HG12	2.11	0.50
10:D:201:TYR:CD1	10:D:201:TYR:C	2.89	0.50
14:T:411:VAL:HG12	14:T:415:HIS:HD2	1.77	0.50
5:A:80:ARG:NH2	5:A:223:SER:OG	2.45	0.50
5:A:156:TYR:HD1	5:A:166:PHE:HA	1.77	0.50
5:A:164:ALA:HB2	5:A:197:PHE:HE2	1.77	0.50
8:C:463:GLN:HE22	8:C:481:GLY:N	1.87	0.50
8:C:467:ILE:HD12	8:C:476:ILE:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1252:MET:HE3	8:C:1252:MET:O	2.12	0.50
1:F:205:ARG:NH1	4:E:159:SER:OG	2.45	0.50
1:F:442:LEU:HG	1:F:458:LEU:HD11	1.92	0.50
1:F:695:ALA:HA	1:F:698:THR:HG22	1.94	0.50
2:J:432:LEU:HD21	2:K:255:LYS:HG3	1.94	0.50
6:B:268:LEU:HD22	6:B:280:ALA:HB3	1.92	0.50
8:C:1490:HIS:O	8:C:1493:LYS:HG2	2.12	0.50
10:D:35:TRP:HZ3	10:D:295:MET:HE1	1.77	0.50
10:P:313:ASP:O	10:P:317:ASP:CG	2.55	0.50
10:P:427:ASP:C	10:P:429:LYS:H	2.20	0.50
13:Q:123:LEU:HD12	13:Q:123:LEU:H	1.76	0.50
14:T:579:VAL:HG11	14:T:613:TYR:CD2	2.47	0.50
1:F:646:CYS:SG	1:F:677:LEU:HG	2.52	0.49
4:E:95:PRO:CD	4:E:95:PRO:C	2.63	0.49
5:A:80:ARG:HH12	5:A:223:SER:H	1.60	0.49
5:A:83:ASN:HD21	5:A:218:ARG:HD2	1.75	0.49
5:A:205:ASN:ND2	5:A:211:ASP:O	2.44	0.49
6:B:474:ILE:HG12	6:B:490:HIS:CE1	2.47	0.49
8:C:1359:VAL:O	8:C:1363:LEU:HB2	2.12	0.49
8:C:1557:LYS:HA	8:C:1564:ALA:HA	1.92	0.49
8:C:1715:GLU:O	8:C:1719:LEU:HG	2.12	0.49
9:O:233:MET:SD	10:D:128:TRP:HB2	2.51	0.49
9:O:329:LYS:HE2	9:O:337:TYR:HE2	1.77	0.49
10:D:28:LYS:NZ	10:D:97:ASP:OD2	2.40	0.49
10:P:141:THR:O	10:P:421:ARG:HG3	2.11	0.49
13:Q:325:ILE:O	13:Q:329:ILE:HB	2.12	0.49
13:Q:366:VAL:CG2	13:Q:467:ILE:CD1	2.89	0.49
8:C:1020:LEU:O	8:C:1020:LEU:HD12	2.11	0.49
9:O:363:GLU:C	9:O:363:GLU:OE2	2.55	0.49
10:P:352:PHE:HD2	10:P:369:TYR:HD1	1.59	0.49
6:B:506:ASP:OD1	6:B:506:ASP:N	2.44	0.49
11:I:36:ASP:OD2	11:I:37:GLU:OE1	2.29	0.49
12:N:108:LEU:HB3	12:N:109:PRO:HD3	1.93	0.49
2:J:245:MET:CG	2:K:394:GLU:OE1	2.60	0.49
8:C:454:LEU:CD2	8:C:459:PRO:HB3	2.29	0.49
8:C:1367:GLN:H	8:C:1384:ASN:HD21	1.59	0.49
9:O:507:SER:O	9:O:511:GLN:HG2	2.12	0.49
10:D:38:GLU:HB3	10:D:328:PHE:HE1	1.77	0.49
10:D:255:LEU:HD21	10:D:268:LEU:HD21	1.94	0.49
13:Q:501:LEU:HD22	13:Q:567:SER:HA	1.94	0.49
2:J:546:ARG:NH2	11:I:37:GLU:OE2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:362:CYS:HA	2:K:365:ARG:HE	1.77	0.49
1:H:533:MET:HE3	4:E:252:LYS:HE3	1.94	0.49
1:H:611:TYR:CD2	1:H:637:ILE:CD1	2.96	0.49
8:C:1228:VAL:HG13	8:C:1229:THR:HG23	1.94	0.49
8:C:1740:TYR:HD1	14:T:119:PHE:CD2	2.30	0.49
13:Q:285:LEU:HD12	13:Q:289:GLY:HA2	1.95	0.49
15:U:71:HIS:HE1	15:U:94:CYS:HB3	1.77	0.49
1:F:127:ILE:HG13	1:F:160:LEU:HD11	1.94	0.49
1:F:629:LEU:HD12	4:E:207:TRP:HE1	1.78	0.49
2:J:479:PHE:HA	2:J:482:CYS:HB3	1.95	0.49
2:K:585:LEU:N	2:K:608:GLN:HE22	2.11	0.49
2:K:728:ILE:O	2:K:732:HIS:ND1	2.45	0.49
1:H:490:MET:HA	1:H:493:LYS:NZ	2.28	0.49
4:E:250:ARG:O	4:E:250:ARG:NH1	2.42	0.49
6:B:109:GLU:C	6:B:109:GLU:OE2	2.55	0.49
8:C:919:LEU:HD11	8:C:960:GLY:HA3	1.95	0.49
8:C:1540:GLU:OE2	8:C:1540:GLU:N	2.23	0.49
9:O:54:TRP:HZ3	9:O:303:ILE:HD13	1.77	0.49
10:D:422:ARG:NH1	11:I:27:TRP:NE1	2.61	0.49
13:Q:239:ILE:HG22	13:Q:464:GLU:HG3	1.95	0.49
2:J:517:PHE:HB2	2:J:540:TYR:CE2	2.48	0.49
2:J:667:ASP:O	2:J:673:THR:OG1	2.19	0.49
8:C:127:GLU:HG3	8:C:152:TYR:HE1	1.75	0.49
8:C:202:ILE:HG21	8:C:411:LEU:HD11	1.94	0.49
8:C:861:TYR:HE2	13:Q:135:ILE:HD12	1.78	0.49
8:C:1724:SER:OG	8:C:1724:SER:O	2.29	0.49
9:O:315:TYR:HA	9:O:352:PHE:HE2	1.77	0.49
14:T:237:PHE:HB2	14:T:240:MET:HE2	0.60	0.49
14:T:610:SER:OG	15:U:14:TRP:NE1	2.45	0.49
14:T:702:LEU:HG	14:T:736:TYR:HE1	1.78	0.49
2:J:286:ILE:HB	2:J:302:LEU:HD12	1.93	0.49
1:H:174:ALA:HB2	1:H:197:MET:HE3	1.95	0.49
6:B:513:GLY:O	6:B:540:ARG:NH2	2.43	0.49
8:C:78:ILE:HD13	8:C:119:TRP:CE3	2.48	0.49
8:C:461:ARG:HG2	8:C:461:ARG:O	2.13	0.49
8:C:752:VAL:HG23	8:C:757:PHE:CE2	2.47	0.49
13:Q:368:VAL:HB	13:Q:463:MET:HE2	1.94	0.49
2:K:448:LYS:HB2	2:K:448:LYS:HZ3	1.78	0.49
2:K:706:LYS:HD3	2:K:737:LEU:HD23	1.95	0.49
5:A:113:TRP:CZ2	5:A:115:SER:HB3	2.48	0.49
6:B:269:ILE:HG12	6:B:520:HIS:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1167:TYR:HD2	8:C:1167:TYR:C	2.21	0.49
8:C:1602:ILE:HG22	8:C:1616:PHE:HE1	1.78	0.49
9:O:51:SER:HB2	12:N:90:LEU:HD21	1.94	0.49
9:O:606:SER:O	9:O:610:ILE:HG22	2.13	0.49
13:Q:327:THR:HG22	13:Q:384:ILE:HD13	1.94	0.49
1:H:649:GLY:HA3	1:H:665:TYR:CE1	2.48	0.49
9:O:162:ASP:OD1	9:O:164:GLU:N	2.42	0.49
10:D:134:GLU:HG2	10:P:395:PHE:HD2	1.77	0.49
10:D:352:PHE:HB3	10:D:369:TYR:CD2	2.47	0.49
10:P:614:GLU:HA	10:P:617:MET:HE2	1.94	0.49
14:T:63:ILE:O	14:T:67:PHE:HD1	1.96	0.49
14:T:181:LEU:CB	14:T:196:LEU:HD21	2.31	0.49
1:F:103:TYR:CE2	1:F:107:ARG:HG3	2.47	0.48
2:J:504:ILE:HG23	2:J:539:THR:HG21	1.94	0.48
4:E:97:CYS:SG	4:E:99:ARG:HB2	2.53	0.48
6:B:280:ALA:HB2	6:B:308:LEU:HD21	1.95	0.48
6:B:368:HIS:HE1	6:B:400:LEU:HD22	1.77	0.48
8:C:211:LYS:CB	8:C:380:LEU:HD12	2.43	0.48
8:C:429:LEU:O	8:C:433:LEU:HG	2.11	0.48
8:C:699:GLU:OE1	8:C:699:GLU:N	2.46	0.48
8:C:722:ILE:HD12	8:C:726:ARG:HD2	1.95	0.48
8:C:907:SER:OG	8:C:908:GLU:N	2.36	0.48
8:C:1061:ASN:OD1	8:C:1061:ASN:N	2.46	0.48
9:O:12:PHE:HB3	9:O:165:MET:SD	2.53	0.48
10:D:553:GLN:HG3	10:D:557:LYS:HZ1	1.78	0.48
10:P:91:LEU:O	10:P:95:LEU:HD12	2.13	0.48
13:Q:572:VAL:HG21	13:Q:644:VAL:HG23	1.93	0.48
2:J:644:PHE:CD2	2:J:683:THR:HG22	2.47	0.48
2:K:479:PHE:HD1	2:K:506:CYS:SG	2.35	0.48
2:K:644:PHE:CE2	2:K:686:LYS:HG3	2.48	0.48
1:H:93:GLU:CD	1:H:94:PHE:CE2	2.91	0.48
6:B:365:ARG:HE	6:B:382:GLU:CD	2.21	0.48
8:C:194:PHE:CG	8:C:195:PRO:HD2	2.48	0.48
14:T:665:ILE:HD12	14:T:667:LEU:HD21	1.95	0.48
1:F:453:PHE:HE1	4:E:96:PHE:HE1	1.61	0.48
1:F:490:MET:HE3	1:F:494:TYR:CE2	2.48	0.48
2:K:432:LEU:HD23	2:K:435:ILE:HD12	1.95	0.48
2:K:441:ILE:HD12	2:K:442:ASN:H	1.77	0.48
2:K:457:TYR:C	2:K:458:LYS:HG2	2.38	0.48
4:E:99:ARG:HA	4:E:99:ARG:CZ	2.42	0.48
6:B:407:ASN:HA	6:B:426:HIS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1065:TRP:CD1	8:C:1065:TRP:C	2.91	0.48
8:C:1691:ILE:HD12	9:O:607:LEU:HD13	1.95	0.48
13:Q:199:ILE:HG23	13:Q:207:GLN:HB2	1.95	0.48
14:T:387:LEU:HG	14:T:389:LEU:CD2	2.43	0.48
14:T:595:HIS:CD2	14:T:600:LEU:HB2	2.45	0.48
1:F:716:LEU:HB3	1:F:732:GLU:HG2	1.95	0.48
2:J:736:TYR:O	2:J:736:TYR:HD2	1.97	0.48
2:K:594:PHE:CZ	6:B:218:LEU:HD23	2.48	0.48
6:B:276:VAL:HG13	6:B:287:LEU:HD11	1.95	0.48
6:B:366:ILE:HB	6:B:381:ILE:HB	1.95	0.48
9:O:338:PHE:HB3	10:D:480:MET:SD	2.53	0.48
10:P:313:ASP:O	10:P:317:ASP:OD2	2.31	0.48
13:Q:298:TRP:HE3	13:Q:299:LEU:HD22	1.77	0.48
14:T:315:TYR:O	14:T:318:ILE:HG22	2.13	0.48
14:T:628:PHE:CE1	14:T:658:LYS:HB3	2.49	0.48
1:F:188:TRP:CE3	1:F:437:MET:HE1	2.48	0.48
1:F:617:SER:O	1:F:620:LYS:HG2	2.14	0.48
2:J:319:ILE:HD12	2:J:361:LEU:HD22	1.93	0.48
2:J:644:PHE:HD2	2:J:683:THR:HG22	1.79	0.48
1:H:119:ALA:O	1:H:123:LEU:HD12	2.13	0.48
1:H:555:ASP:OD1	1:H:555:ASP:N	2.45	0.48
1:H:607:HIS:O	1:H:637:ILE:HD13	2.13	0.48
1:H:635:ARG:HE	1:H:645:ILE:HD13	1.77	0.48
10:D:557:LYS:H	10:D:557:LYS:HD2	1.78	0.48
1:F:740:ASP:OD2	1:F:740:ASP:C	2.57	0.48
2:K:390:ILE:HD11	2:K:417:LEU:HB2	1.96	0.48
2:K:735:LEU:O	1:H:599:LYS:HE3	2.12	0.48
5:A:142:MET:N	5:A:176:ASN:OD1	2.47	0.48
6:B:61:ARG:NH1	10:D:473:GLN:OE1	2.46	0.48
6:B:527:GLY:O	6:B:544:LEU:HD21	2.14	0.48
8:C:1278:ASN:O	8:C:1279:ILE:HG22	2.13	0.48
9:O:374:ASP:HB2	9:O:376:GLU:OE1	2.12	0.48
10:D:14:ARG:HE	10:D:43:LEU:HD22	1.79	0.48
10:D:417:ILE:HD11	10:D:437:MET:HG3	1.96	0.48
14:T:40:TRP:HA	14:T:49:ASN:HA	1.96	0.48
1:F:495:PHE:HE1	1:F:512:PHE:CD1	2.31	0.48
2:K:485:LEU:O	2:K:488:THR:OG1	2.22	0.48
5:A:219:LEU:HD23	5:A:219:LEU:HA	1.69	0.48
6:B:222:PHE:HD1	6:B:222:PHE:O	1.96	0.48
6:B:480:SER:OG	6:B:481:LYS:N	2.47	0.48
8:C:776:LEU:HD11	8:C:787:LEU:HD22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:127:TYR:CZ	13:Q:291:ILE:HB	2.49	0.48
9:O:565:SER:O	9:O:569:ILE:HG22	2.13	0.48
10:P:9:ILE:CG1	10:P:292:PHE:CZ	2.96	0.48
14:T:135:GLU:HG2	14:T:159:LEU:HD11	1.95	0.48
2:K:728:ILE:O	2:K:732:HIS:CE1	2.67	0.48
6:B:122:SER:O	6:B:123:GLU:HG2	2.14	0.48
6:B:281:LEU:HD12	6:B:286:PHE:HD2	1.79	0.48
8:C:930:PHE:CE2	14:T:459:LEU:HD21	2.49	0.48
10:D:17:LEU:HB3	10:D:40:LEU:HD12	1.95	0.48
10:D:128:TRP:CE3	10:D:187:ILE:HD11	2.49	0.48
1:F:202:ASP:O	1:F:206:VAL:HG23	2.14	0.48
2:J:246:TYR:CZ	2:J:275:ASN:HB3	2.48	0.48
2:J:541:TYR:CE2	2:J:549:GLU:OE1	2.67	0.48
2:K:300:TYR:CD1	2:K:357:MET:HE3	2.49	0.48
2:K:648:GLU:HB3	2:K:651:LYS:NZ	2.28	0.48
8:C:946:PHE:N	8:C:946:PHE:CD1	2.81	0.48
9:O:65:ARG:NH2	9:O:260:ASP:OD2	2.39	0.48
10:D:201:TYR:HD1	10:D:203:ILE:H	1.57	0.48
2:J:607:MET:CE	2:J:638:GLU:OE2	2.61	0.48
2:K:397:GLU:OE2	2:K:398:MET:N	2.47	0.48
2:K:736:TYR:CA	1:H:599:LYS:HG3	2.39	0.48
1:H:663:GLN:HA	1:H:666:GLU:OE2	2.14	0.48
5:A:126:MET:SD	5:A:197:PHE:CD1	3.07	0.48
6:B:210:ARG:HG2	10:D:573:VAL:O	2.14	0.48
6:B:428:ALA:HB3	6:B:448:GLY:HA3	1.96	0.48
8:C:463:GLN:CD	8:C:463:GLN:H	2.21	0.48
14:T:315:TYR:O	14:T:319:VAL:HG13	2.13	0.48
2:J:578:GLU:OE1	2:J:578:GLU:N	2.47	0.47
2:K:242:MET:HG2	2:K:243:GLN:CD	2.39	0.47
5:A:33:VAL:HA	5:A:173:ARG:HH22	1.78	0.47
5:A:142:MET:HG3	5:A:175:VAL:H	1.79	0.47
6:B:488:THR:OG1	6:B:498:THR:OG1	2.29	0.47
8:C:1321:LEU:HD13	8:C:1376:PHE:CE1	2.48	0.47
10:D:277:GLN:OE1	10:D:277:GLN:N	2.47	0.47
10:P:193:GLU:C	10:P:193:GLU:OE1	2.56	0.47
12:N:127:THR:HG23	12:N:129:TYR:H	1.77	0.47
1:F:608:TYR:HB3	1:F:637:ILE:HD11	1.94	0.47
2:J:238:PHE:C	2:J:238:PHE:CD1	2.92	0.47
2:K:637:ASN:OD1	2:K:679:ASN:ND2	2.44	0.47
1:H:93:GLU:CG	1:H:94:PHE:CD2	2.97	0.47
8:C:1491:TYR:OH	8:C:1539:GLN:NE2	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:296:THR:HG21	10:D:456:ARG:NH2	2.29	0.47
10:D:390:SER:HB2	10:D:403:ILE:HD11	1.95	0.47
11:I:147:ASP:OD1	11:I:150:ILE:HG22	2.14	0.47
13:Q:94:SER:HB3	13:Q:167:GLU:HB3	1.96	0.47
1:F:51:GLU:OE2	1:H:472:PRO:CD	2.62	0.47
1:F:165:MET:HE2	1:F:165:MET:HA	1.95	0.47
1:F:699:PHE:HB3	1:F:716:LEU:HD22	1.97	0.47
2:J:541:TYR:OH	11:I:88:TRP:HD1	1.97	0.47
2:K:617:LEU:O	2:K:621:TYR:CD2	2.68	0.47
3:G:21:ASP:HA	3:G:24:ASN:HD22	1.80	0.47
4:E:250:ARG:HH11	4:E:250:ARG:C	2.21	0.47
9:O:107:GLY:CA	9:O:170:TRP:HE1	2.28	0.47
9:O:364:GLU:HG2	9:O:367:ARG:HH21	1.80	0.47
9:O:390:GLU:HB2	9:O:428:PHE:CE1	2.49	0.47
14:T:12:LYS:O	14:T:12:LYS:HD3	2.14	0.47
14:T:464:LEU:O	14:T:468:ILE:HG12	2.13	0.47
2:J:257:TYR:CE1	2:J:266:ALA:HB2	2.49	0.47
2:K:455:LYS:HD3	2:K:456:ASP:H	1.79	0.47
2:K:523:LEU:HD23	2:K:533:THR:HA	1.96	0.47
6:B:62:THR:OG1	6:B:201:LEU:O	2.32	0.47
6:B:366:ILE:HD11	6:B:384:HIS:CD2	2.49	0.47
8:C:475:LEU:HD12	8:C:476:ILE:N	2.28	0.47
10:D:201:TYR:CD1	10:D:203:ILE:N	2.78	0.47
10:P:334:TYR:CE1	10:P:338:ILE:HD11	2.50	0.47
13:Q:436:ILE:HG23	13:Q:437:LEU:HG	1.95	0.47
1:F:49:LEU:HD21	1:H:186:TYR:HB3	1.97	0.47
1:F:175:PHE:O	1:F:178:SER:OG	2.31	0.47
1:F:555:ASP:OD1	1:F:556:HIS:N	2.47	0.47
2:K:617:LEU:O	2:K:621:TYR:CE2	2.68	0.47
1:H:682:MET:O	1:H:686:LEU:HG	2.15	0.47
6:B:97:GLN:O	6:B:100:GLU:HG3	2.14	0.47
6:B:521:LEU:HD23	6:B:532:SER:HA	1.96	0.47
8:C:1379:THR:O	8:C:1383:ILE:HG13	2.14	0.47
8:C:1396:MET:HE1	8:C:1503:PHE:CE2	2.50	0.47
10:D:304:PHE:CD2	10:D:311:LEU:HA	2.50	0.47
10:P:367:GLU:N	10:P:367:GLU:OE2	2.47	0.47
13:Q:345:ARG:HB2	13:Q:366:VAL:HG11	1.95	0.47
1:F:168:ASP:HB3	1:F:169:HIS:CD2	2.49	0.47
1:F:598:ARG:NH1	1:F:630:TYR:OH	2.47	0.47
2:J:571:PHE:CE2	11:I:105:LEU:HD23	2.49	0.47
2:K:603:LEU:HD11	2:K:635:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ASP:O	1:H:156:LEU:HG	2.15	0.47
1:H:171:LYS:H	1:H:171:LYS:CD	2.27	0.47
4:E:232:LEU:O	4:E:236:TYR:CD1	2.67	0.47
4:E:236:TYR:CD1	4:E:236:TYR:N	2.82	0.47
6:B:478:VAL:O	6:B:486:LEU:HD12	2.15	0.47
8:C:483:ASN:HB2	8:C:486:GLU:HG2	1.96	0.47
9:O:170:TRP:O	9:O:170:TRP:HE3	1.91	0.47
10:P:328:PHE:CE2	10:P:330:PHE:HB3	2.50	0.47
10:P:625:HIS:HD1	10:P:625:HIS:H	1.63	0.47
14:T:616:TYR:OH	14:T:659:ASP:OD1	2.27	0.47
2:J:255:LYS:NZ	2:K:464:ASP:OD2	2.40	0.47
2:J:288:ARG:HG3	2:J:289:ASN:N	2.30	0.47
2:J:685:ARG:HH11	2:J:685:ARG:HG2	1.79	0.47
2:K:615:LEU:HD21	2:K:645:LYS:HB2	1.95	0.47
2:K:749:LYS:O	2:K:753:GLU:HG2	2.14	0.47
5:A:189:ASP:OD1	5:A:189:ASP:N	2.47	0.47
6:B:124:SER:HB2	6:B:232:ASP:OD1	2.13	0.47
8:C:77:TYR:HA	8:C:87:PHE:HA	1.97	0.47
8:C:197:ASP:N	8:C:197:ASP:OD1	2.48	0.47
8:C:454:LEU:HD23	8:C:454:LEU:H	1.80	0.47
8:C:760:ASP:OD1	8:C:761:TYR:N	2.48	0.47
8:C:783:ILE:HD12	8:C:783:ILE:H	1.80	0.47
8:C:1698:GLU:OE2	9:O:605:ARG:NH1	2.48	0.47
10:D:23:GLU:HA	10:D:26:ARG:HB3	1.97	0.47
10:D:134:GLU:HG2	10:P:395:PHE:CD2	2.50	0.47
10:D:235:MET:O	10:D:239:LEU:HG	2.15	0.47
10:P:345:TYR:HB2	10:P:376:MET:CE	2.44	0.47
10:P:389:VAL:HG12	10:P:399:THR:HG23	1.96	0.47
14:T:352:LEU:HD21	14:T:489:THR:O	2.14	0.47
2:J:392:ASN:OD1	2:J:393:PHE:N	2.47	0.47
2:J:523:LEU:HB3	2:J:533:THR:OG1	2.15	0.47
2:J:551:GLN:HG3	2:J:571:PHE:HE1	1.80	0.47
2:J:595:PHE:HB3	2:J:598:MET:HE2	1.96	0.47
2:K:484:GLU:O	2:K:488:THR:HG23	2.15	0.47
1:H:53:LEU:HD12	1:H:53:LEU:O	2.15	0.47
4:E:209:ASP:OD2	4:E:209:ASP:O	2.33	0.47
8:C:1328:ILE:HD12	8:C:1328:ILE:H	1.80	0.47
10:P:595:GLN:HA	10:P:626:MET:CE	2.41	0.47
14:T:44:ASN:HB2	14:T:113:GLN:HE22	1.79	0.47
14:T:128:LEU:O	14:T:131:ILE:HG22	2.15	0.47
1:H:473:TRP:CE2	1:H:477:GLN:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:324:ASN:OD1	10:D:455:ARG:NH2	2.48	0.47
10:D:96:PHE:C	10:D:96:PHE:CD1	2.93	0.47
10:P:556:LYS:CA	10:P:583:TRP:HH2	2.27	0.47
14:T:613:TYR:O	14:T:615:LYS:HE2	2.13	0.47
1:F:123:LEU:O	1:F:127:ILE:HG12	2.15	0.47
1:F:495:PHE:HB2	1:F:498:LEU:HD13	1.96	0.47
1:H:99:LEU:CD2	1:H:151:PRO:HD2	2.44	0.47
1:H:198:ARG:NE	1:H:606:GLN:OE1	2.46	0.47
1:H:482:HIS:HA	1:H:485:ILE:HG22	1.97	0.47
5:A:108:ASN:ND2	5:A:111:THR:HG23	2.30	0.47
6:B:308:LEU:HD13	6:B:319:VAL:HG22	1.97	0.47
6:B:343:HIS:CE1	6:B:367:LEU:HD22	2.50	0.47
8:C:118:PHE:CD2	8:C:191:LEU:HD23	2.50	0.47
9:O:57:LEU:O	9:O:58:LEU:HB2	2.13	0.47
9:O:181:LYS:HA	9:O:186:TRP:CD1	2.49	0.47
9:O:375:MET:HE3	9:O:375:MET:C	2.40	0.47
10:D:306:GLU:HA	10:D:306:GLU:OE2	2.15	0.47
2:J:620:SER:O	2:J:623:VAL:HG12	2.16	0.46
2:K:263:PRO:HB2	2:K:295:ASN:HD21	1.77	0.46
5:A:6:ILE:HD12	5:A:6:ILE:N	2.30	0.46
6:B:274:THR:HG23	6:B:276:VAL:HB	1.96	0.46
6:B:400:LEU:HD23	6:B:412:TYR:HD2	1.80	0.46
10:D:23:GLU:O	10:D:27:TRP:N	2.48	0.46
13:Q:60:LYS:HA	13:Q:77:PHE:CE1	2.50	0.46
13:Q:180:TYR:HE1	13:Q:468:ALA:HB1	1.80	0.46
1:H:116:VAL:O	1:H:120:ILE:HG12	2.15	0.46
6:B:300:ASP:N	6:B:300:ASP:OD1	2.46	0.46
6:B:504:SER:HA	6:B:505:MET:HE1	1.96	0.46
8:C:114:ILE:HD12	8:C:114:ILE:N	2.30	0.46
9:O:512:ASP:HB3	9:O:531:TYR:CE2	2.51	0.46
14:T:42:SER:O	14:T:49:ASN:HB3	2.15	0.46
1:F:41:LEU:O	1:F:41:LEU:HD23	2.15	0.46
1:F:196:LYS:NZ	1:F:197:MET:CE	2.79	0.46
2:J:248:THR:OG1	2:K:393:PHE:HB3	2.15	0.46
2:J:397:GLU:OE2	2:J:398:MET:N	2.49	0.46
3:G:19:LEU:HD23	3:G:20:ILE:HD13	1.97	0.46
6:B:69:ILE:HD12	6:B:201:LEU:HD22	1.97	0.46
6:B:492:TYR:H	6:B:495:TYR:HE1	1.63	0.46
6:B:532:SER:HB3	6:B:542:TRP:CH2	2.35	0.46
8:C:83:THR:N	8:C:84:PRO:HD3	2.30	0.46
8:C:149:LYS:HD2	8:C:150:HIS:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:458:VAL:HG21	10:D:468:TRP:CE2	2.51	0.46
10:P:256:MET:HE1	10:P:299:PHE:HE1	1.81	0.46
10:P:398:GLU:OE1	10:P:398:GLU:N	2.49	0.46
13:Q:37:ARG:HD2	13:Q:40:VAL:HG23	1.98	0.46
13:Q:118:ASP:N	13:Q:118:ASP:OD1	2.47	0.46
13:Q:489:PHE:CE2	13:Q:516:ILE:HG21	2.48	0.46
14:T:33:ASP:O	14:T:37:LEU:HG	2.15	0.46
1:F:516:LEU:HD11	1:F:524:LYS:HB2	1.98	0.46
2:J:390:ILE:HD12	2:J:419:PHE:HA	1.98	0.46
2:J:605:LEU:HD22	2:J:621:TYR:CE2	2.49	0.46
2:K:380:ASP:OD2	2:K:380:ASP:C	2.58	0.46
2:K:531:ALA:HB2	2:K:560:LEU:HB3	1.97	0.46
4:E:255:ARG:NH2	4:E:256:HIS:CB	2.51	0.46
5:A:114:GLN:HB2	5:A:213:HIS:CE1	2.50	0.46
6:B:255:LEU:HD23	6:B:541:TYR:CZ	2.50	0.46
6:B:367:LEU:HD23	6:B:369:ARG:HE	1.78	0.46
8:C:157:ASP:OD1	8:C:157:ASP:N	2.47	0.46
8:C:662:MET:HE3	8:C:664:TRP:NE1	2.29	0.46
8:C:1167:TYR:O	8:C:1167:TYR:CD2	2.66	0.46
10:D:247:PHE:CA	10:D:295:MET:HE3	2.36	0.46
10:D:340:TYR:OH	10:D:371:ASN:ND2	2.48	0.46
10:D:468:TRP:HB3	10:D:491:ALA:HB2	1.97	0.46
10:P:290:ILE:O	10:P:296:ILE:HG21	2.15	0.46
13:Q:337:ILE:O	13:Q:341:VAL:HG12	2.15	0.46
14:T:517:LEU:O	14:T:607:LYS:NZ	2.47	0.46
1:F:163:LEU:HD12	1:F:164:TYR:N	2.31	0.46
1:F:489:ASP:OD1	1:F:490:MET:N	2.49	0.46
2:K:490:LEU:HD22	2:K:494:GLU:HA	1.98	0.46
2:K:500:LEU:O	2:K:504:ILE:HG12	2.16	0.46
3:W:15:ASP:OD1	3:W:16:VAL:N	2.48	0.46
1:H:459:PHE:CD1	1:H:478:LEU:CD1	2.84	0.46
6:B:189:THR:HA	11:I:97:TRP:HH2	1.81	0.46
8:C:711:THR:HG23	8:C:753:HIS:HE1	1.80	0.46
8:C:1154:LEU:HB3	8:C:1161:MET:SD	2.55	0.46
9:O:58:LEU:HD23	9:O:380:LEU:HD21	1.97	0.46
10:P:231:ILE:HG21	10:P:260:GLN:HE22	1.80	0.46
10:P:621:GLU:O	10:P:625:HIS:CE1	2.68	0.46
13:Q:439:LYS:O	13:Q:442:THR:OG1	2.32	0.46
14:T:201:LYS:HZ2	14:T:201:LYS:HB3	1.80	0.46
14:T:263:ASP:O	14:T:263:ASP:OD2	2.34	0.46
14:T:290:ILE:CG2	14:T:302:LEU:HD21	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:669:PHE:CD2	15:U:1:MET:SD	3.08	0.46
1:F:453:PHE:CE1	4:E:96:PHE:HE1	2.33	0.46
2:J:539:THR:HA	2:J:542:MET:HB2	1.97	0.46
2:K:483:LEU:HD11	2:K:507:LEU:HD23	1.97	0.46
2:K:566:ALA:CA	3:W:1:MET:CE	2.93	0.46
2:K:727:ALA:O	2:K:731:LEU:HD13	2.16	0.46
3:G:1:MET:N	3:G:1:MET:SD	2.89	0.46
8:C:860:ILE:HD13	13:Q:121:PRO:HB2	1.97	0.46
8:C:1106:LEU:HD23	8:C:1109:PHE:CD2	2.51	0.46
8:C:1164:ASP:OD1	8:C:1164:ASP:C	2.58	0.46
9:O:397:ASN:OD1	9:O:398:ARG:N	2.48	0.46
9:O:561:ASP:OD1	9:O:561:ASP:N	2.47	0.46
10:D:9:ILE:O	10:D:13:ILE:HG12	2.16	0.46
10:D:533:ASP:C	10:D:533:ASP:OD2	2.58	0.46
11:I:103:MET:O	11:I:103:MET:HE3	2.14	0.46
13:Q:204:GLY:CA	13:Q:220:LEU:HB2	2.45	0.46
13:Q:514:TYR:OH	13:Q:552:GLU:OE2	2.27	0.46
14:T:701:SER:OG	14:T:704:GLN:HG2	2.16	0.46
2:J:504:ILE:CG2	2:J:539:THR:HG21	2.46	0.46
2:J:605:LEU:HD22	2:J:621:TYR:CZ	2.50	0.46
1:H:478:LEU:HD22	1:H:494:TYR:CD2	2.51	0.46
8:C:454:LEU:HD12	8:C:456:LEU:CD2	2.46	0.46
8:C:927:THR:HG22	8:C:950:MET:HG3	1.97	0.46
8:C:1139:ARG:HH21	8:C:1182:ALA:HA	1.80	0.46
8:C:1642:PHE:HZ	9:O:611:ILE:HD12	1.81	0.46
10:D:608:THR:O	10:D:612:ILE:HG12	2.16	0.46
14:T:44:ASN:HB2	14:T:113:GLN:NE2	2.31	0.46
14:T:665:ILE:HD11	14:T:723:TRP:HH2	1.80	0.46
1:F:197:MET:HA	1:F:197:MET:HE3	1.96	0.46
1:H:577:TYR:HB3	1:H:600:ALA:HB2	1.98	0.46
6:B:477:MET:HB2	6:B:486:LEU:HD11	1.97	0.46
8:C:1117:LEU:HD23	8:C:1117:LEU:H	1.81	0.46
8:C:1253:PHE:HE1	8:C:1522:ALA:HA	1.81	0.46
8:C:1257:LYS:HG3	8:C:1298:TRP:CD1	2.50	0.46
9:O:386:ILE:O	9:O:390:GLU:N	2.40	0.46
9:O:590:GLU:HG2	9:O:613:LEU:HD11	1.98	0.46
10:D:16:GLN:HG2	10:D:247:PHE:CE2	2.51	0.46
10:D:304:PHE:HE2	10:D:312:GLU:H	1.63	0.46
14:T:738:VAL:HG11	15:U:1:MET:SD	2.56	0.46
1:F:30:LEU:HB3	1:F:53:LEU:HD21	1.98	0.46
1:F:733:LEU:HD12	1:F:747:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:242:MET:HG2	2:K:243:GLN:NE2	2.31	0.46
2:K:288:ARG:C	2:K:288:ARG:CD	2.77	0.46
2:K:481:GLU:HA	2:K:481:GLU:OE2	2.16	0.46
2:K:658:LYS:O	2:K:661:GLU:HG3	2.16	0.46
1:H:563:PHE:O	1:H:567:THR:HG23	2.16	0.46
9:O:170:TRP:CE3	9:O:174:GLN:HG2	2.51	0.46
14:T:10:ASP:O	14:T:14:ILE:HG12	2.16	0.46
15:U:73:PHE:HZ	15:U:93:MET:HG2	1.81	0.46
1:F:568:GLN:OE1	4:E:259:ASN:HB3	2.16	0.46
2:J:749:LYS:HA	2:J:752:LEU:CD2	2.26	0.46
3:G:28:LEU:HD12	3:G:31:GLN:HE22	1.81	0.46
5:A:109:TYR:O	5:A:215:ARG:NH2	2.47	0.46
5:A:114:GLN:NE2	5:A:115:SER:O	2.31	0.46
5:A:124:ASP:C	5:A:124:ASP:OD1	2.59	0.46
5:A:167:TYR:HA	8:C:1374:LEU:HD21	1.98	0.46
8:C:791:LEU:O	8:C:795:GLU:HG2	2.16	0.46
8:C:1303:ASP:HB2	8:C:1351:ILE:HD11	1.98	0.46
10:P:235:MET:SD	10:P:258:CYS:CB	3.02	0.46
14:T:309:MET:CE	14:T:315:TYR:HE1	2.10	0.46
14:T:612:LEU:HD23	14:T:613:TYR:HE1	1.80	0.46
2:J:750:ASN:HD21	3:G:23:LEU:HD23	1.80	0.45
2:K:255:LYS:HD3	2:K:255:LYS:HA	1.64	0.45
5:A:90:TRP:CZ3	5:A:123:LEU:HD21	2.51	0.45
6:B:355:HIS:CD2	6:B:356:VAL:HG23	2.51	0.45
8:C:805:LEU:HB3	8:C:814:GLN:HG3	1.97	0.45
8:C:1016:VAL:HG22	8:C:1051:LEU:HB3	1.97	0.45
10:P:448:HIS:CD2	12:N:128:MET:HB3	2.51	0.45
2:J:414:PHE:CZ	2:J:434:LYS:HG3	2.50	0.45
2:J:581:GLN:HE22	2:J:585:LEU:HD21	1.80	0.45
2:K:428:ILE:HD13	2:K:457:TYR:CZ	2.51	0.45
2:K:566:ALA:CB	3:W:1:MET:CE	2.87	0.45
3:G:15:ASP:OD1	3:G:16:VAL:N	2.50	0.45
1:H:591:ASP:OD1	1:H:592:SER:N	2.49	0.45
8:C:524:TYR:CD1	8:C:525:PRO:HD2	2.51	0.45
8:C:530:THR:HG21	8:C:575:GLU:HB3	1.98	0.45
9:O:385:ILE:HG23	9:O:399:PHE:CE2	2.52	0.45
10:P:108:LEU:O	10:P:120:LYS:HD3	2.16	0.45
12:N:99:MET:HG3	12:N:100:LEU:N	2.32	0.45
13:Q:124:ILE:HD12	13:Q:135:ILE:HG21	1.98	0.45
14:T:103:PHE:CE2	14:T:147:ILE:CA	2.99	0.45
14:T:196:LEU:HD12	14:T:200:LEU:CD2	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:207:LEU:HD12	14:T:207:LEU:HA	1.78	0.45
2:J:657:LYS:O	2:J:661:GLU:HG2	2.15	0.45
2:K:466:VAL:O	2:K:470:VAL:HG23	2.15	0.45
2:K:632:ASP:OD1	2:K:632:ASP:N	2.49	0.45
5:A:139:PHE:HD2	5:A:215:ARG:HB2	1.81	0.45
6:B:112:GLY:O	6:B:116:SER:N	2.41	0.45
6:B:498:THR:HG22	6:B:510:ILE:HD12	1.97	0.45
8:C:1308:ILE:O	8:C:1309:MET:HE2	2.16	0.45
13:Q:514:TYR:O	13:Q:538:ILE:HG13	2.16	0.45
1:F:74:TYR:CE2	1:F:78:LEU:HD11	2.52	0.45
2:J:263:PRO:HB2	2:J:295:ASN:ND2	2.31	0.45
2:J:288:ARG:NH2	2:K:493:ASP:HB2	2.32	0.45
2:J:300:TYR:CE1	2:J:364:LEU:HD22	2.52	0.45
1:H:71:VAL:HG11	1:H:94:PHE:HD2	1.82	0.45
5:A:190:ASP:HB3	5:A:192:LEU:HG	1.99	0.45
8:C:391:LEU:O	8:C:395:LEU:HG	2.16	0.45
8:C:498:ILE:H	8:C:498:ILE:HD12	1.82	0.45
9:O:7:LEU:HD11	9:O:242:ILE:HD12	1.98	0.45
10:D:18:ARG:O	10:D:22:THR:OG1	2.31	0.45
10:D:32:SER:OG	10:D:250:SER:N	2.29	0.45
10:D:458:VAL:HG21	10:D:468:TRP:CZ2	2.51	0.45
10:P:601:ALA:HB1	10:P:619:ALA:HB2	1.97	0.45
14:T:43:PRO:CB	14:T:137:TYR:HE1	2.30	0.45
14:T:666:GLN:OE1	14:T:667:LEU:N	2.49	0.45
1:F:89:GLN:O	1:F:93:GLU:HG2	2.17	0.45
1:F:527:ASN:OD1	2:K:514:ASN:ND2	2.29	0.45
2:J:642:MET:HE2	2:J:646:LYS:HE2	1.98	0.45
2:K:443:THR:O	2:K:446:ILE:HG22	2.16	0.45
1:H:127:ILE:HD11	1:H:153:LEU:HD11	1.97	0.45
1:H:650:GLY:O	1:H:653:GLU:HG3	2.16	0.45
8:C:956:THR:HG23	8:C:1498:ASN:ND2	2.32	0.45
9:O:188:ARG:HD3	9:O:189:PHE:CE1	2.51	0.45
9:O:569:ILE:HD11	9:O:589:PHE:O	2.17	0.45
10:P:252:TRP:CZ3	10:P:295:MET:HG3	2.50	0.45
14:T:35:ASN:HA	14:T:38:LEU:HG	1.98	0.45
14:T:102:LEU:O	14:T:106:LEU:HG	2.16	0.45
14:T:510:ARG:NH1	14:T:573:ASN:HA	2.32	0.45
1:F:625:GLU:HG2	4:E:227:LEU:CD1	2.46	0.45
1:F:689:MET:SD	1:F:691:ARG:HG3	2.57	0.45
2:J:752:LEU:HB3	10:P:482:LEU:CG	2.47	0.45
2:K:533:THR:O	2:K:537:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:697:PHE:HA	2:K:700:VAL:HG12	1.99	0.45
5:A:34:LEU:H	5:A:173:ARG:NH1	2.14	0.45
8:C:1254:LEU:HD23	8:C:1254:LEU:HA	1.86	0.45
8:C:1513:LEU:HD23	8:C:1524:LEU:HD21	1.98	0.45
10:D:76:GLN:OE1	10:D:76:GLN:N	2.50	0.45
10:P:252:TRP:HZ3	10:P:295:MET:HG3	1.81	0.45
11:I:36:ASP:OD1	11:I:88:TRP:NE1	2.49	0.45
13:Q:101:ILE:HG21	13:Q:224:LEU:HD11	1.97	0.45
13:Q:196:LYS:HE2	13:Q:211:GLU:HB3	1.98	0.45
1:F:51:GLU:HG3	1:H:471:MET:HE3	1.89	0.45
1:F:477:GLN:O	1:F:481:LEU:HG	2.17	0.45
1:F:751:LEU:HB3	2:J:617:LEU:HD22	1.98	0.45
2:J:736:TYR:C	2:J:736:TYR:CD2	2.93	0.45
1:H:36:GLN:NE2	1:H:40:GLN:OE1	2.48	0.45
1:H:112:LEU:HB3	1:H:114:GLN:HG2	1.99	0.45
5:A:4:ILE:O	5:A:8:LYS:HG2	2.15	0.45
8:C:972:ILE:O	8:C:972:ILE:CG2	2.65	0.45
9:O:49:ARG:NH1	13:Q:419:PHE:O	2.49	0.45
10:P:32:SER:HB3	10:P:250:SER:HB2	1.99	0.45
11:I:43:MET:HE3	11:I:43:MET:HB3	1.84	0.45
12:N:121:PRO:HG2	12:N:124:ILE:HB	1.99	0.45
15:U:100:LEU:CD2	15:U:111:VAL:HA	2.47	0.45
2:K:375:PHE:O	2:K:379:ARG:HG3	2.17	0.45
2:K:444:GLU:O	2:K:448:LYS:HG3	2.17	0.45
2:K:692:ILE:HA	2:K:695:LYS:HG2	1.99	0.45
1:H:103:TYR:CD2	1:H:151:PRO:HG3	2.51	0.45
1:H:490:MET:HA	1:H:493:LYS:HZ1	1.81	0.45
1:H:575:TYR:HA	1:H:578:THR:HG22	1.98	0.45
8:C:1133:MET:HE2	8:C:1133:MET:HB2	1.84	0.45
8:C:1295:MET:HE1	8:C:1341:ILE:HG21	1.99	0.45
9:O:96:LEU:HA	9:O:99:MET:HB2	1.99	0.45
9:O:254:GLN:HE21	9:O:284:PHE:HE1	1.65	0.45
9:O:298:PHE:O	9:O:301:ILE:HG22	2.17	0.45
10:D:301:LEU:HB3	10:D:334:TYR:CE2	2.52	0.45
10:P:142:THR:HG22	10:P:144:LYS:H	1.81	0.45
11:I:157:ARG:O	11:I:157:ARG:HG2	2.16	0.45
13:Q:77:PHE:CD2	14:T:333:PRO:HD2	2.52	0.45
2:J:486:CYS:HB3	2:J:503:TYR:CD1	2.52	0.45
2:J:509:GLU:C	2:J:509:GLU:CD	2.85	0.45
2:K:479:PHE:HA	2:K:482:CYS:SG	2.57	0.45
2:K:562:PRO:HB3	6:B:215:ALA:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:591:ASP:O	1:H:594:LYS:HG2	2.17	0.45
5:A:156:TYR:CD1	5:A:166:PHE:HA	2.52	0.45
8:C:760:ASP:OD1	8:C:761:TYR:CD2	2.70	0.45
8:C:1086:MET:HG2	8:C:1098:LEU:HD11	1.99	0.45
9:O:397:ASN:OD1	9:O:397:ASN:C	2.60	0.45
9:O:513:ILE:HG12	9:O:548:LEU:HD11	1.97	0.45
14:T:102:LEU:HG	14:T:106:LEU:HD21	1.99	0.45
4:E:89:LYS:O	4:E:135:ARG:NH2	2.50	0.45
8:C:1043:ASP:N	8:C:1043:ASP:OD1	2.48	0.45
8:C:1595:ASP:OD1	8:C:1595:ASP:N	2.49	0.45
9:O:115:MET:HG2	9:O:158:TYR:CD2	2.52	0.45
9:O:320:ASP:OD1	10:D:486:TYR:OH	2.20	0.45
10:P:488:PHE:HB3	10:P:505:LEU:HD12	1.98	0.45
10:P:519:ILE:N	10:P:519:ILE:HD13	2.32	0.45
12:N:116:TRP:CZ2	12:N:128:MET:HE1	2.52	0.45
14:T:44:ASN:H	14:T:113:GLN:NE2	2.15	0.45
14:T:186:MET:HA	14:T:186:MET:HE3	1.99	0.45
1:F:99:LEU:HD23	1:F:143:LEU:HA	1.98	0.44
1:F:171:LYS:HD3	4:E:176:LEU:HD11	1.99	0.44
2:J:444:GLU:H	2:J:444:GLU:CD	2.26	0.44
2:K:523:LEU:HD21	2:K:532:ILE:HG22	1.98	0.44
1:H:489:ASP:OD1	1:H:490:MET:N	2.51	0.44
6:B:190:ARG:CD	11:I:97:TRP:CE3	2.98	0.44
6:B:486:LEU:HB3	6:B:500:TRP:HB3	1.99	0.44
6:B:504:SER:CA	6:B:505:MET:HE2	2.36	0.44
8:C:1373:ASN:O	8:C:1377:ARG:N	2.42	0.44
9:O:519:ALA:HB1	9:O:524:ASP:HB3	1.99	0.44
10:D:81:LEU:HD12	10:D:85:GLU:HG3	1.98	0.44
10:D:228:GLU:OE1	10:D:230:ASN:HB2	2.17	0.44
10:D:231:ILE:H	10:D:231:ILE:HD12	1.82	0.44
13:Q:105:TYR:OH	13:Q:227:LYS:CA	2.65	0.44
1:F:617:SER:HA	1:F:620:LYS:HD3	1.99	0.44
2:K:231:GLU:O	2:K:235:LEU:HG	2.17	0.44
2:K:626:TYR:CE1	2:K:630:PRO:HA	2.52	0.44
1:H:686:LEU:HD22	1:H:691:ARG:HG2	1.99	0.44
5:A:141:SER:HB2	5:A:144:ALA:HB3	1.99	0.44
6:B:505:MET:CE	6:B:505:MET:N	2.74	0.44
8:C:968:THR:OG1	8:C:969:GLU:N	2.49	0.44
8:C:1072:SER:HB3	8:C:1073:PRO:HD3	1.99	0.44
9:O:381:ILE:O	9:O:385:ILE:HG13	2.17	0.44
10:D:29:LEU:HD21	10:D:216:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:301:LEU:HD11	10:D:321:LEU:HD12	1.99	0.44
11:I:145:ILE:HD12	11:I:145:ILE:HA	1.89	0.44
14:T:38:LEU:HD12	14:T:39:THR:HG23	1.98	0.44
14:T:490:ASN:HD22	14:T:539:LYS:HE3	1.83	0.44
1:F:645:ILE:HG21	1:F:668:ALA:HB2	2.00	0.44
2:J:485:LEU:O	2:J:489:VAL:HG23	2.18	0.44
8:C:1364:PRO:HB3	14:T:460:TYR:CE1	2.53	0.44
10:D:418:MET:HE2	11:I:27:TRP:CZ3	2.53	0.44
14:T:492:PHE:CZ	14:T:496:LEU:HD11	2.52	0.44
2:J:642:MET:CE	2:J:646:LYS:HE2	2.47	0.44
1:H:611:TYR:CE2	1:H:637:ILE:CD1	3.01	0.44
6:B:257:ALA:HB2	6:B:539:LEU:HD11	1.99	0.44
6:B:370:ASP:O	6:B:376:PRO:HA	2.17	0.44
6:B:490:HIS:NE2	6:B:498:THR:OG1	2.45	0.44
8:C:655:LEU:HD23	8:C:655:LEU:HA	1.84	0.44
8:C:707:LEU:HD12	8:C:749:TYR:HD1	1.82	0.44
8:C:925:THR:HB	8:C:953:ARG:HH12	1.82	0.44
8:C:1225:LEU:HA	8:C:1228:VAL:HG12	2.00	0.44
9:O:191:ASP:OD1	9:O:191:ASP:N	2.48	0.44
10:D:553:GLN:HG3	10:D:557:LYS:NZ	2.33	0.44
10:D:602:MET:HE2	10:D:602:MET:HA	1.98	0.44
10:P:486:TYR:CZ	10:P:490:LYS:HD2	2.52	0.44
2:K:263:PRO:HB3	2:K:291:LEU:HD23	2.00	0.44
2:K:390:ILE:O	2:K:390:ILE:CG2	2.66	0.44
4:E:170:LYS:O	4:E:174:GLU:HG2	2.17	0.44
5:A:20:LYS:HA	8:C:1368:TYR:OH	2.17	0.44
5:A:154:LYS:HD3	5:A:166:PHE:HE2	1.83	0.44
6:B:403:GLY:HA3	6:B:433:MET:HE3	1.99	0.44
6:B:477:MET:HE2	6:B:477:MET:HB3	1.74	0.44
8:C:424:TRP:HE1	8:C:449:ILE:HG23	1.81	0.44
8:C:1260:ASN:CG	8:C:1263:ILE:HG12	2.43	0.44
10:D:331:LEU:HD12	10:D:331:LEU:HA	1.79	0.44
10:P:198:LEU:HD13	10:P:198:LEU:HA	1.86	0.44
10:P:304:PHE:CZ	10:P:311:LEU:HA	2.52	0.44
11:I:34:LEU:HD11	11:I:37:GLU:OE2	2.16	0.44
14:T:140:PHE:HB3	14:T:141:PRO:HD3	2.00	0.44
1:F:453:PHE:CE1	4:E:96:PHE:CE1	3.06	0.44
2:J:541:TYR:CD2	2:J:549:GLU:OE1	2.71	0.44
2:K:262:ASP:OD1	2:K:262:ASP:N	2.49	0.44
6:B:482:ASN:HB2	6:B:545:PHE:CE2	2.51	0.44
8:C:610:PHE:CD1	8:C:610:PHE:C	2.92	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:616:ASP:OD1	8:C:616:ASP:N	2.50	0.44
10:P:509:TYR:CE1	10:P:517:GLU:OE1	2.71	0.44
12:N:13:ASP:C	12:N:13:ASP:OD2	2.60	0.44
13:Q:447:ILE:HG23	13:Q:448:ILE:H	1.82	0.44
14:T:163:ARG:HG2	14:T:199:TRP:CZ2	2.53	0.44
1:F:532:LEU:HB3	1:F:542:THR:HG22	1.99	0.44
2:J:356:LYS:HE3	2:J:357:MET:H	1.82	0.44
2:J:399:LEU:HD21	2:J:405:LEU:HD12	2.00	0.44
5:A:26:HIS:CE1	5:A:28:LYS:HB2	2.53	0.44
6:B:237:LEU:HD13	8:C:1110:LEU:HD21	1.99	0.44
6:B:257:ALA:HB1	6:B:281:LEU:HD21	2.00	0.44
8:C:1414:HIS:HE1	8:C:1498:ASN:OD1	2.01	0.44
9:O:27:HIS:HE2	13:Q:288:LEU:HD11	1.83	0.44
10:P:16:GLN:NE2	10:P:247:PHE:CE2	2.86	0.44
10:P:187:ILE:HA	10:P:190:ILE:HD12	1.99	0.44
13:Q:19:PHE:CZ	13:Q:30:TYR:HB2	2.52	0.44
13:Q:103:LEU:HD11	13:Q:230:VAL:HG11	1.99	0.44
1:F:43:TYR:HE2	1:F:80:LEU:HD13	1.82	0.44
2:K:711:HIS:HB3	2:K:734:SER:HB2	1.99	0.44
1:H:532:LEU:HB3	1:H:542:THR:HG22	2.00	0.44
8:C:1344:ALA:HB3	8:C:1515:THR:HG21	2.00	0.44
8:C:1582:GLU:OE1	8:C:1583:VAL:C	2.61	0.44
9:O:377:THR:O	9:O:381:ILE:HG12	2.18	0.44
10:D:26:ARG:O	10:D:89:TYR:OH	2.31	0.44
10:P:27:TRP:HZ2	10:P:115:TYR:HH	0.57	0.44
14:T:44:ASN:N	14:T:113:GLN:NE2	2.66	0.44
14:T:225:CYS:HB3	14:T:229:MET:HE3	1.99	0.44
14:T:265:HIS:ND1	14:T:266:GLU:N	2.66	0.44
14:T:389:LEU:HD12	14:T:393:GLU:OE1	2.17	0.44
1:H:721:ARG:HG2	1:H:753:LYS:HZ3	1.83	0.44
6:B:363:ASP:OD1	6:B:363:ASP:N	2.50	0.44
8:C:415:HIS:CE1	8:C:417:PRO:HD2	2.53	0.44
8:C:1398:MET:HA	8:C:1398:MET:HE2	1.99	0.44
8:C:1514:ASN:HA	8:C:1552:ARG:NH2	2.33	0.44
9:O:131:LYS:NZ	13:Q:296:GLU:OE1	2.46	0.44
10:P:481:HIS:HB3	10:P:508:CYS:SG	2.58	0.44
14:T:342:LEU:HD23	14:T:343:ARG:HD3	1.99	0.44
1:F:495:PHE:CE1	1:F:512:PHE:CD1	3.01	0.43
2:J:571:PHE:O	2:J:574:THR:OG1	2.29	0.43
1:H:84:TYR:HB3	1:H:112:LEU:HD21	1.99	0.43
1:H:694:VAL:O	1:H:698:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:287:LEU:HD12	6:B:288:THR:N	2.33	0.43
8:C:34:ILE:HG13	8:C:35:THR:OG1	2.18	0.43
8:C:574:MET:HA	8:C:574:MET:HE2	2.00	0.43
8:C:1125:THR:O	8:C:1129:ILE:HG22	2.17	0.43
8:C:1589:THR:HB	8:C:1590:PRO:HD3	1.98	0.43
10:P:23:GLU:O	10:P:27:TRP:HD1	2.01	0.43
1:F:40:GLN:OE1	1:H:151:PRO:HA	2.17	0.43
2:J:255:LYS:HD3	2:K:432:LEU:CD1	2.42	0.43
2:J:295:ASN:N	2:J:295:ASN:OD1	2.50	0.43
2:J:513:LYS:HB2	2:J:513:LYS:HE3	1.87	0.43
1:H:72:TYR:OH	1:H:148:VAL:O	2.30	0.43
6:B:245:ARG:HH11	6:B:247:ILE:HD11	1.81	0.43
6:B:297:HIS:O	6:B:334:ARG:NH2	2.51	0.43
8:C:799:SER:O	8:C:799:SER:OG	2.34	0.43
8:C:1582:GLU:OE1	8:C:1584:ILE:N	2.51	0.43
10:P:139:ILE:HD11	12:N:119:PHE:CE1	2.48	0.43
14:T:682:GLU:OE2	14:T:715:ARG:NH2	2.51	0.43
2:J:658:LYS:O	2:J:661:GLU:HG3	2.18	0.43
2:K:303:GLY:O	2:K:307:VAL:HG23	2.18	0.43
2:K:486:CYS:SG	2:K:503:TYR:HB2	2.58	0.43
1:H:721:ARG:HG2	1:H:753:LYS:NZ	2.33	0.43
6:B:222:PHE:CD1	6:B:222:PHE:O	2.71	0.43
6:B:271:TRP:CZ2	6:B:525:ASN:HB3	2.53	0.43
6:B:403:GLY:HA3	6:B:433:MET:CE	2.47	0.43
8:C:64:ARG:NH2	9:O:352:PHE:O	2.51	0.43
8:C:644:CYS:HB2	8:C:647:GLU:OE2	2.17	0.43
8:C:760:ASP:O	8:C:802:ARG:NH1	2.48	0.43
8:C:1596:PHE:HB3	8:C:1622:ALA:HB3	2.00	0.43
2:J:306:PHE:HB3	2:J:315:ALA:HB2	2.01	0.43
6:B:441:GLY:O	6:B:459:VAL:N	2.43	0.43
8:C:468:HIS:CE1	8:C:470:LEU:HB3	2.53	0.43
8:C:606:GLU:OE1	8:C:606:GLU:N	2.48	0.43
8:C:1260:ASN:OD1	8:C:1263:ILE:HG12	2.19	0.43
8:C:1581:GLU:HG2	8:C:1582:GLU:H	1.84	0.43
9:O:375:MET:HE3	9:O:376:GLU:N	2.32	0.43
10:D:108:LEU:HD23	10:D:108:LEU:HA	1.85	0.43
10:D:417:ILE:CD1	10:D:437:MET:HG3	2.49	0.43
14:T:103:PHE:CZ	14:T:147:ILE:CA	2.91	0.43
14:T:591:CYS:SG	14:T:606:PRO:HD2	2.58	0.43
1:F:721:ARG:NH2	1:F:750:GLU:OE1	2.51	0.43
2:J:538:ALA:HB2	2:J:553:TYR:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:435:ILE:HA	2:K:446:ILE:HD11	2.00	0.43
2:K:653:LYS:HG3	2:K:684:TYR:CE1	2.50	0.43
2:K:709:GLU:CD	3:W:10:GLN:OE1	2.61	0.43
5:A:128:SER:CB	8:C:1235:GLU:HG3	2.49	0.43
8:C:722:ILE:CD1	8:C:726:ARG:HD2	2.48	0.43
8:C:741:ARG:NH2	8:C:775:GLU:OE1	2.51	0.43
8:C:774:ASP:HB2	9:O:570:ASN:ND2	2.33	0.43
8:C:861:TYR:CE2	13:Q:135:ILE:HB	2.54	0.43
10:P:137:GLU:O	10:P:141:THR:HG22	2.19	0.43
11:I:99:LEU:HD22	11:I:155:TYR:CE1	2.53	0.43
12:N:128:MET:HA	12:N:131:LEU:HD12	2.00	0.43
1:F:686:LEU:HG	1:F:691:ARG:HB2	2.00	0.43
2:K:734:SER:HA	2:K:737:LEU:HD13	2.00	0.43
1:H:459:PHE:HD1	1:H:478:LEU:CD1	2.29	0.43
1:H:533:MET:CE	4:E:252:LYS:HD2	2.48	0.43
6:B:271:TRP:HB2	6:B:522:THR:CG2	2.48	0.43
6:B:271:TRP:N	6:B:522:THR:HG21	2.33	0.43
8:C:974:THR:HG23	9:O:378:LEU:HD12	1.99	0.43
9:O:42:LEU:O	9:O:46:SER:OG	2.28	0.43
9:O:127:TYR:O	9:O:130:MET:HB2	2.18	0.43
9:O:173:LEU:O	9:O:177:LYS:N	2.43	0.43
9:O:418:ASP:O	9:O:420:ASN:N	2.50	0.43
10:D:304:PHE:HE2	10:D:312:GLU:N	2.17	0.43
13:Q:95:LYS:HB3	13:Q:95:LYS:HE2	1.78	0.43
14:T:38:LEU:HB2	14:T:109:PHE:CZ	2.54	0.43
14:T:309:MET:HB3	14:T:315:TYR:HE1	1.84	0.43
15:U:82:LEU:HD11	15:U:98:PHE:CD2	2.53	0.43
1:F:123:LEU:HA	1:F:126:ILE:CG2	2.49	0.43
2:J:526:THR:HG23	2:K:280:VAL:HG21	2.01	0.43
2:K:229:ALA:N	2:K:231:GLU:OE1	2.52	0.43
2:K:658:LYS:HB2	2:K:658:LYS:HE3	1.81	0.43
2:K:736:TYR:HA	1:H:599:LYS:HE2	1.96	0.43
1:H:90:ILE:HD13	1:H:90:ILE:HA	1.91	0.43
1:H:485:ILE:HG23	1:H:487:ASN:HB2	2.01	0.43
6:B:445:THR:OG1	6:B:455:LYS:HB2	2.19	0.43
8:C:80:PHE:CD2	8:C:158:PRO:HD3	2.54	0.43
8:C:1082:LEU:HD12	8:C:1086:MET:HE3	2.01	0.43
8:C:1593:LEU:HD21	8:C:1596:PHE:HE1	1.82	0.43
9:O:101:TYR:O	9:O:105:ILE:HG12	2.19	0.43
9:O:391:VAL:HG12	9:O:392:HIS:CD2	2.54	0.43
9:O:500:SER:O	9:O:501:LEU:HG	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:146:ARG:NH1	13:Q:177:ASN:HB3	2.33	0.43
13:Q:423:LEU:HG	13:Q:424:TYR:CD1	2.54	0.43
13:Q:489:PHE:HE1	13:Q:541:LEU:HD11	1.83	0.43
13:Q:504:ILE:HG12	13:Q:571:PHE:CG	2.54	0.43
1:F:169:HIS:ND1	1:F:172:GLU:OE1	2.51	0.43
2:K:364:LEU:HD23	2:K:364:LEU:O	2.18	0.43
1:H:751:LEU:O	1:H:755:HIS:ND1	2.37	0.43
6:B:59:PRO:HB3	6:B:204:TYR:CE1	2.53	0.43
6:B:214:ALA:H	6:B:217:LEU:HD13	1.84	0.43
8:C:662:MET:HE3	8:C:664:TRP:HE1	1.84	0.43
8:C:1352:ARG:NH1	8:C:1403:ASP:OD2	2.51	0.43
8:C:1642:PHE:CD2	8:C:1694:LEU:HD21	2.53	0.43
9:O:347:THR:HG23	9:O:501:LEU:HB3	2.00	0.43
9:O:636:VAL:O	9:O:640:VAL:HG23	2.18	0.43
10:D:121:LEU:HD21	10:D:193:GLU:HG2	2.00	0.43
10:D:130:LYS:O	10:D:134:GLU:OE1	2.37	0.43
10:P:519:ILE:HD11	10:P:545:LEU:CD2	2.40	0.43
13:Q:281:GLU:OE1	13:Q:295:LEU:HD13	2.17	0.43
14:T:209:SER:O	14:T:213:ILE:HG12	2.19	0.43
1:F:563:PHE:CE2	1:F:579:LEU:HB3	2.53	0.43
2:J:545:ASP:O	2:J:545:ASP:OD1	2.37	0.43
1:H:611:TYR:CD2	1:H:637:ILE:HD13	2.54	0.43
1:H:718:GLN:O	1:H:722:ILE:HG12	2.19	0.43
5:A:20:LYS:HG2	8:C:1368:TYR:CE2	2.54	0.43
6:B:71:SER:O	8:C:1068:TYR:HE2	2.02	0.43
6:B:190:ARG:HD3	11:I:97:TRP:HE3	1.81	0.43
8:C:37:LYS:NZ	8:C:79:ASP:OD1	2.51	0.43
8:C:54:VAL:HG11	8:C:87:PHE:HZ	1.84	0.43
8:C:1165:GLU:HG3	8:C:1242:ASN:CG	2.42	0.43
10:D:106:PHE:HB2	10:P:361:TYR:HD2	1.82	0.43
14:T:177:LEU:HD13	14:T:200:LEU:HD21	2.01	0.43
14:T:612:LEU:HD23	14:T:613:TYR:CE1	2.54	0.43
1:F:435:GLU:OE1	1:F:435:GLU:N	2.44	0.43
2:J:292:ASP:HA	2:J:298:CYS:SG	2.59	0.43
2:J:699:CYS:O	2:J:702:GLU:HG3	2.19	0.43
1:H:47:GLU:OE1	1:H:78:LEU:CD2	2.66	0.43
8:C:404:ARG:HA	8:C:409:GLU:HA	2.01	0.43
8:C:903:GLY:O	8:C:907:SER:HB3	2.19	0.43
9:O:46:SER:OG	9:O:47:PRO:HD3	2.18	0.43
11:I:81:GLU:O	11:I:84:SER:OG	2.32	0.43
14:T:110:TYR:O	14:T:114:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:403:ASP:OD2	14:T:406:ALA:N	2.46	0.43
2:K:486:CYS:HA	2:K:489:VAL:CG1	2.48	0.42
2:K:718:TYR:HB3	2:K:727:ALA:HB2	2.00	0.42
1:H:640:VAL:HG13	1:H:671:LEU:HD21	2.01	0.42
5:A:65:LEU:HA	5:A:68:MET:HG3	2.01	0.42
5:A:164:ALA:HB2	5:A:197:PHE:CE2	2.54	0.42
8:C:636:GLU:OE1	8:C:636:GLU:HA	2.19	0.42
8:C:763:LEU:HB3	8:C:804:ASN:OD1	2.19	0.42
8:C:987:VAL:HG22	8:C:993:LYS:HG3	2.01	0.42
10:D:11:HIS:NE2	10:D:15:ILE:HD11	2.34	0.42
10:D:530:GLN:NE2	10:D:534:GLN:HE22	2.17	0.42
10:D:602:MET:HE3	10:D:619:ALA:HB2	2.01	0.42
10:P:294:ILE:HD11	10:P:325:PHE:CZ	2.54	0.42
13:Q:318:ALA:O	13:Q:322:THR:OG1	2.27	0.42
1:F:594:LYS:O	1:F:598:ARG:HG2	2.19	0.42
1:F:731:LYS:O	1:F:735:VAL:HG23	2.19	0.42
2:J:304:LEU:HA	2:J:307:VAL:HG12	2.00	0.42
2:J:461:ASP:C	2:J:461:ASP:OD1	2.62	0.42
2:J:536:SER:O	2:J:539:THR:HG22	2.19	0.42
2:J:581:GLN:NE2	2:J:585:LEU:HD21	2.34	0.42
2:K:390:ILE:O	2:K:390:ILE:HG22	2.17	0.42
2:K:566:ALA:HA	3:W:1:MET:HE3	2.01	0.42
1:H:43:TYR:HB3	1:H:81:ASN:OD1	2.18	0.42
1:H:92:LYS:HD3	1:H:105:PHE:CE1	2.53	0.42
4:E:165:VAL:HB	4:E:168:CYS:SG	2.60	0.42
4:E:255:ARG:CZ	4:E:256:HIS:N	2.82	0.42
5:A:10:LEU:HD21	8:C:1309:MET:SD	2.59	0.42
5:A:153:VAL:HB	5:A:170:LEU:HD22	2.01	0.42
8:C:867:ILE:CD1	9:O:453:ILE:HD11	2.49	0.42
8:C:1007:VAL:O	8:C:1011:GLN:HG3	2.19	0.42
8:C:1122:LYS:HD2	8:C:1540:GLU:OE1	2.19	0.42
8:C:1321:LEU:H	8:C:1321:LEU:HD12	1.85	0.42
9:O:209:SER:HA	9:O:213:GLN:HG3	2.01	0.42
10:P:128:TRP:CZ3	10:P:187:ILE:HD13	2.54	0.42
10:P:198:LEU:HD11	10:P:214:LEU:HD11	2.01	0.42
13:Q:338:ILE:HD13	13:Q:338:ILE:HA	1.89	0.42
13:Q:368:VAL:HB	13:Q:463:MET:CE	2.50	0.42
13:Q:542:LYS:NZ	13:Q:547:GLY:HA3	2.34	0.42
13:Q:620:GLU:O	13:Q:624:ASN:HB2	2.19	0.42
14:T:411:VAL:HG12	14:T:415:HIS:CD2	2.53	0.42
1:F:442:LEU:HD13	1:F:445:ARG:NH2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:649:PHE:HB3	2:J:687:LEU:HD13	2.02	0.42
2:K:257:TYR:CE1	2:K:266:ALA:HB2	2.54	0.42
5:A:90:TRP:HH2	5:A:217:ILE:HG12	1.84	0.42
8:C:213:LEU:HD13	8:C:380:LEU:CD2	2.46	0.42
8:C:603:GLU:H	8:C:603:GLU:CD	2.27	0.42
8:C:1016:VAL:HG11	8:C:1543:HIS:CG	2.54	0.42
8:C:1096:SER:O	8:C:1100:LYS:HG3	2.18	0.42
9:O:644:MET:HE2	9:O:644:MET:HB3	1.73	0.42
10:D:187:ILE:HD13	10:D:187:ILE:HA	1.89	0.42
10:P:9:ILE:CG1	10:P:292:PHE:HZ	2.27	0.42
13:Q:300:CYS:SG	13:Q:301:ASN:N	2.92	0.42
1:F:28:ILE:HD13	1:F:28:ILE:HA	1.93	0.42
1:F:748:ILE:HD13	1:F:748:ILE:HA	1.86	0.42
2:J:754:LEU:CD2	3:G:27:LYS:HD3	2.50	0.42
3:G:26:GLN:C	3:G:26:GLN:OE1	2.62	0.42
1:H:691:ARG:HD3	1:H:693:ASN:OD1	2.20	0.42
6:B:270:ASP:OD1	6:B:310:TRP:CD1	2.73	0.42
9:O:133:ARG:HA	9:O:133:ARG:HD2	1.75	0.42
9:O:523:ASP:N	9:O:523:ASP:OD1	2.52	0.42
10:P:15:ILE:HD11	10:P:76:GLN:HG3	2.02	0.42
10:P:110:ASP:OD1	10:P:110:ASP:O	2.38	0.42
13:Q:249:HIS:HB3	13:Q:325:ILE:HD11	2.02	0.42
14:T:181:LEU:CD1	14:T:196:LEU:CD2	2.80	0.42
14:T:196:LEU:CD1	14:T:200:LEU:CD2	2.96	0.42
1:F:738:ASN:ND2	2:J:590:THR:OG1	2.44	0.42
2:J:398:MET:SD	2:J:402:LYS:HE2	2.60	0.42
2:K:724:LEU:HD21	2:K:754:LEU:HG	2.01	0.42
1:H:91:SER:OG	1:H:105:PHE:HB2	2.18	0.42
1:H:92:LYS:HD3	1:H:105:PHE:HE1	1.84	0.42
1:H:144:ASN:C	1:H:144:ASN:OD1	2.61	0.42
4:E:231:GLU:O	4:E:235:VAL:HG23	2.19	0.42
5:A:138:ILE:HD11	5:A:214:LEU:HD11	2.02	0.42
6:B:432:ALA:C	6:B:477:MET:CE	2.90	0.42
8:C:32:ILE:HG23	8:C:33:ASN:H	1.84	0.42
8:C:707:LEU:HD13	8:C:707:LEU:HA	1.83	0.42
8:C:752:VAL:HG13	8:C:753:HIS:HD2	1.84	0.42
9:O:127:TYR:CE1	13:Q:291:ILE:HB	2.54	0.42
13:Q:383:SER:O	13:Q:387:LEU:CD2	2.61	0.42
14:T:389:LEU:CD1	14:T:390:PRO:HD2	2.50	0.42
1:F:492:LEU:O	1:F:496:ASN:CB	2.66	0.42
2:K:264:ASP:OD1	2:K:265:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:721:THR:HG22	2:K:722:LYS:N	2.33	0.42
1:H:514:THR:O	1:H:518:HIS:ND1	2.52	0.42
1:H:665:TYR:HB3	1:H:682:MET:CE	2.49	0.42
5:A:148:TYR:HD2	5:A:213:HIS:CD2	2.38	0.42
5:A:162:SER:O	8:C:1534:THR:OG1	2.38	0.42
6:B:55:ASP:HB2	10:D:343:LEU:HD21	2.02	0.42
8:C:956:THR:HG23	8:C:1498:ASN:HD22	1.84	0.42
9:O:167:GLU:O	9:O:171:ILE:HD12	2.19	0.42
10:D:198:LEU:HD21	10:D:218:TYR:CZ	2.55	0.42
10:D:469:PHE:HZ	10:D:504:VAL:HG21	1.85	0.42
10:P:111:VAL:HG11	10:P:116:LEU:HB3	2.01	0.42
13:Q:12:TYR:HB2	13:Q:574:ASN:HB2	2.02	0.42
14:T:407:LEU:O	14:T:410:LEU:HG	2.20	0.42
15:U:101:GLN:HB3	15:U:104:LEU:HD12	2.02	0.42
1:F:191:TYR:HA	1:F:194:ILE:HG22	2.01	0.42
1:F:202:ASP:OD1	1:F:202:ASP:N	2.41	0.42
2:J:462:ASN:O	2:J:466:VAL:HG13	2.20	0.42
2:J:693:ALA:O	2:J:697:PHE:HD1	2.02	0.42
2:J:716:TYR:CZ	3:G:19:LEU:HD13	2.54	0.42
2:K:246:TYR:CZ	2:K:275:ASN:HB3	2.55	0.42
2:K:653:LYS:O	2:K:657:LYS:HG3	2.20	0.42
1:H:662:LEU:HD11	1:H:689:MET:CE	2.33	0.42
6:B:268:LEU:O	6:B:308:LEU:HB2	2.20	0.42
8:C:561:LEU:HD23	8:C:561:LEU:HA	1.87	0.42
8:C:1326:LEU:N	8:C:1327:PRO:HD2	2.35	0.42
8:C:1517:THR:OG1	8:C:1520:SER:OG	2.34	0.42
13:Q:237:MET:HE3	13:Q:237:MET:HB3	1.93	0.42
14:T:580:MET:HA	14:T:583:ASP:HB2	2.02	0.42
1:F:457:ARG:HD3	1:F:457:ARG:HA	1.73	0.42
2:J:397:GLU:HG3	2:K:247:ARG:NE	2.35	0.42
2:K:254:ASP:OD2	2:K:255:LYS:NZ	2.52	0.42
2:K:736:TYR:CA	1:H:599:LYS:HE2	2.48	0.42
1:H:532:LEU:HD12	1:H:542:THR:HG22	2.02	0.42
6:B:504:SER:HA	6:B:505:MET:CE	2.49	0.42
8:C:1174:SER:O	8:C:1178:ILE:HG13	2.19	0.42
8:C:1526:MET:HE3	8:C:1526:MET:HB3	1.84	0.42
8:C:1557:LYS:HD3	8:C:1631:ILE:HD12	2.02	0.42
9:O:9:ILE:HD11	9:O:247:LEU:HD23	2.00	0.42
10:P:205:ILE:HD11	10:P:244:CYS:HB2	2.02	0.42
10:P:404:ALA:HB1	10:P:420:PHE:CD2	2.55	0.42
13:Q:104:ARG:CD	13:Q:156:ASN:HD22	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:131:LYS:HD3	13:Q:131:LYS:N	2.35	0.42
14:T:590:LEU:HG	14:T:594:MET:HE3	2.01	0.42
1:F:165:MET:HE2	1:F:165:MET:CA	2.49	0.42
2:K:705:ASP:OD1	2:K:706:LYS:N	2.52	0.42
1:H:165:MET:HG2	1:H:165:MET:H	1.66	0.42
6:B:197:ARG:HD3	10:D:377:GLN:HE22	1.85	0.42
6:B:412:TYR:HD1	6:B:419:PRO:HA	1.85	0.42
8:C:997:LYS:HG2	8:C:1000:GLU:OE1	2.20	0.42
8:C:1135:TYR:HB3	8:C:1178:ILE:HG23	2.01	0.42
8:C:1574:VAL:HG23	8:C:1576:GLU:H	1.85	0.42
9:O:10:THR:OG1	9:O:241:LEU:HD13	2.20	0.42
9:O:409:TYR:CD1	9:O:409:TYR:C	2.98	0.42
10:D:566:GLU:HA	10:D:572:ILE:HG22	2.00	0.42
10:P:91:LEU:HD21	10:P:107:PHE:HD2	1.84	0.42
12:N:119:PHE:O	12:N:127:THR:OG1	2.35	0.42
13:Q:124:ILE:O	13:Q:245:TYR:OH	2.38	0.42
13:Q:396:LYS:NZ	13:Q:428:ASP:OD2	2.37	0.42
15:U:41:CYS:HB3	15:U:44:CYS:SG	2.60	0.42
1:F:187:LEU:HD13	1:H:42:ASN:ND2	2.29	0.42
5:A:91:LYS:HD3	5:A:91:LYS:HA	1.80	0.42
8:C:741:ARG:CZ	8:C:775:GLU:OE2	2.68	0.42
8:C:1541:LEU:CD1	8:C:1544:PHE:CD2	2.98	0.42
9:O:343:LEU:HD21	9:O:381:ILE:HD13	2.01	0.42
10:D:299:PHE:O	10:D:303:VAL:HG12	2.20	0.42
10:P:186:ASN:O	10:P:190:ILE:HG13	2.20	0.42
10:P:218:TYR:HE1	10:P:221:ARG:HH11	1.67	0.42
10:P:483:TYR:HD1	10:P:483:TYR:HA	1.76	0.42
12:N:133:MET:HE2	12:N:133:MET:HB2	1.85	0.42
14:T:37:LEU:HD21	14:T:62:ILE:CD1	2.50	0.42
1:F:187:LEU:HG	1:F:190:SER:OG	2.20	0.41
2:K:617:LEU:HD23	2:K:621:TYR:OH	2.19	0.41
3:W:17:THR:HA	3:W:20:ILE:HG22	2.01	0.41
1:H:473:TRP:CZ2	1:H:477:GLN:HG3	2.54	0.41
1:H:591:ASP:HA	1:H:594:LYS:HG2	2.01	0.41
6:B:289:ASP:HB2	6:B:292:THR:OG1	2.20	0.41
6:B:298:LEU:HD23	6:B:334:ARG:HG2	2.01	0.41
6:B:406:ASP:OD1	6:B:406:ASP:N	2.52	0.41
8:C:819:ILE:O	8:C:823:ILE:HG12	2.20	0.41
8:C:952:LEU:O	8:C:956:THR:HG22	2.19	0.41
9:O:107:GLY:HA3	10:P:384:TYR:CE1	2.54	0.41
10:D:321:LEU:HD23	10:D:321:LEU:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:129:TYR:C	12:N:129:TYR:CD2	2.98	0.41
13:Q:51:ASN:ND2	13:Q:95:LYS:HG3	2.35	0.41
1:F:664:TYR:OH	4:E:212:LEU:HD23	2.20	0.41
1:F:675:SER:OG	1:F:678:SER:OG	2.20	0.41
1:F:699:PHE:HB3	1:F:716:LEU:CD2	2.51	0.41
2:J:264:ASP:OD1	2:J:265:ASP:N	2.53	0.41
2:K:600:LEU:HD12	2:K:600:LEU:HA	1.83	0.41
2:K:682:HIS:O	2:K:685:ARG:HG2	2.20	0.41
2:K:710:ILE:HD13	2:K:710:ILE:HA	1.94	0.41
1:H:43:TYR:CZ	1:H:80:LEU:HD13	2.55	0.41
1:H:478:LEU:HD22	1:H:494:TYR:HD2	1.84	0.41
5:A:129:LYS:HB3	5:A:131:MET:CE	2.51	0.41
6:B:478:VAL:HB	6:B:487:VAL:HG22	2.02	0.41
8:C:869:LYS:HE2	8:C:869:LYS:HB3	1.86	0.41
8:C:944:LYS:NZ	8:C:1001:ASP:OD1	2.48	0.41
8:C:1238:TRP:CD1	8:C:1238:TRP:H	2.36	0.41
8:C:1269:VAL:HG11	8:C:1286:LEU:HD22	2.01	0.41
8:C:1735:GLN:NE2	14:T:5:ILE:HG13	2.35	0.41
9:O:481:GLY:CA	9:O:624:LEU:HD22	2.50	0.41
9:O:624:LEU:HD21	9:O:662:PHE:HE1	1.84	0.41
10:D:499:ARG:NH1	10:D:534:GLN:OE1	2.53	0.41
13:Q:92:LYS:O	13:Q:166:ASN:ND2	2.48	0.41
14:T:302:LEU:HD12	14:T:354:LEU:HB2	2.00	0.41
14:T:344:TYR:O	14:T:348:ILE:HG12	2.19	0.41
15:U:1:MET:HE3	15:U:1:MET:CA	2.46	0.41
15:U:100:LEU:HD22	15:U:111:VAL:HA	2.02	0.41
1:F:539:LYS:HA	1:F:539:LYS:HD2	1.84	0.41
1:F:714:TYR:CE1	1:F:747:ILE:HG12	2.50	0.41
2:J:397:GLU:HG3	2:K:247:ARG:HE	1.85	0.41
2:J:516:LEU:HD23	2:J:540:TYR:HA	2.02	0.41
2:K:738:LYS:NZ	2:K:740:ASN:O	2.50	0.41
1:H:452:SER:HA	1:H:481:LEU:HD11	2.02	0.41
1:H:508:ASP:OD1	1:H:508:ASP:N	2.51	0.41
1:H:611:TYR:CE2	1:H:637:ILE:HD13	2.55	0.41
1:H:635:ARG:HB2	1:H:644:LEU:HD21	2.02	0.41
6:B:97:GLN:O	6:B:101:THR:HG22	2.20	0.41
6:B:252:TYR:CZ	6:B:543:LYS:HB2	2.55	0.41
6:B:473:GLN:O	6:B:490:HIS:ND1	2.53	0.41
8:C:722:ILE:O	8:C:722:ILE:CG1	2.64	0.41
8:C:806:GLU:OE1	8:C:806:GLU:N	2.29	0.41
9:O:78:LEU:HB2	9:O:176:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:88:LEU:HD23	10:D:88:LEU:HA	1.88	0.41
10:D:352:PHE:HB3	10:D:369:TYR:HD2	1.86	0.41
10:D:435:THR:HG22	10:D:439:HIS:CE1	2.55	0.41
10:P:16:GLN:HE21	10:P:16:GLN:HB3	1.52	0.41
10:P:431:THR:O	10:P:433:ALA:N	2.46	0.41
10:P:509:TYR:OH	10:P:517:GLU:HB3	2.20	0.41
10:P:551:ASP:HB3	10:P:554:GLU:HB2	2.01	0.41
13:Q:536:LEU:HD22	13:Q:557:ILE:HD11	2.02	0.41
14:T:130:ASP:O	14:T:133:ARG:HG2	2.20	0.41
2:K:252:ILE:O	2:K:256:VAL:HG23	2.21	0.41
2:K:571:PHE:O	2:K:574:THR:OG1	2.29	0.41
5:A:14:ALA:HB1	8:C:1365:LEU:CD1	2.50	0.41
6:B:478:VAL:CG1	6:B:523:LEU:HB3	2.51	0.41
8:C:153:ILE:HG23	8:C:162:PHE:HB3	2.02	0.41
8:C:386:PHE:HB2	8:C:394:ILE:HG23	2.02	0.41
8:C:1233:ASP:N	8:C:1233:ASP:OD1	2.52	0.41
10:P:20:ALA:O	10:P:24:LEU:HB2	2.20	0.41
10:P:509:TYR:CZ	10:P:517:GLU:HB3	2.56	0.41
13:Q:73:ILE:HD11	13:Q:84:SER:HB3	2.01	0.41
13:Q:536:LEU:HD23	13:Q:536:LEU:H	1.84	0.41
14:T:174:LYS:HE3	14:T:207:LEU:HD22	2.01	0.41
14:T:231:ARG:HD3	14:T:233:TRP:CZ2	2.54	0.41
14:T:582:TRP:NE1	14:T:586:CYS:SG	2.93	0.41
1:F:178:SER:O	4:E:161:LEU:HD12	2.21	0.41
1:F:196:LYS:NZ	1:F:197:MET:HE1	2.36	0.41
1:F:471:MET:HG3	1:F:474:CYS:H	1.86	0.41
2:K:477:CYS:HB3	2:K:479:PHE:CE2	2.55	0.41
1:H:499:LYS:HE2	1:H:503:PRO:HA	2.02	0.41
1:H:565:LYS:HD2	4:E:257:TYR:HE1	1.86	0.41
6:B:281:LEU:HD12	6:B:286:PHE:CD2	2.55	0.41
8:C:745:ILE:HD11	8:C:779:TYR:CZ	2.56	0.41
8:C:748:LEU:HD23	8:C:748:LEU:HA	1.88	0.41
10:D:421:ARG:HB2	10:D:437:MET:HE1	2.00	0.41
1:F:95:LYS:HD3	1:F:105:PHE:CE2	2.55	0.41
1:F:439:ASN:O	1:F:443:ILE:HG12	2.20	0.41
1:F:446:SER:OG	1:F:455:ALA:HB2	2.20	0.41
2:J:398:MET:HE2	2:J:398:MET:HB2	1.84	0.41
2:J:485:LEU:HA	2:J:488:THR:HG22	2.03	0.41
2:J:545:ASP:OD1	2:J:545:ASP:C	2.63	0.41
2:J:552:LYS:O	2:J:555:SER:OG	2.26	0.41
2:J:635:VAL:O	2:J:639:MET:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:432:LEU:HD23	2:K:432:LEU:HA	1.82	0.41
1:H:486:ILE:HG23	1:H:488:TYR:HE1	1.86	0.41
6:B:73:SER:HB2	6:B:134:PRO:C	2.46	0.41
6:B:265:TYR:HE1	6:B:405:ASN:HD21	1.69	0.41
8:C:454:LEU:HD11	8:C:462:ILE:HD11	2.02	0.41
8:C:605:TYR:HD1	8:C:610:PHE:CE2	2.38	0.41
8:C:807:LEU:H	8:C:807:LEU:HD12	1.85	0.41
8:C:972:ILE:O	8:C:972:ILE:HG22	2.20	0.41
8:C:1169:LEU:O	8:C:1173:ILE:HG22	2.21	0.41
9:O:604:ILE:HD12	9:O:607:LEU:HD11	2.02	0.41
9:O:647:GLU:HA	9:O:650:ILE:HG22	2.02	0.41
13:Q:29:ILE:HD13	13:Q:39:ALA:HB3	2.02	0.41
13:Q:242:LEU:HA	13:Q:245:TYR:HB3	2.02	0.41
14:T:326:PHE:CD1	14:T:330:ILE:HB	2.56	0.41
1:F:748:ILE:HD13	1:F:751:LEU:HD12	2.03	0.41
2:K:407:PRO:HB3	2:K:438:SER:CB	2.50	0.41
2:K:583:GLN:HE21	8:C:1142:ARG:NH2	2.17	0.41
1:H:679:LYS:HB3	1:H:679:LYS:HE3	1.62	0.41
6:B:472:SER:HG	6:B:490:HIS:CE1	2.32	0.41
8:C:1332:MET:O	8:C:1336:ILE:HG12	2.20	0.41
8:C:1386:LEU:O	8:C:1390:ILE:HG22	2.20	0.41
8:C:1731:ILE:O	8:C:1735:GLN:HG3	2.20	0.41
13:Q:264:PHE:HD1	13:Q:267:ARG:HH22	1.67	0.41
14:T:309:MET:HE1	14:T:311:ASP:O	2.20	0.41
1:F:461:SER:HG	1:F:462:GLN:CD	2.26	0.41
1:F:469:ASP:OD1	1:F:470:THR:N	2.53	0.41
1:F:543:TRP:HB3	1:F:566:ALA:HB2	2.03	0.41
1:F:543:TRP:CE2	1:F:565:LYS:HG2	2.56	0.41
2:K:678:LEU:HD12	2:K:697:PHE:HE1	1.86	0.41
1:H:185:PRO:HG2	1:H:186:TYR:CE1	2.55	0.41
1:H:601:LEU:HD13	1:H:601:LEU:HA	1.92	0.41
1:H:753:LYS:HG3	1:H:754:CYS:N	2.35	0.41
5:A:14:ALA:HB1	8:C:1365:LEU:HD11	2.02	0.41
5:A:88:ALA:HB1	5:A:126:MET:O	2.21	0.41
6:B:194:ASN:OD1	6:B:194:ASN:N	2.53	0.41
6:B:252:TYR:HE1	6:B:543:LYS:N	2.18	0.41
6:B:431:LYS:HB3	6:B:475:CYS:HA	2.03	0.41
8:C:1097:LYS:HD3	8:C:1097:LYS:HA	1.74	0.41
8:C:1504:LEU:HA	8:C:1504:LEU:HD23	1.79	0.41
9:O:172:ASN:O	9:O:176:PHE:N	2.41	0.41
10:D:259:LEU:HD11	10:D:268:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:311:LEU:HD23	10:D:311:LEU:H	1.84	0.41
10:P:518:ALA:O	10:P:522:TYR:N	2.37	0.41
10:P:543:ALA:O	10:P:547:GLU:HG2	2.21	0.41
15:U:78:ILE:HG12	15:U:98:PHE:CZ	2.56	0.41
1:F:35:GLN:HE22	1:F:148:VAL:N	2.10	0.41
1:F:205:ARG:NH1	4:E:159:SER:O	2.54	0.41
1:F:591:ASP:OD1	1:F:592:SER:N	2.54	0.41
2:K:419:PHE:CE2	2:K:430:LYS:HA	2.55	0.41
3:G:16:VAL:O	3:G:20:ILE:HG12	2.21	0.41
1:H:60:LEU:CD2	1:H:64:SER:HB3	2.33	0.41
1:H:597:TYR:CZ	1:H:613:GLY:HA3	2.56	0.41
1:H:723:VAL:HG12	1:H:725:ARG:NH1	2.27	0.41
5:A:124:ASP:OD2	5:A:126:MET:HE2	2.20	0.41
6:B:190:ARG:N	11:I:97:TRP:CZ2	2.75	0.41
6:B:562:PHE:C	6:B:562:PHE:CD2	2.99	0.41
8:C:527:THR:O	8:C:531:LYS:NZ	2.51	0.41
8:C:1063:GLU:HG2	8:C:1066:HIS:CE1	2.56	0.41
8:C:1248:VAL:HA	8:C:1251:ILE:HG22	2.02	0.41
8:C:1569:PRO:O	8:C:1570:ILE:HD13	2.21	0.41
9:O:255:ILE:HG13	9:O:256:VAL:N	2.35	0.41
9:O:364:GLU:HG2	9:O:367:ARG:NH2	2.35	0.41
10:D:201:TYR:CD1	10:D:202:GLU:N	2.89	0.41
10:P:25:SER:HB3	10:P:33:SER:OG	2.21	0.41
10:P:301:LEU:HD21	10:P:334:TYR:CE2	2.36	0.41
13:Q:69:GLY:HA2	13:Q:93:ILE:HD11	2.03	0.41
13:Q:101:ILE:O	13:Q:159:LEU:N	2.46	0.41
13:Q:377:LEU:HA	13:Q:380:THR:HG22	2.03	0.41
14:T:103:PHE:CE2	14:T:147:ILE:HG23	2.56	0.41
14:T:609:ILE:HB	14:T:614:TRP:NE1	2.36	0.41
1:F:116:VAL:O	1:F:120:ILE:HG13	2.21	0.41
1:F:527:ASN:ND2	2:K:518:LEU:HD21	2.36	0.41
1:H:514:THR:HG23	5:A:250:ARG:HB3	2.02	0.41
1:H:594:LYS:HG3	1:H:598:ARG:HH21	1.86	0.41
1:H:633:LYS:HD2	1:H:636:SER:OG	2.20	0.41
9:O:4:TYR:HA	9:O:286:LEU:HD21	2.03	0.41
9:O:21:LEU:HA	9:O:24:ILE:HG22	2.02	0.41
9:O:93:LYS:CD	9:O:93:LYS:H	2.34	0.41
9:O:552:ARG:HD2	9:O:568:LEU:HD21	2.03	0.41
10:D:515:LYS:HD2	10:D:545:LEU:HD22	2.03	0.41
13:Q:156:ASN:OD1	13:Q:156:ASN:N	2.53	0.41
13:Q:336:ARG:O	13:Q:339:ILE:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:129:LYS:O	14:T:133:ARG:NE	2.54	0.41
14:T:288:PHE:CE1	14:T:326:PHE:HA	2.56	0.41
14:T:459:LEU:O	14:T:463:ILE:HB	2.21	0.41
14:T:634:LEU:HD21	15:U:5:ILE:HD13	2.02	0.41
2:J:282:ALA:O	2:J:286:ILE:HG12	2.21	0.40
2:J:432:LEU:HD12	2:J:432:LEU:HA	1.90	0.40
2:J:514:ASN:HB2	10:D:387:GLN:HG2	2.02	0.40
2:J:607:MET:SD	2:J:638:GLU:OE2	2.79	0.40
2:J:609:PHE:HD1	2:J:609:PHE:HA	1.80	0.40
2:K:697:PHE:HB3	2:K:714:LEU:HD21	2.03	0.40
5:A:16:SER:HB2	8:C:1365:LEU:HG	2.03	0.40
8:C:68:TYR:CD1	8:C:91:LEU:HD11	2.56	0.40
8:C:1285:LEU:CD1	8:C:1289:ARG:HG3	2.51	0.40
8:C:1715:GLU:N	8:C:1715:GLU:OE1	2.54	0.40
9:O:18:LEU:HA	9:O:21:LEU:HB2	2.03	0.40
9:O:41:PHE:O	9:O:45:ILE:HD12	2.21	0.40
10:D:10:ILE:HG23	10:D:43:LEU:HD21	2.03	0.40
10:D:16:GLN:O	10:D:20:ALA:N	2.44	0.40
10:P:434:TRP:HB3	10:P:457:ALA:HB2	2.03	0.40
13:Q:183:PHE:O	13:Q:477:GLN:NE2	2.54	0.40
13:Q:233:LEU:HD23	13:Q:233:LEU:HA	1.87	0.40
2:J:255:LYS:HE2	2:K:432:LEU:HD21	2.04	0.40
2:J:393:PHE:CE2	2:K:251:TYR:CD2	3.08	0.40
2:J:496:ASN:O	2:J:500:LEU:HG	2.21	0.40
1:H:123:LEU:HB3	1:H:160:LEU:HD12	2.03	0.40
1:H:652:LEU:HA	1:H:655:LEU:CD1	2.49	0.40
5:A:187:ARG:NH1	8:C:1322:ASN:HB3	2.35	0.40
6:B:417:LYS:HD2	6:B:417:LYS:H	1.87	0.40
8:C:749:TYR:OH	8:C:783:ILE:HG23	2.21	0.40
8:C:1298:TRP:CH2	8:C:1342:ARG:HA	2.56	0.40
8:C:1363:LEU:HD21	8:C:1412:TYR:HD2	1.86	0.40
9:O:45:ILE:HG23	9:O:150:PHE:CD1	2.55	0.40
9:O:402:THR:N	9:O:405:GLN:OE1	2.50	0.40
9:O:422:PHE:CE2	12:N:5:LEU:HD22	2.56	0.40
9:O:481:GLY:HA2	9:O:624:LEU:HD22	2.03	0.40
10:D:463:ARG:HA	10:D:494:LEU:HD11	2.03	0.40
10:D:533:ASP:O	10:D:536:THR:HG22	2.22	0.40
10:P:44:ALA:HB2	10:P:326:PRO:HG2	2.03	0.40
10:P:499:ARG:HH11	10:P:499:ARG:HG2	1.85	0.40
10:P:539:TYR:HE2	10:P:565:VAL:HG21	1.85	0.40
11:I:16:LEU:HD23	11:I:16:LEU:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:316:CYS:SG	13:Q:317:GLU:N	2.93	0.40
13:Q:328:LEU:O	13:Q:329:ILE:HD13	2.21	0.40
14:T:490:ASN:HD21	14:T:492:PHE:HD2	1.69	0.40
15:U:121:ARG:HD3	15:U:121:ARG:HA	1.96	0.40
1:F:201:VAL:HG12	4:E:162:LEU:HA	2.03	0.40
1:F:436:ILE:HD13	1:F:436:ILE:HA	1.94	0.40
2:J:737:LEU:HD23	2:J:737:LEU:HA	1.89	0.40
2:K:631:ASN:OD1	2:K:631:ASN:N	2.54	0.40
1:H:80:LEU:HD23	1:H:80:LEU:HA	1.92	0.40
1:H:601:LEU:CD1	1:H:611:TYR:CZ	3.04	0.40
6:B:436:SER:OG	6:B:442:VAL:HB	2.22	0.40
6:B:439:LYS:HA	6:B:439:LYS:HD2	1.88	0.40
8:C:546:ASN:O	8:C:550:ILE:HD12	2.21	0.40
8:C:634:ILE:HG13	8:C:635:ARG:N	2.36	0.40
8:C:815:ARG:NH2	8:C:1633:TYR:H	2.20	0.40
8:C:867:ILE:HG21	9:O:449:LYS:HG2	2.03	0.40
8:C:1038:LYS:HA	8:C:1039:PRO:HD3	1.91	0.40
9:O:506:SER:HB2	9:O:544:GLN:HE22	1.85	0.40
10:D:215:ALA:HB2	10:D:244:CYS:SG	2.61	0.40
10:D:305:GLU:HG3	10:D:338:ILE:HD11	2.03	0.40
12:N:116:TRP:HB3	12:N:117:ASN:OD1	2.21	0.40
13:Q:60:LYS:HG3	13:Q:77:PHE:CD1	2.57	0.40
14:T:389:LEU:HD13	14:T:390:PRO:HD2	2.03	0.40
1:F:31:GLN:O	1:F:35:GLN:HG2	2.21	0.40
1:F:88:PHE:CD1	1:F:105:PHE:HE1	2.38	0.40
1:F:519:LEU:HD23	1:F:519:LEU:HA	1.87	0.40
1:F:633:LYS:HA	1:F:633:LYS:HD2	1.87	0.40
2:J:643:TYR:HE2	2:J:655:TYR:HE2	1.68	0.40
2:K:621:TYR:HA	2:K:624:LEU:CG	2.48	0.40
6:B:468:ILE:HG21	6:B:500:TRP:CH2	2.57	0.40
8:C:75:ALA:HB1	8:C:87:PHE:HE1	1.86	0.40
8:C:559:ILE:HG12	8:C:603:GLU:HG3	2.03	0.40
8:C:613:LEU:HD23	8:C:613:LEU:HA	1.87	0.40
8:C:749:TYR:CZ	8:C:783:ILE:HG23	2.56	0.40
8:C:942:GLN:HB3	8:C:946:PHE:CZ	2.57	0.40
8:C:1128:ILE:HD11	8:C:1147:ILE:CD1	2.52	0.40
9:O:128:ARG:HD3	9:O:128:ARG:HA	1.88	0.40
9:O:319:LEU:HD12	9:O:319:LEU:HA	1.94	0.40
9:O:343:LEU:O	9:O:347:THR:N	2.40	0.40
10:D:523:LYS:NZ	10:D:546:TYR:OH	2.53	0.40
10:P:316:GLU:H	10:P:316:GLU:CD	2.24	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:533:ASP:O	10:P:536:THR:HG22	2.22	0.40
13:Q:422:ASP:HB3	13:Q:425:PHE:HB2	2.03	0.40
14:T:27:HIS:O	14:T:27:HIS:ND1	2.50	0.40
14:T:181:LEU:HD23	14:T:212:LEU:HB3	2.03	0.40
14:T:576:SER:HB2	14:T:613:TYR:HB3	2.03	0.40
14:T:626:LEU:HD22	14:T:659:ASP:HB3	2.03	0.40
1:F:745:GLN:HG2	1:F:746:VAL:N	2.37	0.40
2:J:364:LEU:HD12	2:J:364:LEU:HA	1.79	0.40
2:K:728:ILE:HB	2:K:732:HIS:CE1	2.56	0.40
5:A:142:MET:CG	5:A:175:VAL:H	2.34	0.40
5:A:171:GLU:HG2	5:A:173:ARG:CZ	2.51	0.40
6:B:353:ASN:ND2	6:B:395:VAL:O	2.54	0.40
8:C:1524:LEU:O	8:C:1528:VAL:HG13	2.22	0.40
8:C:1541:LEU:HD12	8:C:1544:PHE:HD2	1.80	0.40
10:D:590:LYS:HA	10:D:590:LYS:HD3	1.90	0.40
10:P:16:GLN:NE2	10:P:247:PHE:CD2	2.85	0.40
10:P:331:LEU:HD23	10:P:331:LEU:HA	1.82	0.40
13:Q:423:LEU:HD23	13:Q:424:TYR:N	2.36	0.40
14:T:606:PRO:HG3	14:T:641:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	496/758 (65%)	475 (96%)	21 (4%)	0	100	100
1	H	499/758 (66%)	481 (96%)	16 (3%)	2 (0%)	30	62
2	J	505/850 (59%)	487 (96%)	18 (4%)	0	100	100
2	K	501/850 (59%)	488 (97%)	13 (3%)	0	100	100
3	G	33/124 (27%)	32 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	35/124 (28%)	35 (100%)	0	0	100	100
4	E	120/265 (45%)	119 (99%)	1 (1%)	0	100	100
5	A	213/250 (85%)	201 (94%)	11 (5%)	1 (0%)	24	57
6	B	432/566 (76%)	404 (94%)	27 (6%)	1 (0%)	43	74
7	S	4/1518 (0%)	3 (75%)	1 (25%)	0	100	100
8	C	1384/1748 (79%)	1299 (94%)	81 (6%)	4 (0%)	36	67
9	O	654/685 (96%)	625 (96%)	25 (4%)	4 (1%)	21	54
10	D	554/626 (88%)	540 (98%)	13 (2%)	1 (0%)	43	74
10	P	550/626 (88%)	530 (96%)	20 (4%)	0	100	100
11	I	105/170 (62%)	98 (93%)	7 (7%)	0	100	100
12	N	92/368 (25%)	89 (97%)	3 (3%)	0	100	100
13	Q	619/652 (95%)	596 (96%)	22 (4%)	1 (0%)	43	74
14	T	631/853 (74%)	620 (98%)	11 (2%)	0	100	100
15	U	110/165 (67%)	107 (97%)	3 (3%)	0	100	100
All	All	7537/11956 (63%)	7229 (96%)	294 (4%)	14 (0%)	44	74

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	844	VAL
8	C	1279	ILE
9	O	193	VAL
10	D	205	ILE
1	H	507	LYS
1	H	554	LYS
13	Q	10	ILE
8	C	1416	VAL
9	O	51	SER
9	O	53	GLU
6	B	123	GLU
8	C	801	VAL
9	O	355	CYS
5	A	21	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	433/684 (63%)	433 (100%)	0	100	100
1	H	439/684 (64%)	438 (100%)	1 (0%)	87	85
2	J	451/760 (59%)	451 (100%)	0	100	100
2	K	448/760 (59%)	448 (100%)	0	100	100
3	G	34/115 (30%)	34 (100%)	0	100	100
3	W	36/115 (31%)	36 (100%)	0	100	100
4	E	123/246 (50%)	123 (100%)	0	100	100
5	A	190/226 (84%)	190 (100%)	0	100	100
6	B	375/503 (75%)	375 (100%)	0	100	100
7	S	6/1389 (0%)	6 (100%)	0	100	100
8	C	1180/1568 (75%)	1179 (100%)	1 (0%)	88	87
9	O	598/643 (93%)	598 (100%)	0	100	100
10	D	477/560 (85%)	477 (100%)	0	100	100
10	P	476/560 (85%)	475 (100%)	1 (0%)	87	85
11	I	95/144 (66%)	95 (100%)	0	100	100
12	N	83/332 (25%)	83 (100%)	0	100	100
13	Q	571/598 (96%)	570 (100%)	1 (0%)	87	85
14	T	605/804 (75%)	605 (100%)	0	100	100
15	U	103/149 (69%)	103 (100%)	0	100	100
All	All	6723/10840 (62%)	6719 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	599	LYS
8	C	1105	HIS
10	P	560	MET
13	Q	448	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	35	GLN
1	F	42	ASN
1	F	85	HIS
1	F	111	GLN
1	F	128	ASN
1	F	184	ASN
1	F	663	GLN
2	J	271	GLN
2	J	275	ASN
2	J	408	GLN
2	J	450	ASN
2	J	581	GLN
2	J	647	ASN
2	J	690	ASN
2	J	750	ASN
2	J	755	ASN
2	K	243	GLN
2	K	244	HIS
2	K	290	ASN
2	K	583	GLN
2	K	677	GLN
2	K	750	ASN
3	G	26	GLN
3	W	13	HIS
1	H	39	GLN
1	H	42	ASN
1	H	111	GLN
1	H	157	ASN
1	H	482	HIS
1	H	587	ASN
1	H	638	ASN
4	E	123	HIS
4	E	219	HIS
5	A	208	ASN
6	B	219	GLN
6	B	290	ASN
6	B	354	ASN
6	B	405	ASN
8	C	31	GLN
8	C	419	HIS
8	C	753	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	1058	HIS
8	C	1543	HIS
9	O	11	ASN
9	O	252	ASN
9	O	323	HIS
9	O	333	ASN
9	O	372	ASN
10	D	77	ASN
10	D	377	GLN
10	D	448	HIS
10	D	534	GLN
10	D	610	GLN
10	P	16	GLN
10	P	248	ASN
10	P	260	GLN
10	P	287	GLN
10	P	413	HIS
10	P	489	GLN
10	P	544	GLN
11	I	92	HIS
11	I	98	ASN
11	I	158	ASN
13	Q	254	ASN
13	Q	324	GLN
13	Q	479	HIS
14	T	99	GLN
14	T	113	GLN
14	T	741	HIS
15	U	70	HIS
15	U	101	GLN
15	U	107	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

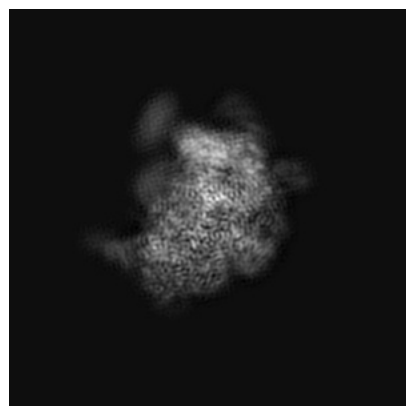
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15123. These allow visual inspection of the internal detail of the map and identification of artifacts.

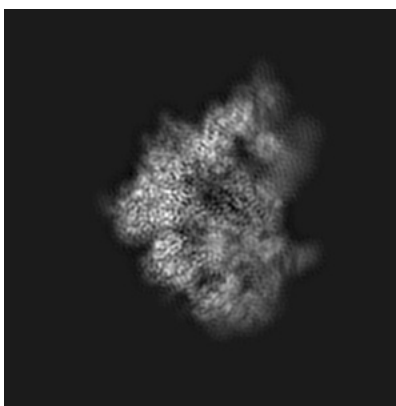
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

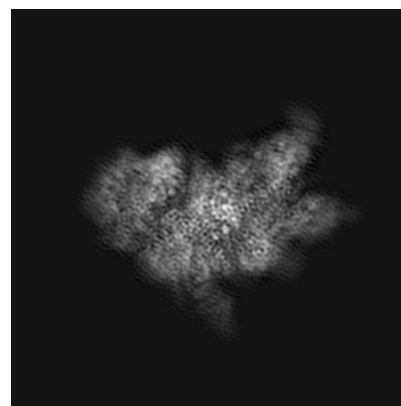
6.1.1 Primary map



X

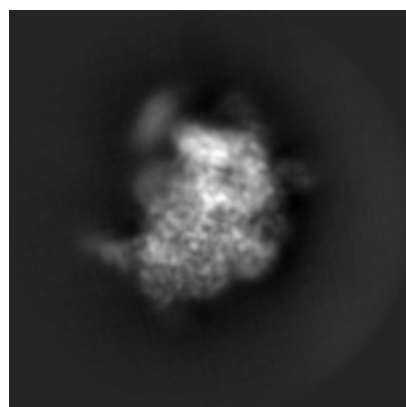


Y

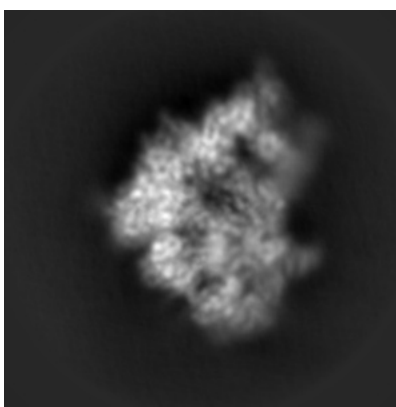


Z

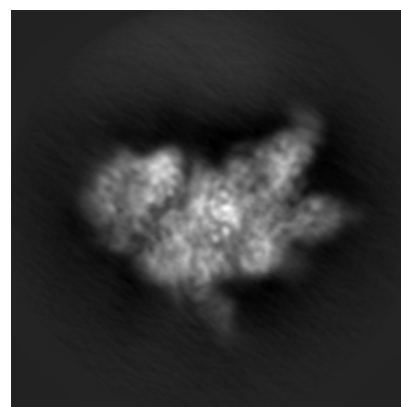
6.1.2 Raw map



X



Y

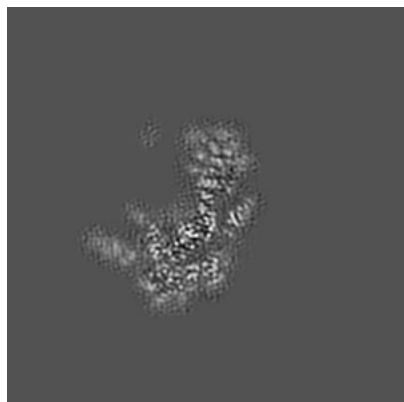


Z

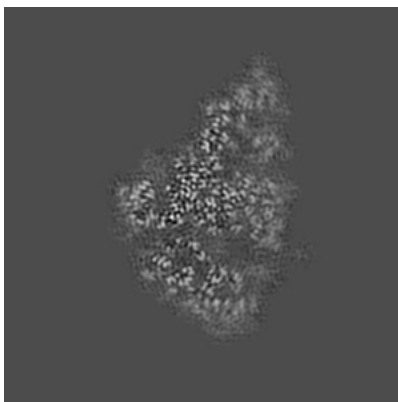
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

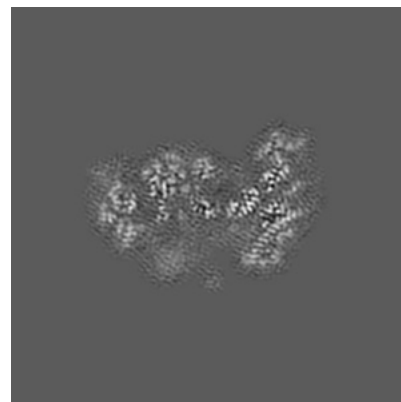
6.2.1 Primary map



X Index: 128

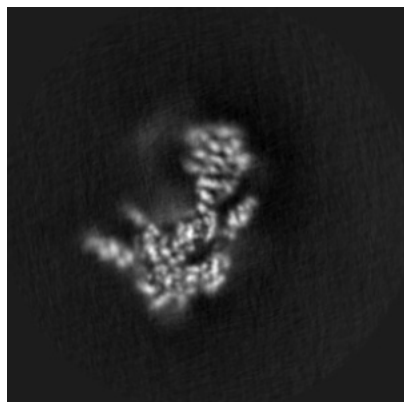


Y Index: 128

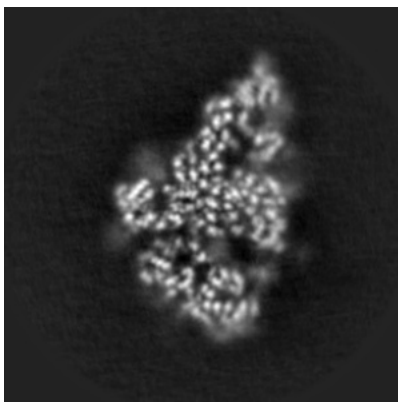


Z Index: 128

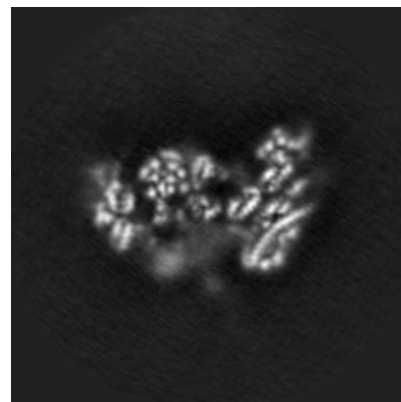
6.2.2 Raw map



X Index: 128



Y Index: 128

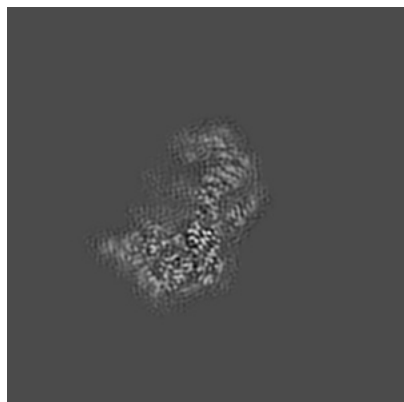


Z Index: 128

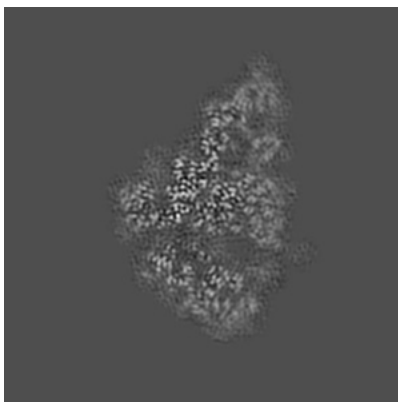
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

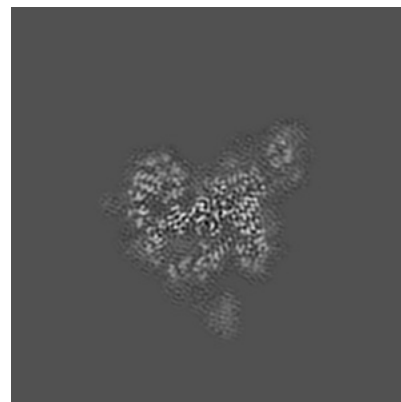
6.3.1 Primary map



X Index: 122

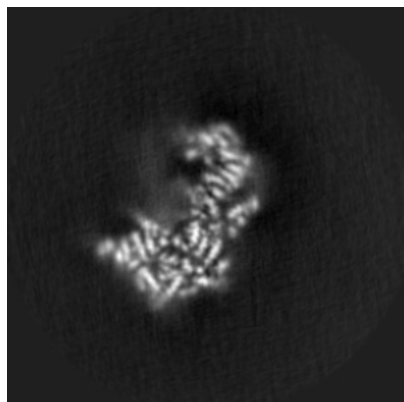


Y Index: 129

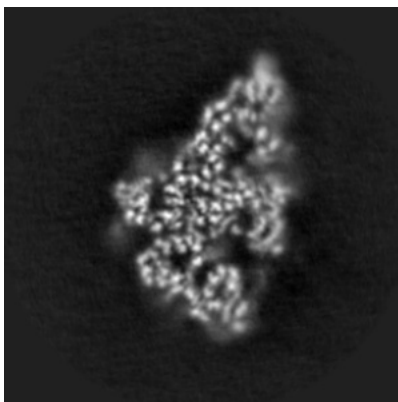


Z Index: 111

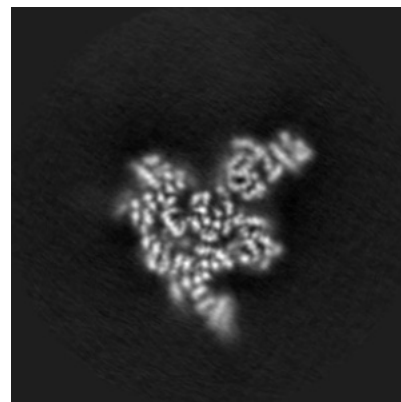
6.3.2 Raw map



X Index: 123



Y Index: 125

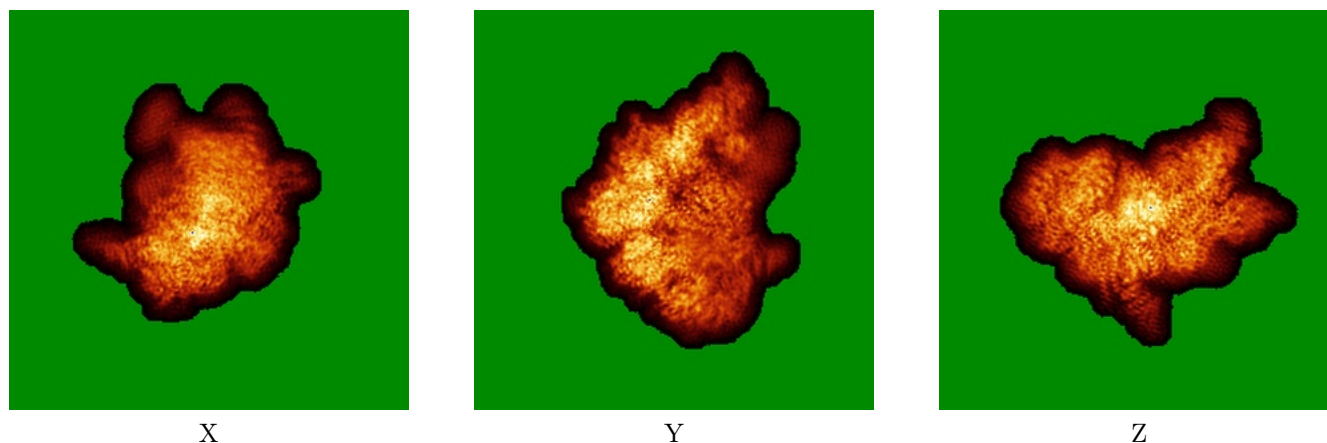


Z Index: 104

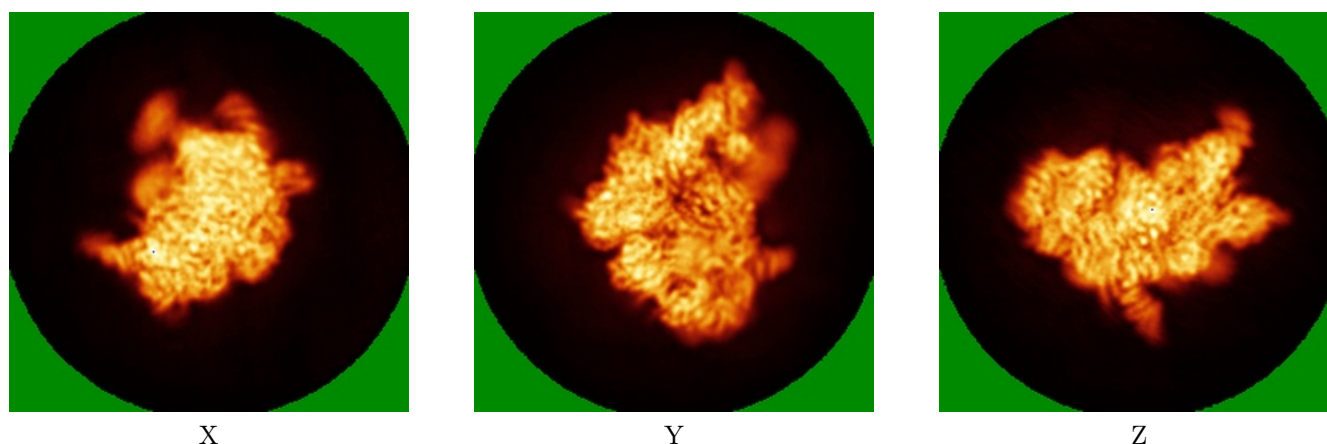
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

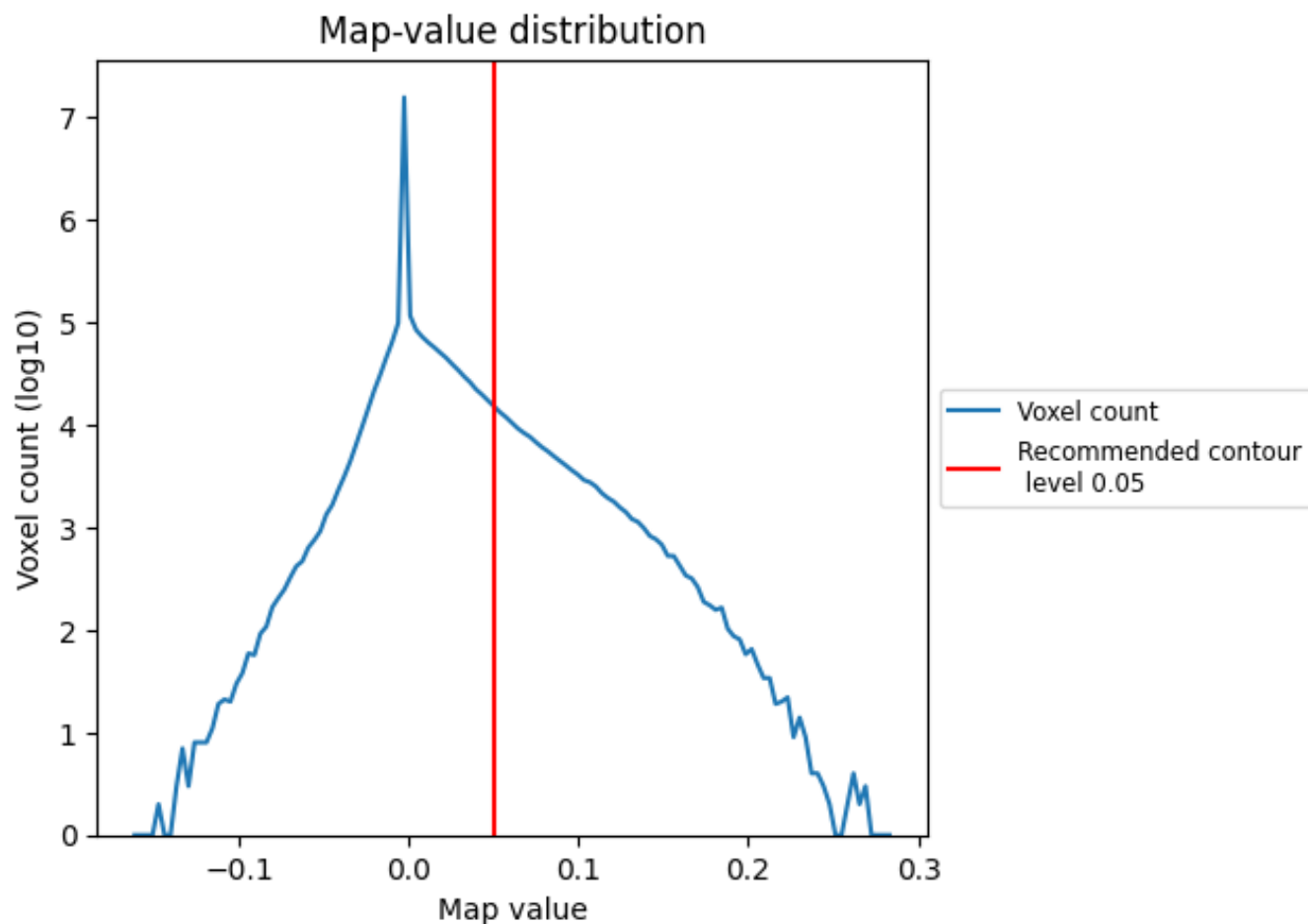
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

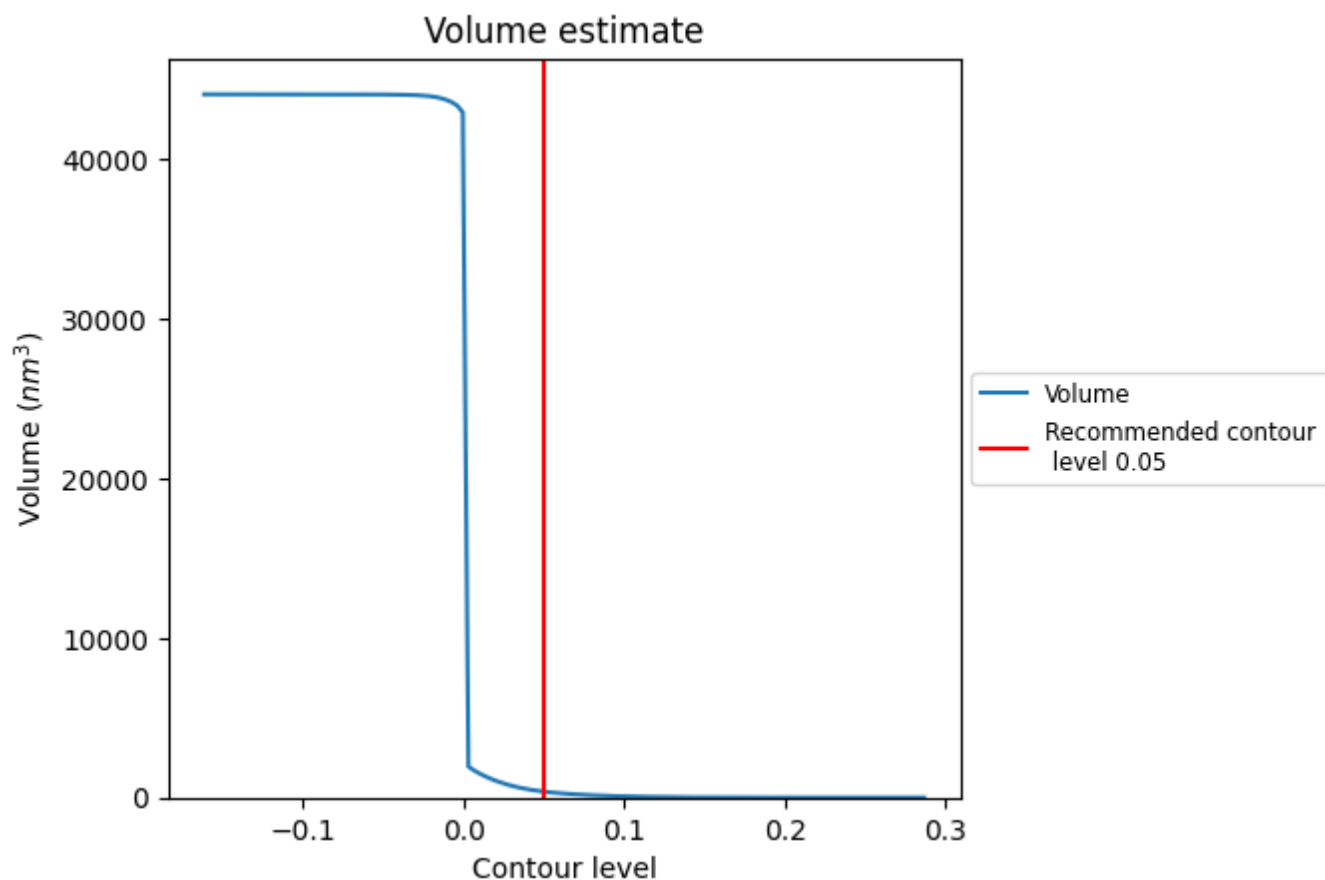
This section contains the results of statistical analysis of the map.

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.

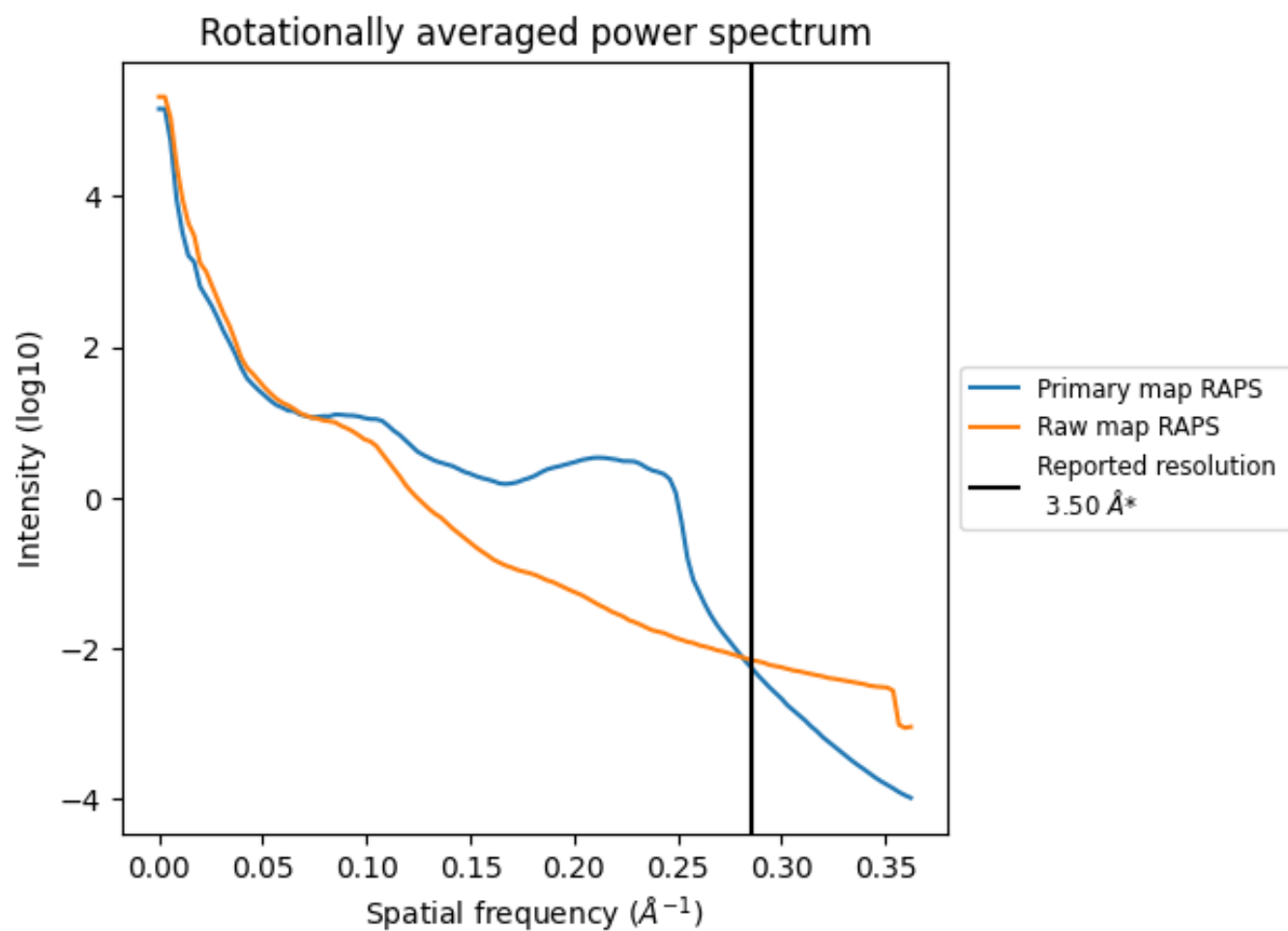
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 339 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 ⓘ

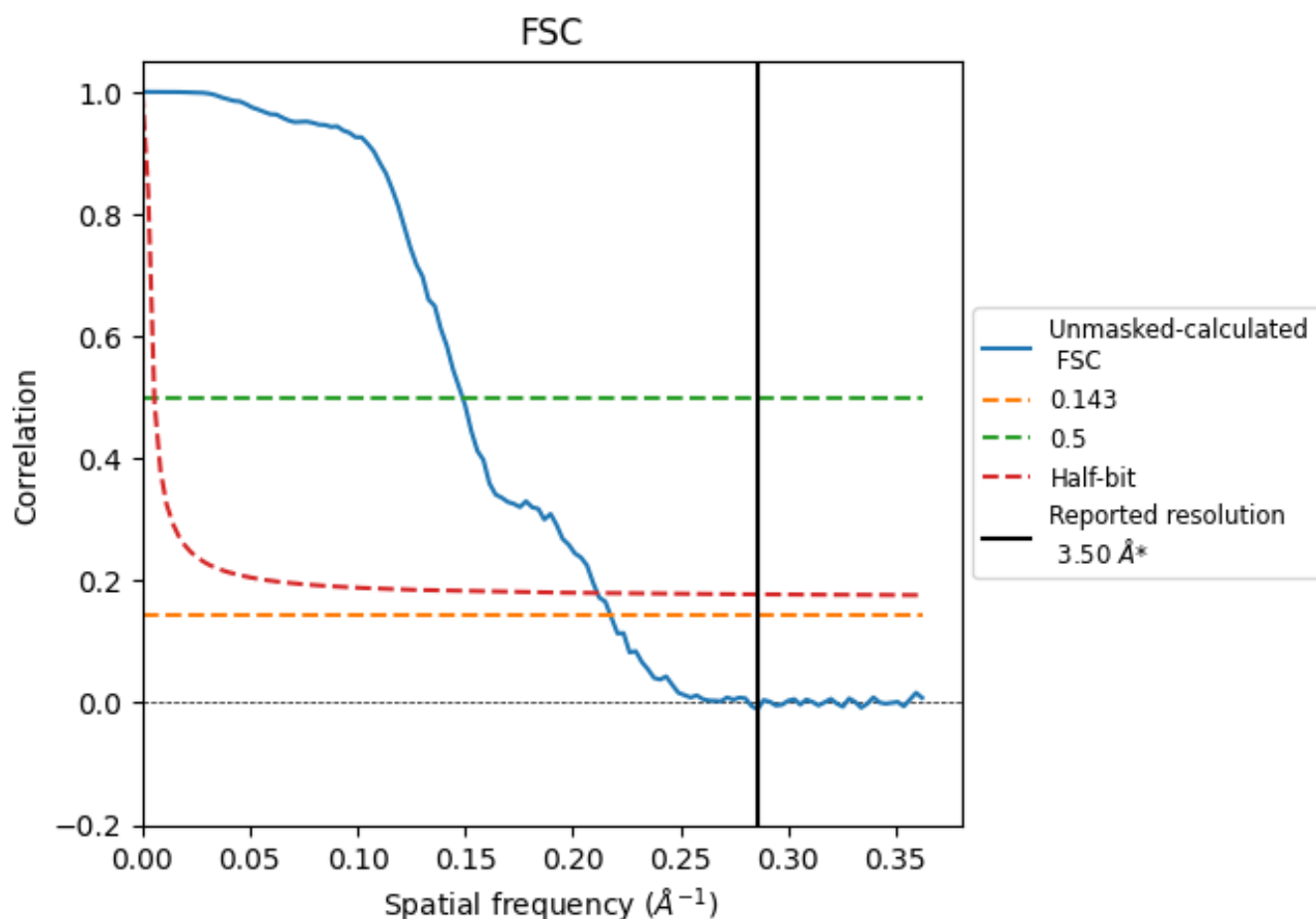


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

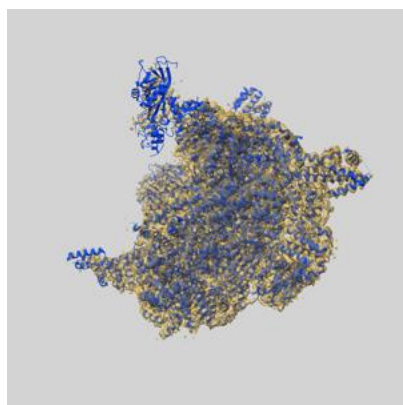
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.60	6.72	4.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.5 by more than 10 %

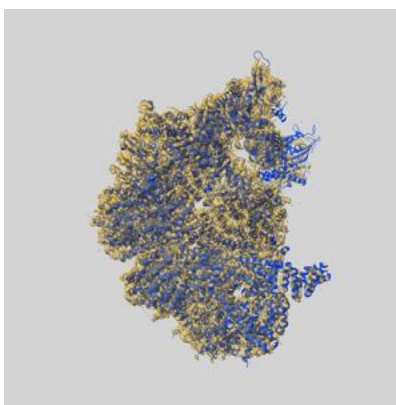
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15123 and PDB model 8A3T. Per-residue inclusion information can be found in section [3](#) on page [8](#).

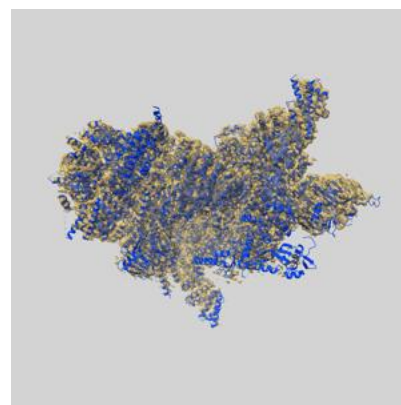
9.1 Map-model overlay [i](#)



X



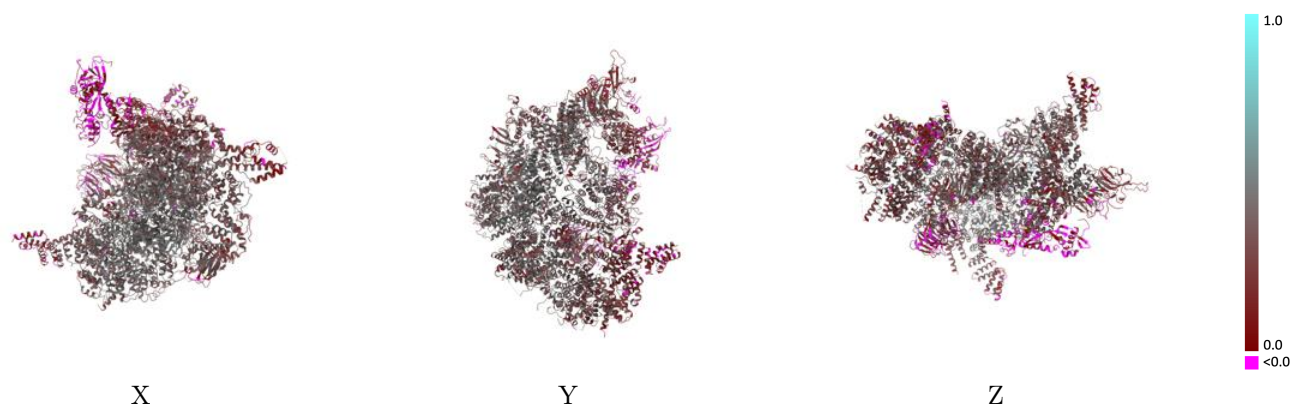
Y



Z

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

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

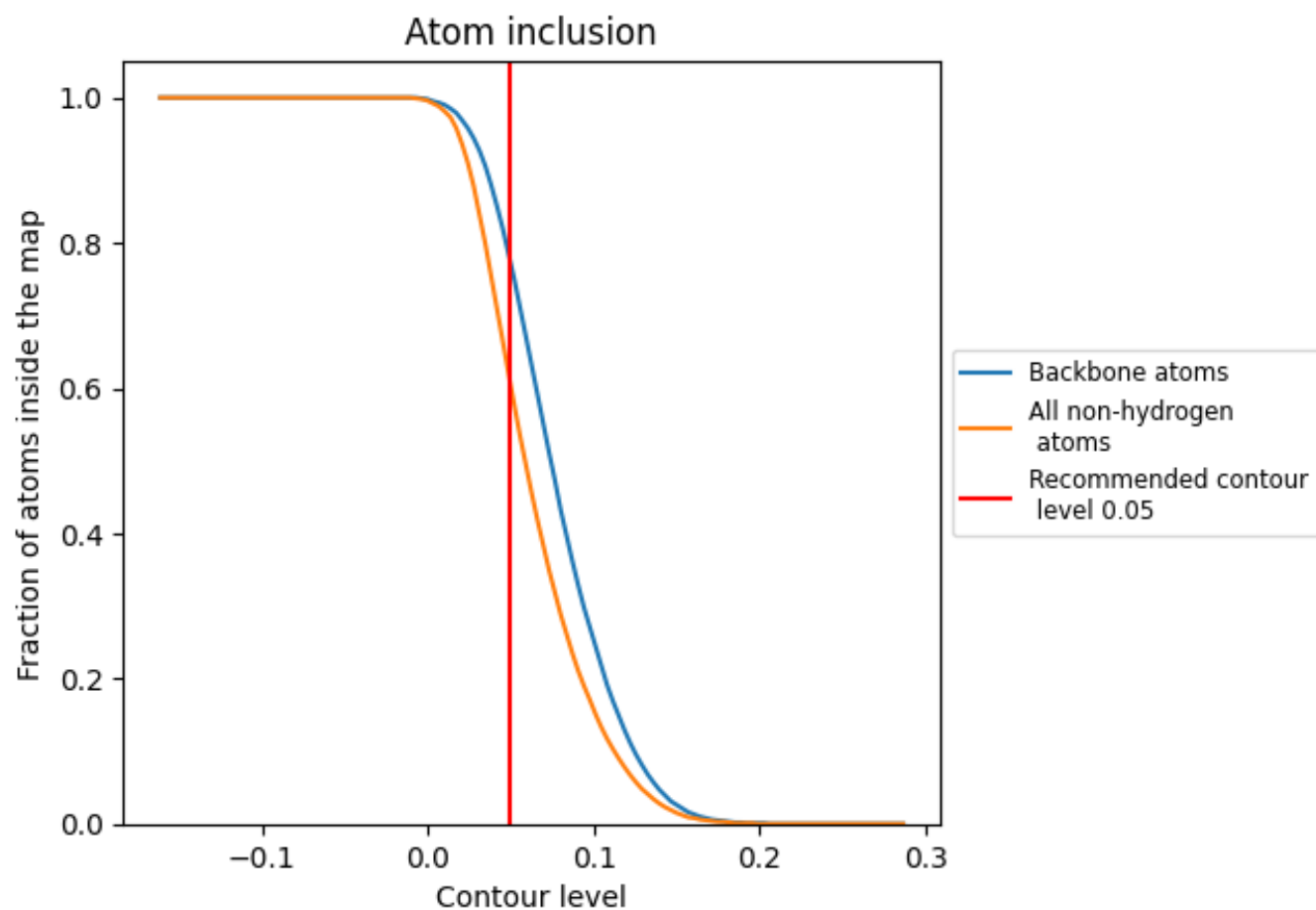


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6040	 0.3360
A	 0.4920	 0.2640
B	 0.3380	 0.2250
C	 0.6640	 0.3690
D	 0.7720	 0.4350
E	 0.4390	 0.3050
F	 0.6580	 0.3470
G	 0.5860	 0.3150
H	 0.4310	 0.2530
I	 0.7310	 0.4370
J	 0.7380	 0.3990
K	 0.6630	 0.3650
N	 0.7000	 0.4200
O	 0.7470	 0.4260
P	 0.7050	 0.3710
Q	 0.6150	 0.3270
S	 0.4890	 0.3190
T	 0.3620	 0.1900
U	 0.0230	 0.0240
W	 0.3110	 0.2370

