Full wwPDB EM Validation Report ⓘ

Oct 8, 2024 – 04:35 PM JST

PDB ID	:	8Y80
EMDB ID	:	EMD-39028
Title	:	Cryo-EM structure of the tetrameric SPARSA gRNA-ssDNA complex
Authors	:	Zhang, J.T.; Cui, N.; Wei, X.Y.; Jia, N.
Deposited on	:	2024-02-05
Resolution	:	3.38 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:

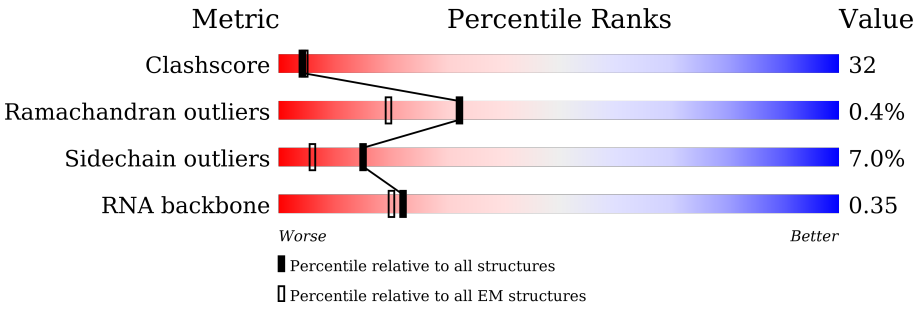
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.38 Å.

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



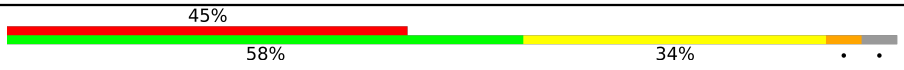
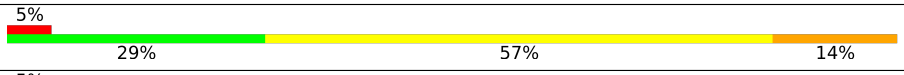
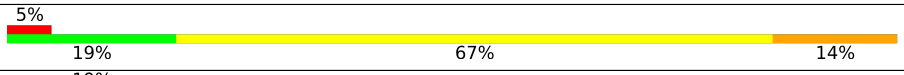
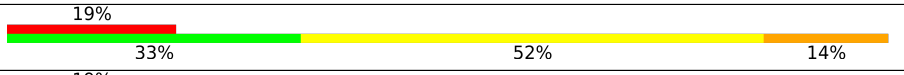
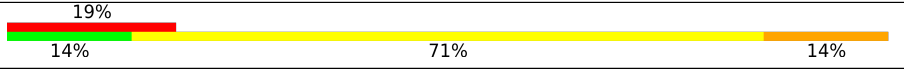
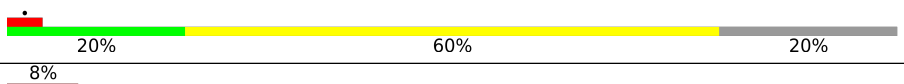
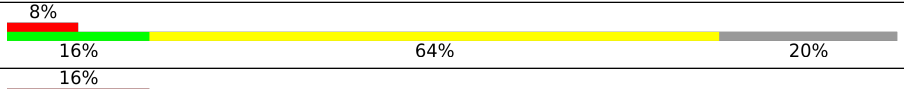
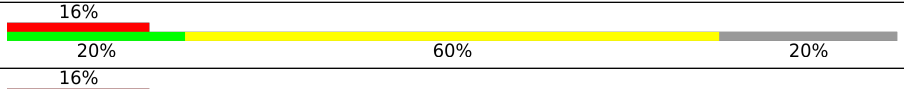
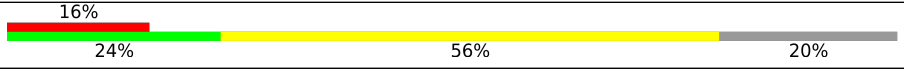
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	587	28% 46% 29% • 21%
1	E	587	31% 51% 41% 6% •
1	I	587	55% 47% 28% • 21%
1	M	587	46% 53% 40% • •
2	B	473	12% 55% 39% • •
2	F	473	20% 60% 34% • •
2	J	473	40% 60% 34% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	473	
3	C	21	
3	G	21	
3	K	21	
3	O	21	
4	D	25	
4	H	25	
4	L	25	
4	P	25	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34473 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 Sir2 superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3655	2346	633	664	12		
1	E	576	Total	C	N	O	S	0	0
			4612	2954	798	846	14		
1	I	463	Total	C	N	O	S	0	0
			3662	2351	634	665	12		
1	M	576	Total	C	N	O	S	0	0
			4612	2954	798	846	14		

- Molecule 2 is a protein called Piwi domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	0	0
			3629	2327	613	671	18		
2	F	456	Total	C	N	O	S	0	0
			3629	2327	613	671	18		
2	J	456	Total	C	N	O	S	0	0
			3629	2327	613	671	18		
2	N	456	Total	C	N	O	S	0	0
			3629	2327	613	671	18		

- Molecule 3 is a RNA chain called RNA (21-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	21	Total	C	N	O	P	0	0
			442	198	73	150	21		
3	G	21	Total	C	N	O	P	0	0
			442	198	73	150	21		
3	K	21	Total	C	N	O	P	0	0
			442	198	73	150	21		
3	O	21	Total	C	N	O	P	0	0
			442	198	73	150	21		

- Molecule 4 is a DNA chain called DNA (25-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	20	Total 411	C 196	N 80	O 115	P 20	0	0
4	H	20	Total 411	C 196	N 80	O 115	P 20	0	0
4	L	20	Total 411	C 196	N 80	O 115	P 20	0	0
4	P	20	Total 411	C 196	N 80	O 115	P 20	0	0

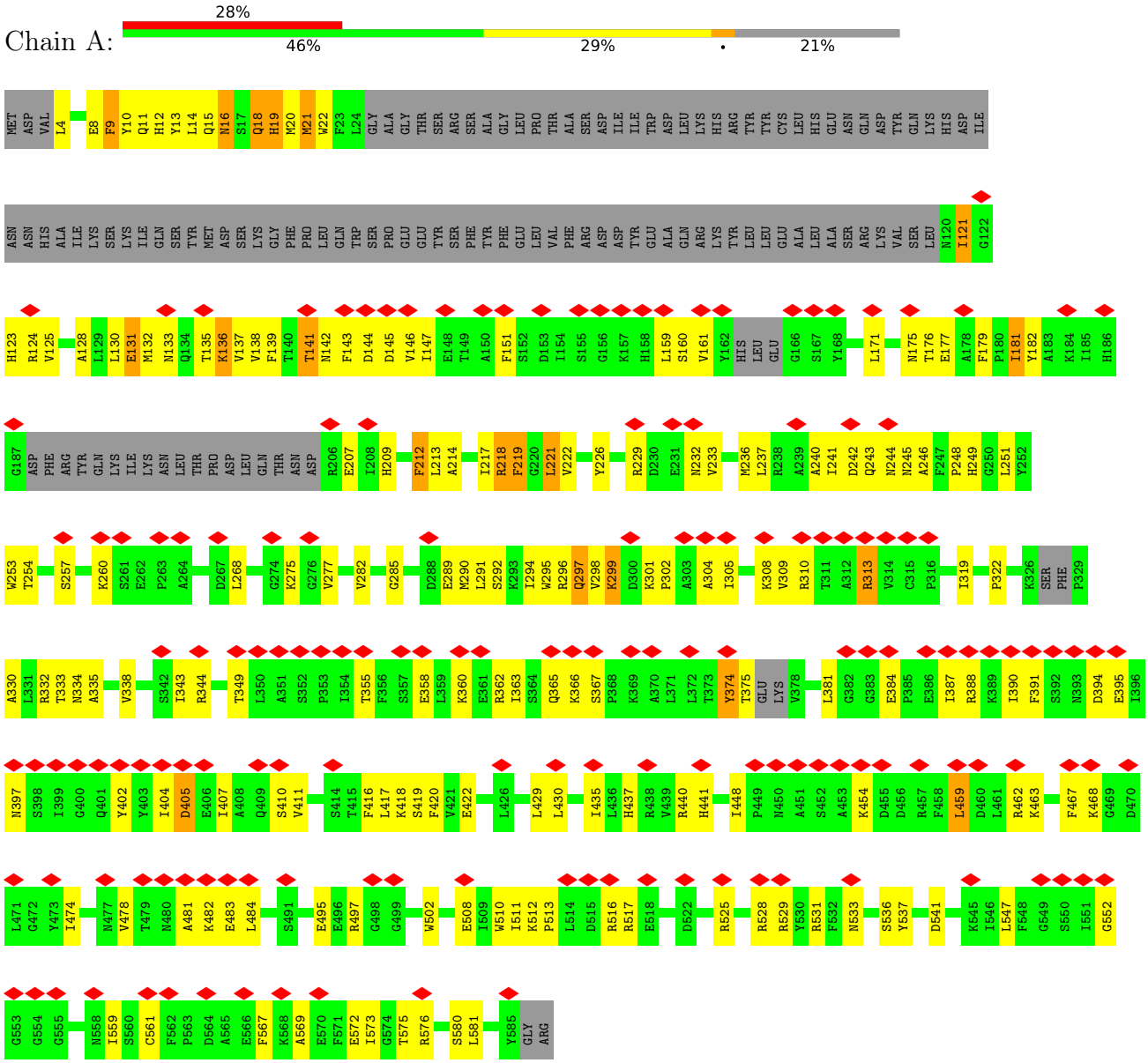
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total 1	Mg 1	0
5	F	1	Total 1	Mg 1	0
5	K	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0

3 Residue-property plots (i)

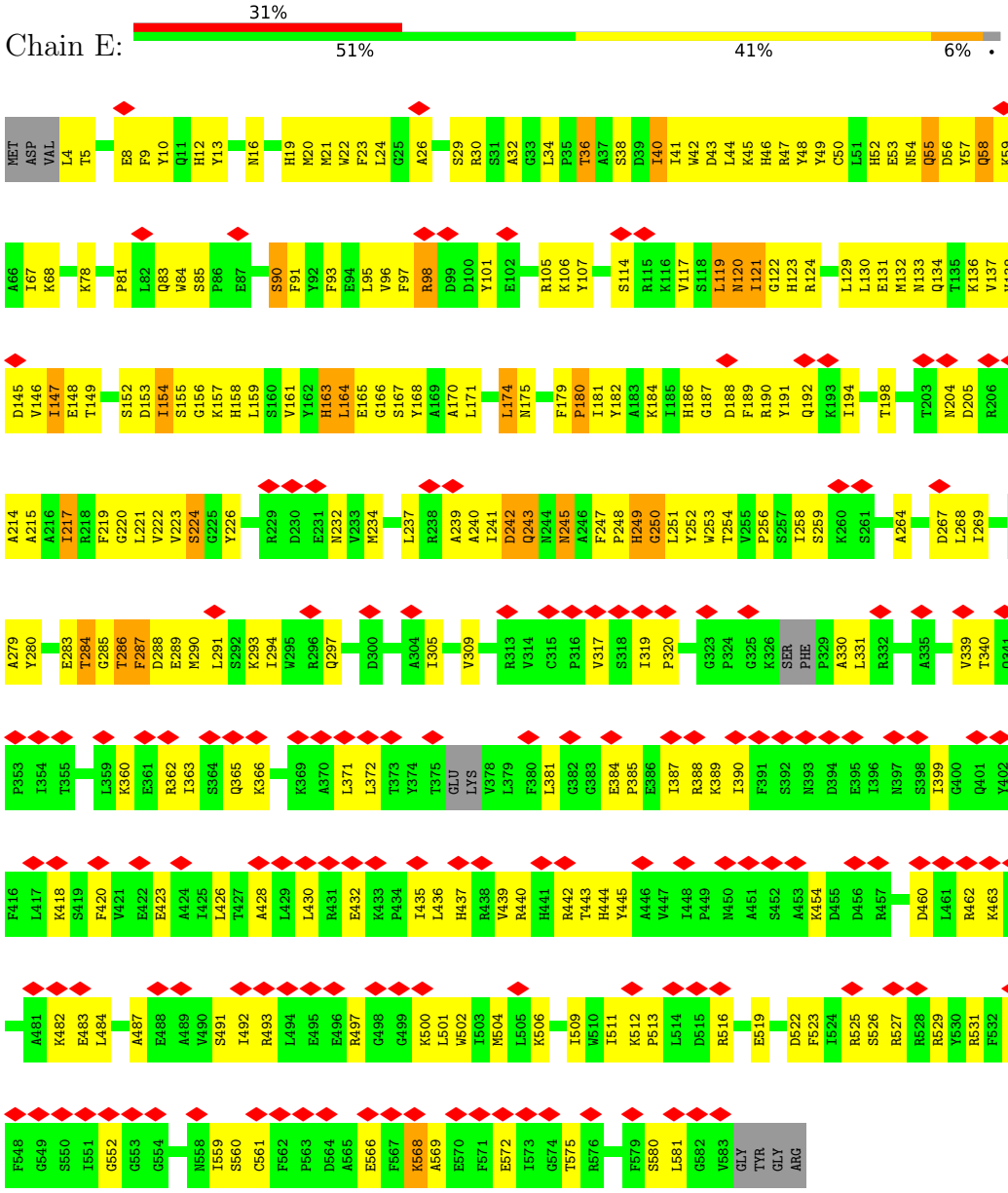
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Sir2 superfamily protein



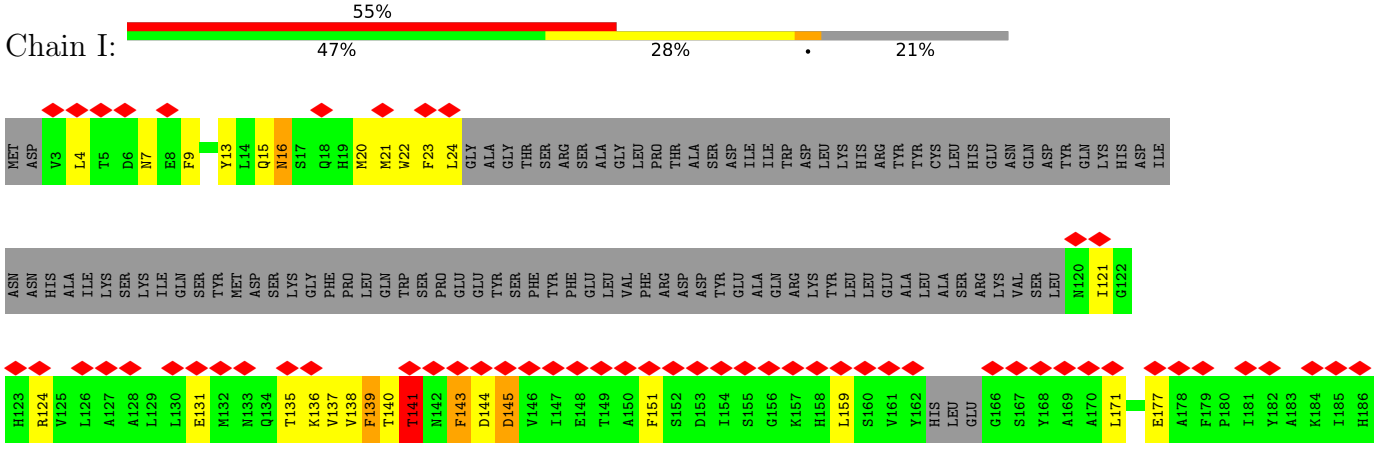
- Molecule 1: Sir2 superfamily protein

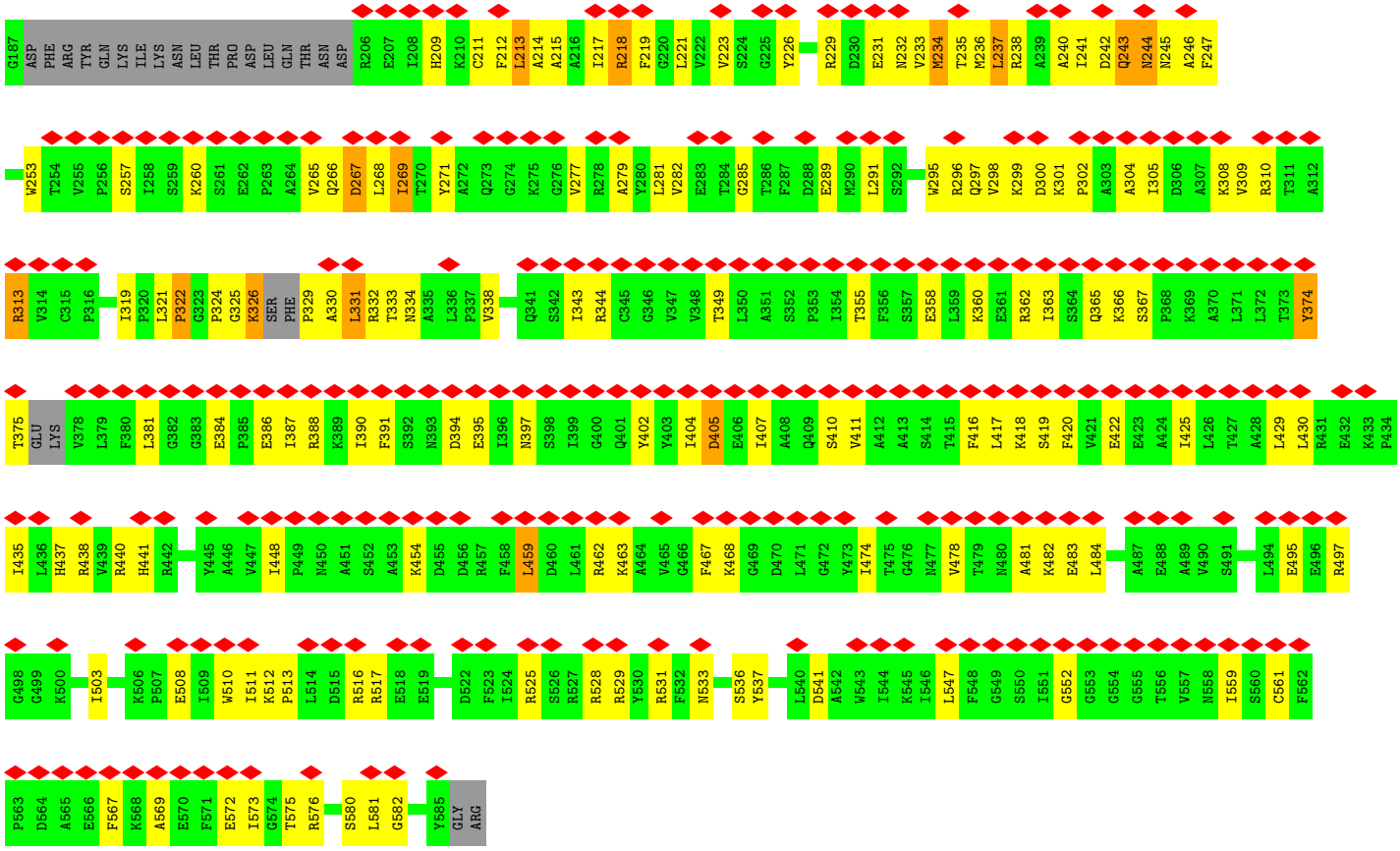
Chain E:



• Molecule 1: Sir2 superfamily protein

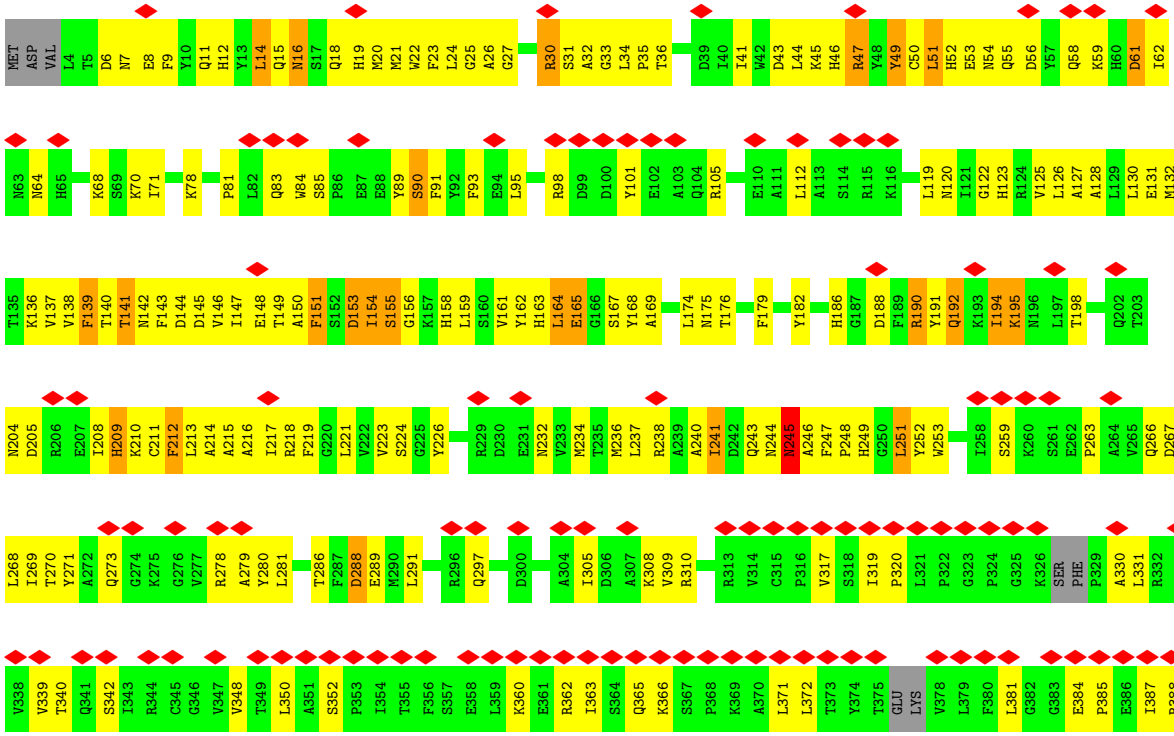
Chain I:





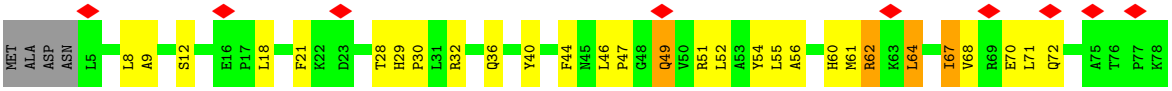
• Molecule 1: Sir2 superfamily protein

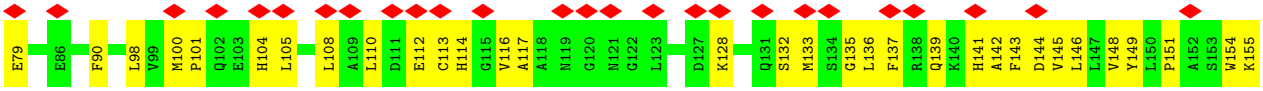
Chain M:

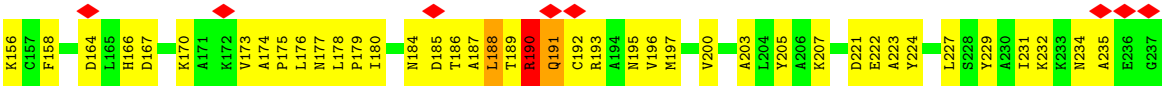


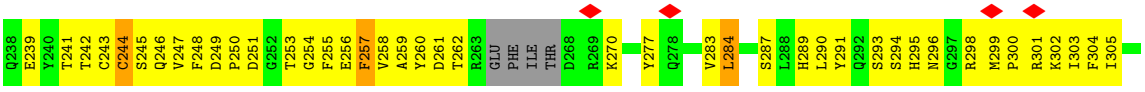
• Molecule 2: Piwi domain protein

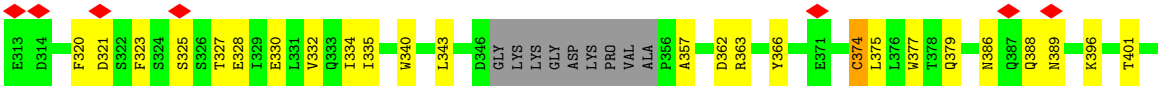
Chain B:

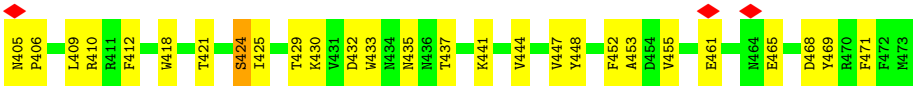






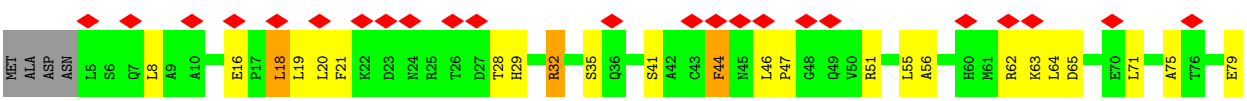


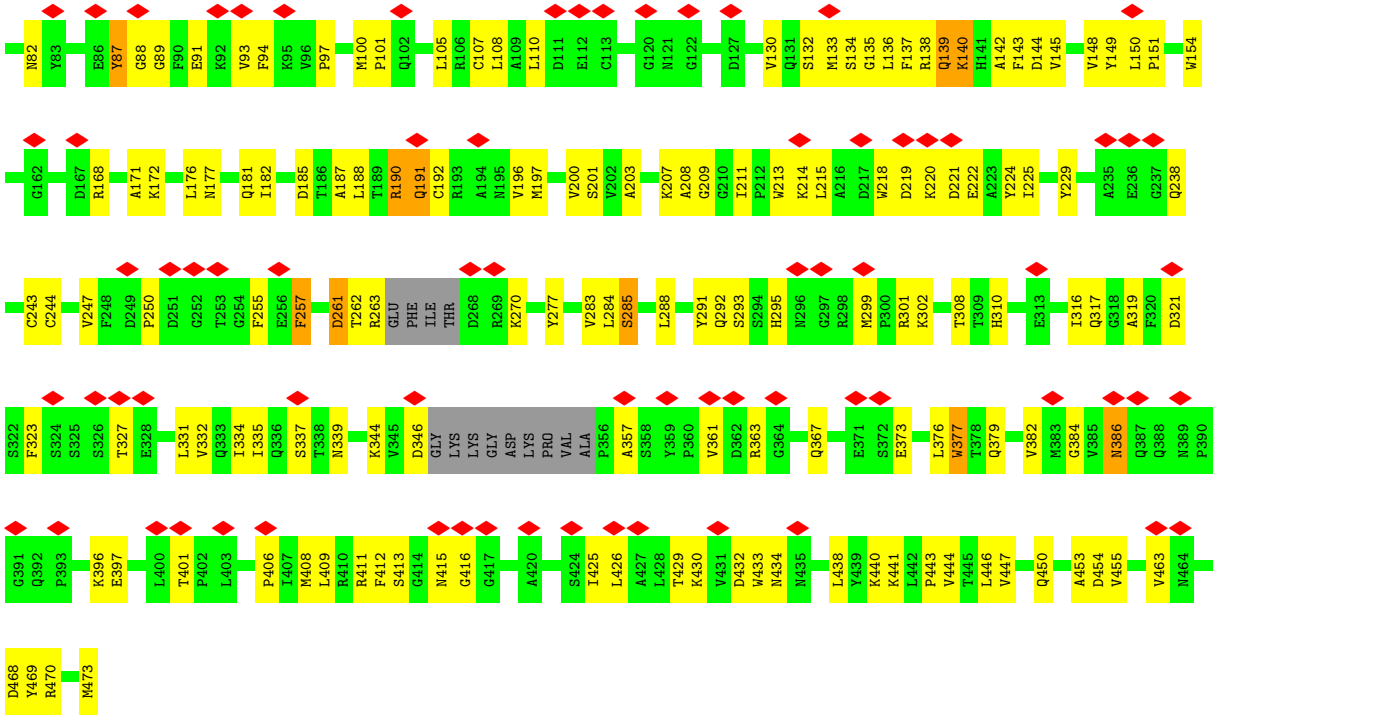




• Molecule 2: Piwi domain protein

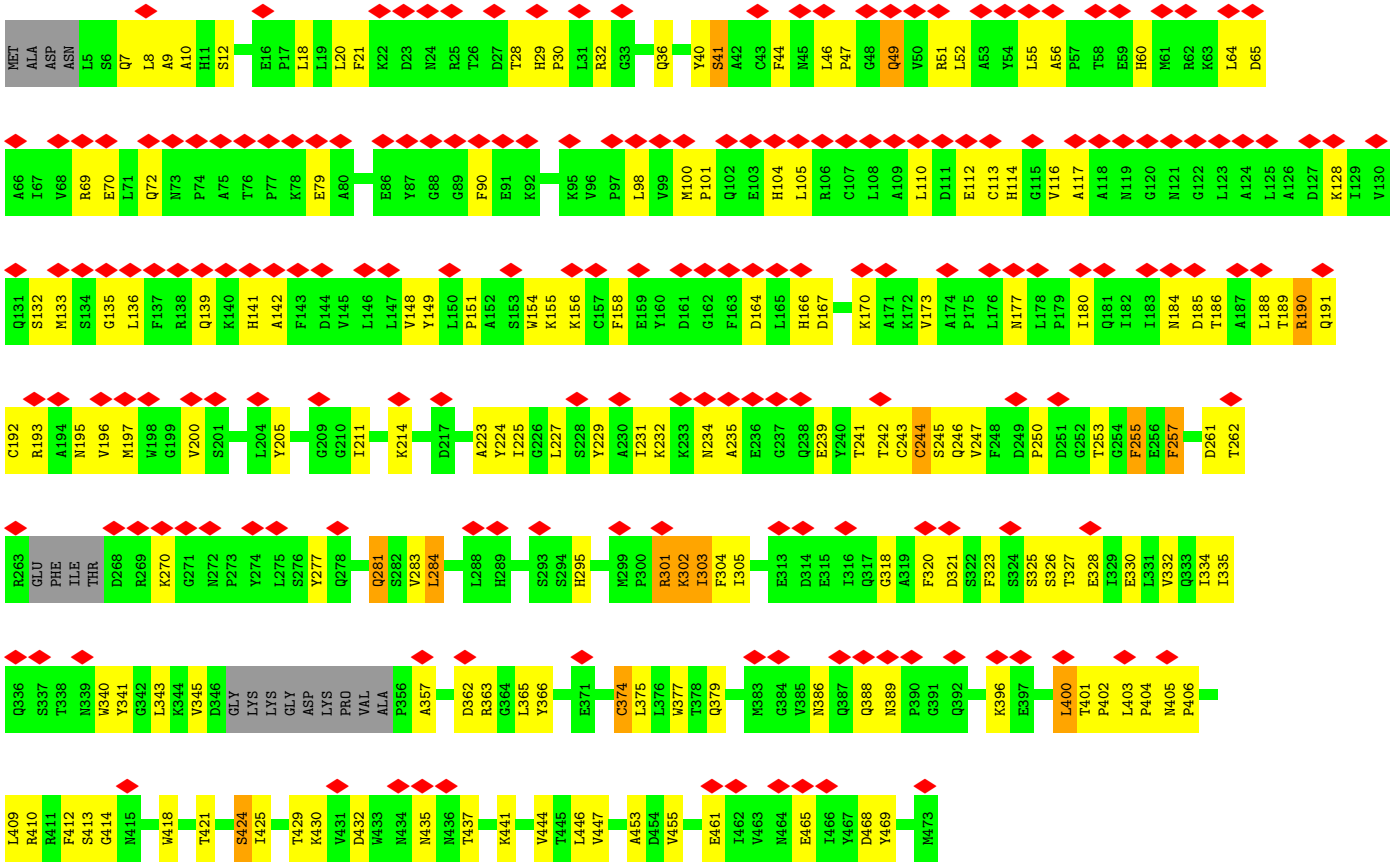
Chain F:





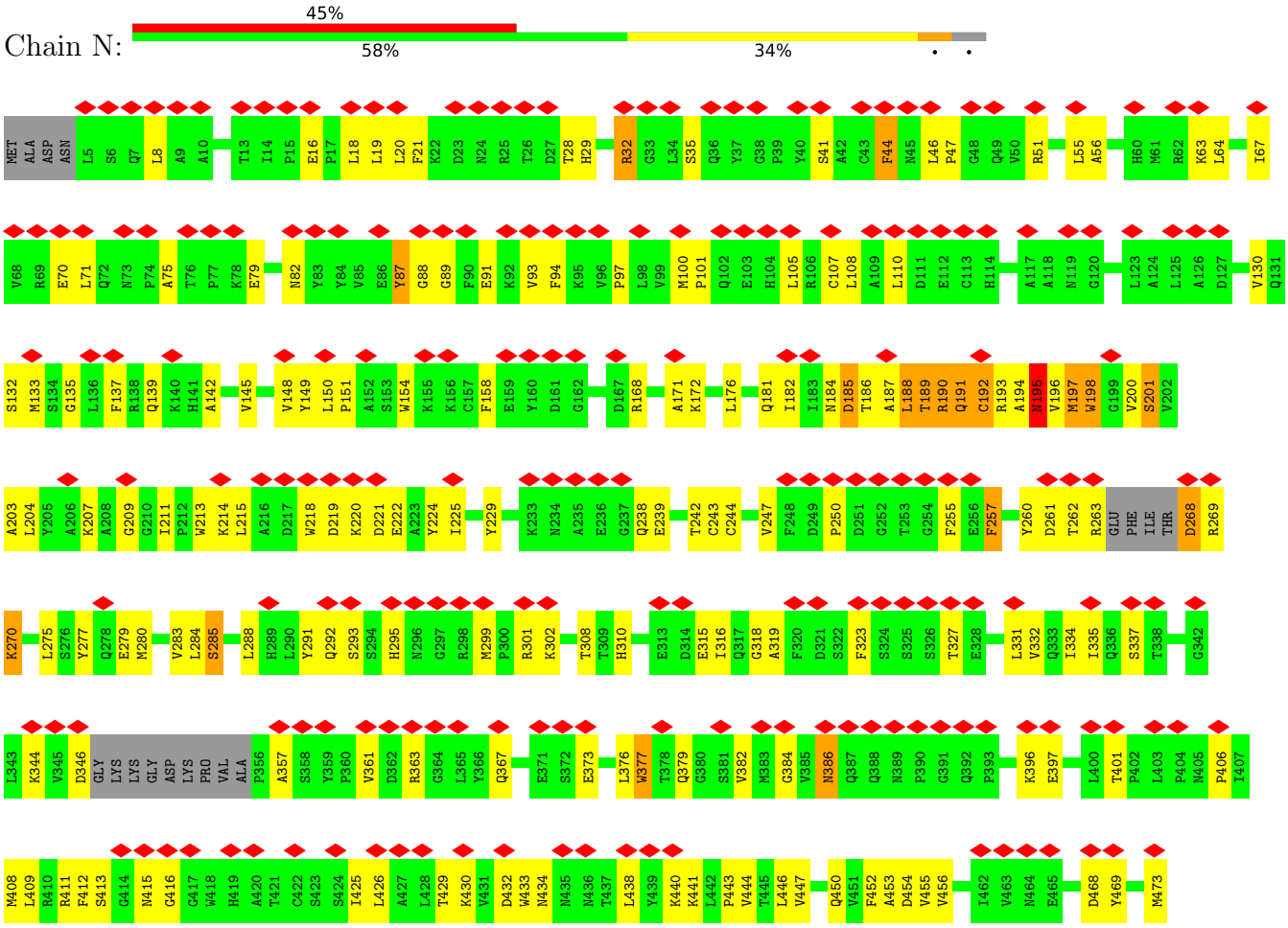
• Molecule 2: Piwi domain protein

Chain J:



• Molecule 2: Piwi domain protein

Chain N:

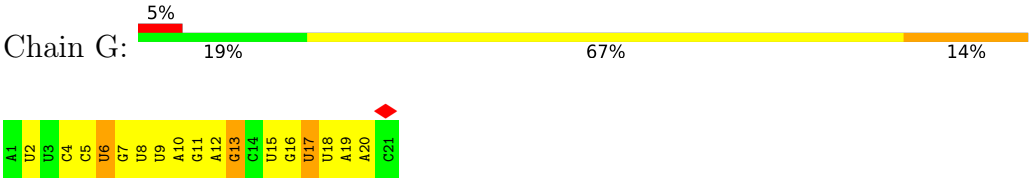


• Molecule 3: RNA (21-mer)

Chain C:

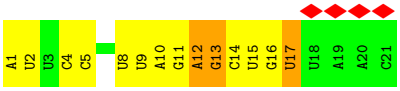
• Molecule 3: RNA (21-mer)

Chain G:



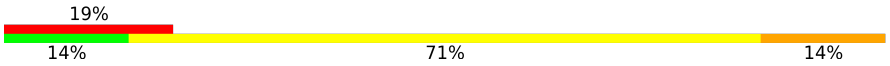
• Molecule 3: RNA (21-mer)

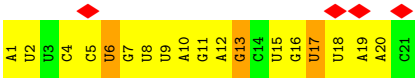
Chain K:



• Molecule 3: RNA (21-mer)

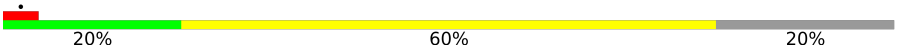
Chain O:

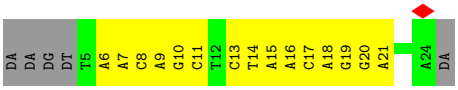




• Molecule 4: DNA (25-mer)

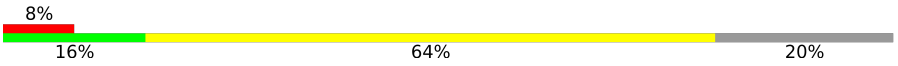
Chain D:





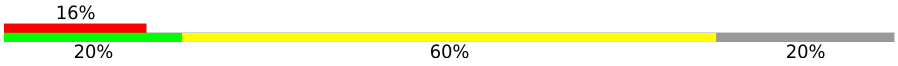
• Molecule 4: DNA (25-mer)

Chain H:



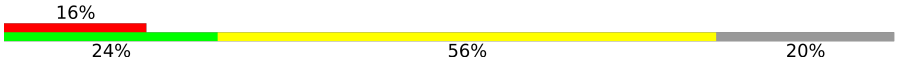
• Molecule 4: DNA (25-mer)

Chain L:



• Molecule 4: DNA (25-mer)

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.002	Depositor
Minimum map value	-1.084	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.375	Depositor
Map size (Å)	380.42, 380.42, 380.42	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/3733	0.54	0/5048
1	E	0.40	0/4719	0.61	2/6386 (0.0%)
1	I	0.31	0/3740	0.55	0/5058
1	M	0.35	0/4719	0.61	1/6386 (0.0%)
2	B	0.33	0/3724	0.53	0/5060
2	F	0.28	0/3724	0.52	0/5060
2	J	0.30	0/3724	0.51	0/5060
2	N	0.33	1/3724 (0.0%)	0.56	2/5060 (0.0%)
3	C	0.29	0/492	0.89	0/763
3	G	0.31	0/492	0.94	0/763
3	K	0.29	0/492	0.89	0/763
3	O	0.31	0/492	0.93	0/763
4	D	0.52	0/462	0.89	0/710
4	H	0.53	0/462	0.88	0/710
4	L	0.52	0/462	0.89	0/710
4	P	0.54	0/462	0.88	0/710
All	All	0.34	1/35623 (0.0%)	0.61	5/49010 (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
2	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	198	TRP	CB-CG	-5.13	1.41	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	213	LEU	CA-CB-CG	-8.02	96.86	115.30
2	N	191	GLN	C-N-CA	-6.33	105.88	121.70
1	M	245	ASN	CB-CA-C	5.93	122.25	110.40
1	E	249	HIS	C-N-CA	-5.19	111.40	122.30
2	N	195	ASN	N-CA-C	-5.19	96.99	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	188	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3655	0	3677	241	0
1	E	4612	0	4595	458	0
1	I	3662	0	3685	245	0
1	M	4612	0	4595	417	0
2	B	3629	0	3564	252	0
2	F	3629	0	3564	180	0
2	J	3629	0	3564	205	0
2	N	3629	0	3564	203	0
3	C	442	0	224	18	0
3	G	442	0	224	21	0
3	K	442	0	224	14	0
3	O	442	0	224	14	0
4	D	411	0	225	15	0
4	H	411	0	225	18	0
4	L	411	0	225	14	0
4	P	411	0	225	16	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34473	0	32604	2113	0

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

All (2113) 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)
1:M:49:TYR:CD2	1:M:71:ILE:HG12	1.32	1.64
1:I:24:LEU:HG	1:I:140:THR:CG2	1.31	1.61
2:B:70:GLU:HG3	2:B:197:MET:CE	1.33	1.57
2:B:250:PRO:HA	2:B:295:HIS:CE1	1.42	1.55
1:E:163:HIS:NE2	1:E:191:TYR:CE2	1.74	1.55
1:E:287:PHE:CE1	1:E:291:LEU:HD11	1.44	1.49
2:F:136:LEU:HB3	2:F:143:PHE:CE2	1.46	1.49
1:I:238:ARG:NH1	1:I:271:TYR:HB3	1.18	1.49
1:E:210:LYS:CD	1:I:244:ASN:ND2	1.74	1.48
1:E:163:HIS:CD2	1:E:191:TYR:CE2	2.00	1.46
1:E:117:VAL:HG21	1:E:146:VAL:CG1	1.44	1.46
1:E:287:PHE:CZ	1:E:291:LEU:HD11	1.51	1.44
1:E:46:HIS:CE1	1:E:57:TYR:CE1	2.07	1.42
2:N:87:TYR:CE2	2:N:197:MET:HB3	1.52	1.41
1:E:46:HIS:CE1	1:E:57:TYR:HE1	1.36	1.40
1:M:21:MET:HE3	1:M:139:PHE:CE1	1.57	1.40
1:M:163:HIS:CD2	1:M:191:TYR:HE2	1.37	1.38
1:E:165:GLU:HG3	1:E:191:TYR:CD1	1.55	1.38
1:E:148:GLU:HG3	1:E:182:TYR:CE2	1.56	1.38
1:M:105:ARG:HD3	1:M:192:GLN:NE2	1.37	1.37
2:B:70:GLU:CG	2:B:197:MET:CE	2.02	1.35
1:I:24:LEU:CG	1:I:140:THR:HG21	1.04	1.34
1:M:49:TYR:CD2	1:M:71:ILE:CG1	2.11	1.33
1:I:137:VAL:HG12	1:I:139:PHE:CE1	1.65	1.32
1:E:114:SER:CB	1:E:145:ASP:OD2	1.77	1.32
1:I:234:MET:SD	1:I:268:LEU:HD12	1.70	1.31
1:E:163:HIS:CD2	1:E:191:TYR:CD2	2.16	1.30
1:M:131:GLU:HG3	1:M:155:SER:OG	1.13	1.30
1:I:137:VAL:HG11	1:I:139:PHE:CZ	1.68	1.28
1:E:192:GLN:HB2	1:M:168:TYR:CZ	1.67	1.27
2:B:250:PRO:CA	2:B:295:HIS:CE1	2.17	1.27
2:B:203:ALA:O	2:B:207:LYS:HG3	1.30	1.27
1:E:163:HIS:HD2	1:E:191:TYR:CD2	1.51	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:330:GLU:OE1	2:J:414:GLY:CA	1.82	1.26
1:M:127:ALA:HB1	1:M:151:PHE:CB	1.64	1.26
1:M:237:LEU:O	1:M:241:ILE:HG12	1.29	1.26
2:N:87:TYR:CD2	2:N:197:MET:HB3	1.70	1.25
1:E:148:GLU:CG	1:E:182:TYR:CE2	2.19	1.25
1:I:23:PHE:HA	1:I:139:PHE:O	1.36	1.25
1:M:49:TYR:HD2	1:M:71:ILE:CG1	1.44	1.25
2:N:262:THR:CG2	2:N:283:VAL:CG2	2.14	1.25
2:N:239:GLU:OE2	2:N:269:ARG:HG2	1.33	1.25
2:J:302:LYS:NZ	2:J:330:GLU:CG	1.98	1.25
1:E:46:HIS:ND1	1:E:57:TYR:HE1	1.34	1.24
1:M:143:PHE:HE2	1:M:194:ILE:CG2	1.48	1.24
1:A:123:HIS:HE1	1:A:144:ASP:OD2	1.16	1.24
1:A:217:ILE:HD13	1:A:245:ASN:O	1.12	1.24
1:I:238:ARG:NH1	1:I:271:TYR:CB	2.01	1.24
1:M:24:LEU:HB2	1:M:140:THR:CG2	1.65	1.24
1:E:168:TYR:OH	1:M:192:GLN:N	1.71	1.23
2:B:249:ASP:O	2:B:295:HIS:NE2	1.72	1.23
1:E:120:ASN:ND2	1:E:288:ASP:OD2	1.72	1.23
1:E:221:LEU:O	1:E:251:LEU:HD12	1.37	1.23
1:M:163:HIS:CD2	1:M:191:TYR:CE2	2.27	1.22
2:N:262:THR:CG2	2:N:283:VAL:HG21	1.67	1.22
2:J:186:THR:HA	2:J:189:THR:OG1	1.37	1.22
1:E:210:LYS:HD3	1:I:244:ASN:ND2	0.89	1.22
1:A:144:ASP:OD1	1:A:146:VAL:HG22	1.38	1.21
1:I:137:VAL:CG1	1:I:139:PHE:CZ	2.22	1.21
1:E:122:GLY:O	1:E:291:LEU:HD13	1.41	1.21
2:J:301:ARG:NH1	1:M:59:LYS:O	1.71	1.21
1:M:127:ALA:CB	1:M:151:PHE:HB2	1.70	1.21
2:F:136:LEU:HB3	2:F:143:PHE:CZ	1.74	1.20
2:J:330:GLU:OE1	2:J:414:GLY:HA3	1.03	1.20
1:E:5:THR:HG22	1:E:8:GLU:CD	1.62	1.20
1:E:221:LEU:CB	1:E:251:LEU:HD13	1.71	1.20
1:E:4:LEU:HD12	1:E:8:GLU:OE1	1.38	1.20
1:E:192:GLN:CB	1:M:168:TYR:OH	1.90	1.19
2:F:261:ASP:OD2	2:F:463:VAL:CG1	1.88	1.19
1:E:148:GLU:CD	1:E:161:VAL:HG11	1.62	1.19
2:F:261:ASP:OD2	2:F:463:VAL:HG12	1.05	1.19
1:E:117:VAL:CG2	1:E:146:VAL:CG1	2.21	1.19
2:N:70:GLU:HB3	2:N:197:MET:CE	1.71	1.19
1:A:217:ILE:CD1	1:A:245:ASN:O	1.89	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:VAL:HG22	1:E:181:ILE:HD11	1.18	1.17
1:M:131:GLU:CG	1:M:155:SER:OG	1.92	1.17
1:I:212:PHE:CD2	1:I:236:MET:SD	2.37	1.17
2:J:302:LYS:HZ3	2:J:330:GLU:CG	1.54	1.17
1:M:127:ALA:HB1	1:M:151:PHE:CA	1.75	1.17
1:M:143:PHE:CE2	1:M:194:ILE:HG22	1.79	1.16
1:E:114:SER:HB3	1:E:145:ASP:OD2	1.00	1.15
1:E:165:GLU:HG3	1:E:191:TYR:CG	1.80	1.15
2:N:239:GLU:CD	2:N:269:ARG:HG2	1.65	1.15
1:I:24:LEU:HB2	1:I:140:THR:HB	1.21	1.15
2:N:280:MET:CE	2:N:315:GLU:HG2	1.76	1.15
1:A:11:GLN:OE1	1:E:96:VAL:HG13	1.45	1.15
1:M:21:MET:CE	1:M:139:PHE:HE1	1.59	1.15
2:B:249:ASP:O	2:B:295:HIS:CE1	2.01	1.14
1:E:287:PHE:CZ	1:E:291:LEU:CD1	2.29	1.14
1:I:212:PHE:CG	1:I:236:MET:SD	2.41	1.14
1:E:156:GLY:O	1:M:153:ASP:HB2	1.48	1.12
1:M:105:ARG:CD	1:M:192:GLN:HE22	1.60	1.13
1:M:127:ALA:HB1	1:M:151:PHE:HB2	1.16	1.12
2:J:223:ALA:CB	2:J:303:ILE:HD11	1.80	1.11
2:B:143:PHE:CZ	2:B:178:LEU:CD1	2.34	1.11
1:E:5:THR:HG23	1:E:8:GLU:CG	1.78	1.11
2:J:185:ASP:HA	2:J:188:LEU:HD21	1.32	1.11
1:M:234:MET:SD	1:M:268:LEU:HD12	1.91	1.11
1:M:252:TYR:HA	1:M:280:TYR:O	1.50	1.11
1:A:123:HIS:CE1	1:A:144:ASP:OD2	2.04	1.10
2:B:143:PHE:HZ	2:B:178:LEU:CD1	1.65	1.10
2:J:223:ALA:O	2:J:303:ILE:CD1	1.99	1.10
1:M:143:PHE:CE2	1:M:194:ILE:CG2	2.34	1.10
1:E:156:GLY:O	1:M:153:ASP:CB	1.99	1.09
1:I:24:LEU:HB2	1:I:140:THR:CB	1.71	1.09
1:M:127:ALA:HB1	1:M:151:PHE:HA	1.34	1.09
2:N:262:THR:HG22	2:N:283:VAL:HG22	1.22	1.09
2:F:136:LEU:CB	2:F:143:PHE:CE2	2.33	1.09
1:I:137:VAL:CG1	1:I:139:PHE:CE1	2.36	1.09
1:M:9:PHE:CE1	1:M:252:TYR:CD2	2.38	1.09
2:B:260:TYR:OH	2:B:287:SER:CB	1.99	1.09
2:N:190:ARG:O	2:N:193:ARG:CG	2.01	1.09
2:N:262:THR:HG22	2:N:283:VAL:CG2	1.80	1.09
2:N:277:TYR:CE1	2:N:318:GLY:HA2	1.88	1.09
2:B:260:TYR:OH	2:B:287:SER:HB2	1.51	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:VAL:CG2	1:E:146:VAL:HG12	1.79	1.08
2:J:302:LYS:HZ3	2:J:330:GLU:HG3	0.94	1.08
1:E:217:ILE:HG21	1:I:217:ILE:HG21	1.36	1.08
2:N:280:MET:HE2	2:N:315:GLU:HG2	1.33	1.08
1:E:5:THR:CG2	1:E:8:GLU:CD	2.21	1.08
2:J:186:THR:CA	2:J:189:THR:OG1	2.00	1.08
1:M:105:ARG:CD	1:M:192:GLN:NE2	2.15	1.08
2:N:190:ARG:O	2:N:193:ARG:HG2	1.53	1.07
1:A:244:ASN:HD21	1:M:213:LEU:HB2	1.18	1.07
2:J:79:GLU:OE1	2:J:190:ARG:NH2	1.87	1.07
1:E:221:LEU:HG	1:E:251:LEU:HD11	1.33	1.07
1:I:330:ALA:HB2	1:I:581:LEU:HA	1.24	1.07
2:N:191:GLN:O	2:N:193:ARG:N	1.86	1.07
2:J:223:ALA:O	2:J:303:ILE:HD12	1.54	1.06
2:J:302:LYS:CE	2:J:330:GLU:HG2	1.83	1.06
2:B:246:GLN:OE1	2:B:287:SER:OG	1.72	1.06
1:M:43:ASP:O	1:M:47:ARG:CG	2.02	1.06
1:E:148:GLU:CD	1:E:161:VAL:CG1	2.25	1.05
1:M:25:GLY:O	1:M:142:ASN:ND2	1.89	1.05
2:B:143:PHE:CZ	2:B:178:LEU:HD11	1.90	1.05
2:B:70:GLU:CG	2:B:197:MET:HE3	1.77	1.04
1:M:21:MET:CE	1:M:139:PHE:CE1	2.35	1.04
2:N:70:GLU:CB	2:N:197:MET:HE3	1.87	1.04
1:A:217:ILE:HG13	1:M:217:ILE:HD13	1.36	1.04
2:J:223:ALA:HB3	2:J:303:ILE:CD1	1.88	1.04
1:M:24:LEU:HB2	1:M:140:THR:HG21	1.38	1.04
1:M:49:TYR:CE2	1:M:71:ILE:HG13	1.91	1.04
1:I:217:ILE:HD12	1:I:245:ASN:O	1.54	1.04
2:J:302:LYS:HE2	2:J:330:GLU:HG2	1.38	1.04
2:N:262:THR:HB	2:N:283:VAL:CG2	1.86	1.04
2:J:40:TYR:HE2	2:J:214:LYS:HD3	1.22	1.04
2:J:190:ARG:HB3	2:J:190:ARG:HH11	1.18	1.03
1:M:24:LEU:CB	1:M:140:THR:CG2	2.36	1.03
1:E:287:PHE:CE1	1:E:291:LEU:CD1	2.40	1.03
1:A:244:ASN:ND2	1:M:213:LEU:HB2	1.74	1.03
2:N:67:ILE:CD1	2:N:187:ALA:HB1	1.88	1.03
1:E:192:GLN:HB2	1:M:168:TYR:OH	1.51	1.03
1:E:5:THR:HG23	1:E:8:GLU:HG3	1.07	1.03
1:E:221:LEU:HB3	1:E:251:LEU:HD13	1.04	1.03
1:A:11:GLN:OE1	1:E:96:VAL:CG1	2.07	1.02
2:B:251:ASP:OD1	2:B:298:ARG:NH2	1.90	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:ASP:OD2	1:E:190:ARG:NH2	1.91	1.02
1:E:21:MET:HE3	1:E:139:PHE:CE1	1.92	1.02
1:I:267:ASP:O	1:I:271:TYR:CD2	2.11	1.02
1:A:12:HIS:HE1	1:A:20:MET:HE1	1.20	1.02
2:B:61:MET:HE3	2:B:108:LEU:CD2	1.88	1.02
2:J:302:LYS:NZ	2:J:330:GLU:HG2	1.73	1.02
2:B:259:ALA:HB2	2:B:448:TYR:CE2	1.94	1.01
1:M:43:ASP:O	1:M:47:ARG:HG2	1.59	1.01
1:A:144:ASP:O	1:A:146:VAL:N	1.90	1.01
1:E:131:GLU:HG3	1:E:155:SER:OG	1.61	1.01
2:F:63:LYS:HB3	2:F:188:LEU:HD11	1.41	1.01
1:E:119:LEU:HD22	1:E:119:LEU:H	1.21	1.01
2:N:67:ILE:HD12	2:N:187:ALA:HB1	1.39	1.01
2:N:262:THR:HG21	2:N:283:VAL:HG21	1.35	1.01
2:B:250:PRO:HA	2:B:295:HIS:ND1	1.75	1.01
1:E:158:HIS:CD2	1:M:148:GLU:HB3	1.96	1.01
2:J:401:THR:OG1	2:J:402:PRO:HD2	1.57	1.01
1:M:9:PHE:HE1	1:M:252:TYR:HD2	1.05	1.01
1:E:5:THR:CG2	1:E:8:GLU:HG3	1.90	1.00
1:M:24:LEU:H	1:M:140:THR:HG22	1.24	1.00
2:N:262:THR:CB	2:N:283:VAL:CG2	2.40	1.00
1:M:163:HIS:CG	1:M:191:TYR:HE2	1.78	1.00
1:A:4:LEU:O	1:A:282:VAL:HG12	1.62	1.00
1:E:192:GLN:N	1:M:168:TYR:OH	1.94	1.00
1:E:137:VAL:HG11	1:E:139:PHE:CZ	1.96	0.99
1:A:121:ILE:H	1:A:121:ILE:HD12	1.28	0.99
1:A:301:LYS:HE2	1:E:58:GLN:CD	1.82	0.99
1:I:24:LEU:CB	1:I:140:THR:HB	1.83	0.99
1:E:13:TYR:OH	1:E:129:LEU:CD1	2.11	0.98
2:N:87:TYR:CE2	2:N:197:MET:CB	2.45	0.98
2:B:188:LEU:HA	2:B:193:ARG:HH12	1.27	0.98
1:M:9:PHE:HE1	1:M:252:TYR:CD2	1.77	0.98
2:B:249:ASP:C	2:B:295:HIS:CE1	2.37	0.98
1:E:137:VAL:CG2	1:E:181:ILE:HD11	1.93	0.98
1:E:217:ILE:HD13	1:I:217:ILE:HG21	1.45	0.98
1:I:24:LEU:CB	1:I:140:THR:CB	2.28	0.98
1:E:114:SER:HB3	1:E:145:ASP:CG	1.83	0.98
1:E:117:VAL:HG21	1:E:146:VAL:HG12	1.00	0.98
1:M:131:GLU:HB2	1:M:151:PHE:CE2	1.99	0.98
1:A:221:LEU:CD2	1:A:251:LEU:CD1	2.42	0.97
1:E:137:VAL:HG22	1:E:181:ILE:CD1	1.93	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:LEU:HD23	1:M:147:ILE:HD12	1.44	0.97
1:M:237:LEU:O	1:M:241:ILE:CG1	2.12	0.97
1:A:124:ARG:HG2	1:A:309:VAL:HG12	1.47	0.97
1:A:137:VAL:HG22	1:A:181:ILE:HG12	1.44	0.97
1:E:156:GLY:O	1:M:153:ASP:CA	2.13	0.97
1:M:49:TYR:CE2	1:M:71:ILE:CG1	2.44	0.97
1:E:5:THR:CG2	1:E:8:GLU:CG	2.43	0.97
1:I:267:ASP:O	1:I:271:TYR:HD2	1.46	0.97
1:M:24:LEU:N	1:M:140:THR:HG22	1.80	0.96
2:J:401:THR:OG1	2:J:402:PRO:CD	2.13	0.96
2:N:280:MET:CE	2:N:315:GLU:CG	2.42	0.96
1:E:148:GLU:OE2	1:E:161:VAL:CG1	2.13	0.96
1:E:148:GLU:OE2	1:E:182:TYR:CD2	2.19	0.96
2:N:277:TYR:HE1	2:N:318:GLY:HA2	1.24	0.96
1:E:221:LEU:HG	1:E:251:LEU:CD1	1.96	0.96
1:M:226:TYR:HD2	1:M:253:TRP:CH2	1.83	0.96
1:E:42:TRP:HB3	1:E:62:ILE:HD11	1.46	0.96
1:M:145:ASP:HB2	1:M:148:GLU:HB2	1.45	0.95
1:I:330:ALA:CB	1:I:581:LEU:HA	1.95	0.95
2:N:262:THR:CG2	2:N:283:VAL:HG22	1.86	0.95
1:E:46:HIS:ND1	1:E:57:TYR:CE1	2.25	0.95
1:E:222:VAL:HG22	1:E:252:TYR:HD2	1.29	0.95
1:I:217:ILE:CD1	1:I:245:ASN:HB3	1.96	0.95
1:M:126:LEU:HD23	1:M:147:ILE:CD1	1.97	0.95
2:B:143:PHE:CE2	2:B:178:LEU:HD11	2.02	0.94
1:M:21:MET:HE3	1:M:139:PHE:HE1	0.78	0.94
1:E:217:ILE:HG21	1:I:217:ILE:CG2	1.97	0.94
2:J:185:ASP:O	2:J:189:THR:HG23	1.66	0.94
1:A:22:TRP:HD1	1:A:135:THR:OG1	1.49	0.94
1:E:148:GLU:CG	1:E:182:TYR:CD2	2.51	0.94
2:J:302:LYS:NZ	2:J:330:GLU:HG3	1.70	0.94
1:E:148:GLU:CG	1:E:182:TYR:HE2	1.66	0.94
1:M:24:LEU:CB	1:M:140:THR:HG22	1.97	0.94
1:E:170:ALA:HB1	1:E:211:CYS:SG	2.08	0.94
1:A:213:LEU:CD1	1:A:240:ALA:HA	1.98	0.94
1:I:21:MET:CG	1:I:139:PHE:HE1	1.79	0.94
2:B:189:THR:O	2:B:191:GLN:N	2.00	0.93
1:A:221:LEU:HD22	1:A:251:LEU:HD13	1.49	0.93
2:J:223:ALA:HB3	2:J:303:ILE:HD11	0.94	0.93
2:B:203:ALA:O	2:B:207:LYS:CG	2.14	0.93
1:A:12:HIS:HE1	1:A:20:MET:CE	1.81	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:PHE:CD1	1:M:252:TYR:CD2	2.55	0.93
1:M:119:LEU:HG	1:M:150:ALA:HB2	1.50	0.93
2:B:145:VAL:HA	2:B:179:PRO:HG2	1.47	0.93
1:M:192:GLN:HA	1:M:192:GLN:HE21	1.34	0.93
2:F:149:TYR:HE2	2:F:188:LEU:HD12	1.29	0.93
1:A:175:ASN:HD21	1:M:245:ASN:HD22	1.07	0.92
1:E:156:GLY:CA	1:M:153:ASP:HA	2.00	0.92
2:B:190:ARG:O	2:B:192:CYS:N	2.02	0.92
2:N:87:TYR:HE2	2:N:197:MET:HB3	1.14	0.92
1:M:226:TYR:CD2	1:M:253:TRP:CH2	2.58	0.92
2:J:188:LEU:HD23	2:J:188:LEU:H	1.32	0.92
2:N:70:GLU:HB3	2:N:197:MET:HE2	1.48	0.92
1:A:125:VAL:CG1	1:A:291:LEU:HB3	1.99	0.92
1:M:128:ALA:HB2	1:M:154:ILE:HD11	1.51	0.92
2:B:258:VAL:HG11	2:B:290:LEU:HD11	1.51	0.91
1:E:222:VAL:HG22	1:E:252:TYR:CD2	2.04	0.91
1:I:21:MET:CG	1:I:139:PHE:CE1	2.53	0.91
2:N:70:GLU:CB	2:N:197:MET:CE	2.44	0.91
1:E:120:ASN:CG	1:E:288:ASP:OD2	2.07	0.91
2:J:341:TYR:CD2	2:J:403:LEU:HD23	2.05	0.91
1:M:105:ARG:HD3	1:M:192:GLN:HE21	1.25	0.91
2:N:87:TYR:CD2	2:N:197:MET:CB	2.54	0.91
1:M:49:TYR:HE2	1:M:71:ILE:HG13	1.32	0.91
1:M:27:GLY:O	1:M:30:ARG:HB3	1.70	0.91
1:A:125:VAL:CG2	1:A:295:TRP:HB2	2.00	0.91
2:B:70:GLU:CG	2:B:197:MET:HE2	1.99	0.91
1:E:237:LEU:O	1:E:241:ILE:HD13	1.69	0.91
2:B:62:ARG:HG2	2:B:62:ARG:HH11	1.33	0.91
1:M:43:ASP:O	1:M:47:ARG:HG3	1.71	0.91
2:B:246:GLN:HG3	2:B:287:SER:OG	1.69	0.90
1:E:210:LYS:CD	1:I:244:ASN:HD21	1.54	0.90
1:I:448:ILE:HD13	1:I:474:ILE:HD12	1.54	0.90
2:B:250:PRO:HD2	2:B:254:GLY:O	1.71	0.90
1:M:148:GLU:CD	1:M:161:VAL:HG11	1.91	0.90
2:B:70:GLU:HG2	2:B:197:MET:CE	1.98	0.90
2:B:249:ASP:C	2:B:295:HIS:HE1	1.73	0.90
1:A:221:LEU:CD2	1:A:251:LEU:HD13	2.00	0.90
2:N:280:MET:HE3	2:N:315:GLU:CG	2.02	0.90
2:B:67:ILE:HD11	2:B:193:ARG:NH2	1.87	0.89
2:B:246:GLN:OE1	2:B:287:SER:O	1.90	0.89
2:B:260:TYR:OH	2:B:287:SER:OG	1.91	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG11	1:A:291:LEU:HB3	1.53	0.89
2:B:61:MET:CE	2:B:108:LEU:CD2	2.50	0.89
1:M:123:HIS:CE1	1:M:146:VAL:HG11	2.07	0.89
1:M:127:ALA:CB	1:M:151:PHE:CA	2.50	0.89
1:A:124:ARG:CG	1:A:309:VAL:HG12	2.03	0.89
1:E:163:HIS:NE2	1:E:191:TYR:HE2	1.62	0.89
2:B:143:PHE:HZ	2:B:178:LEU:HD13	1.37	0.89
1:E:146:VAL:O	1:E:149:THR:N	2.06	0.89
1:E:210:LYS:CG	1:I:244:ASN:HD21	1.85	0.89
1:E:10:TYR:CE2	1:E:293:LYS:HD3	2.08	0.88
1:A:448:ILE:HD13	1:A:474:ILE:HD12	1.54	0.88
1:I:24:LEU:CG	1:I:140:THR:CG2	2.00	0.88
2:N:93:VAL:HG21	2:N:198:TRP:CH2	2.09	0.88
1:E:21:MET:HE3	1:E:139:PHE:HE1	1.33	0.88
2:N:197:MET:O	2:N:201:SER:HB3	1.73	0.88
1:E:165:GLU:CG	1:E:191:TYR:CD1	2.51	0.88
1:M:127:ALA:CB	1:M:151:PHE:CB	2.42	0.88
1:E:5:THR:HG22	1:E:8:GLU:OE1	1.71	0.88
1:M:119:LEU:HD21	1:M:149:THR:CG2	2.04	0.88
2:B:296:ASN:ND2	2:F:470:ARG:CZ	2.37	0.88
2:J:185:ASP:CA	2:J:188:LEU:HD21	2.04	0.88
1:M:127:ALA:CB	1:M:151:PHE:HA	2.03	0.87
2:N:70:GLU:HB2	2:N:197:MET:HE3	1.55	0.87
2:B:144:ASP:O	2:B:179:PRO:HG3	1.73	0.87
1:M:16:ASN:O	1:M:16:ASN:ND2	2.08	0.87
2:N:262:THR:CB	2:N:283:VAL:HG21	2.00	0.87
1:E:221:LEU:CB	1:E:251:LEU:CD1	2.51	0.87
1:E:13:TYR:OH	1:E:129:LEU:HD13	1.74	0.87
1:E:163:HIS:NE2	1:E:191:TYR:CZ	2.12	0.87
2:N:239:GLU:OE2	2:N:269:ARG:CG	2.20	0.87
1:E:161:VAL:HG12	1:E:182:TYR:HD2	1.40	0.87
1:E:210:LYS:CD	1:I:244:ASN:HD22	1.62	0.87
2:F:136:LEU:CB	2:F:143:PHE:CZ	2.57	0.87
2:N:190:ARG:O	2:N:193:ARG:HG3	1.74	0.87
1:I:16:ASN:O	1:I:16:ASN:ND2	2.07	0.86
1:I:234:MET:SD	1:I:268:LEU:CD1	2.59	0.86
1:M:148:GLU:HG2	1:M:161:VAL:HG11	1.54	0.86
2:N:277:TYR:CE1	2:N:318:GLY:CA	2.58	0.86
1:E:46:HIS:CE1	1:E:57:TYR:CD1	2.62	0.86
1:E:117:VAL:HG21	1:E:146:VAL:HG13	1.57	0.86
1:E:226:TYR:HD2	1:E:253:TRP:CZ2	1.93	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:ILE:HD11	1:I:245:ASN:HB3	1.55	0.86
2:B:46:LEU:HD22	2:F:137:PHE:CE2	2.11	0.86
1:E:146:VAL:O	1:E:147:ILE:C	2.12	0.86
2:F:136:LEU:HB3	2:F:143:PHE:HE2	1.40	0.86
1:A:16:ASN:HD21	1:A:20:MET:CE	1.88	0.86
1:M:248:PRO:O	1:M:278:ARG:NH1	2.08	0.86
2:F:221:ASP:HB3	2:F:301:ARG:HG2	1.58	0.86
1:A:14:LEU:HD11	1:A:297:GLN:HB2	1.56	0.86
1:A:16:ASN:ND2	1:A:16:ASN:O	2.07	0.86
2:J:190:ARG:HB3	2:J:190:ARG:NH1	1.89	0.86
1:I:330:ALA:HB1	1:I:580:SER:O	1.74	0.85
2:J:302:LYS:HZ1	2:J:330:GLU:CG	1.88	0.85
1:E:148:GLU:HG3	1:E:182:TYR:HE2	1.06	0.85
1:I:212:PHE:CD2	1:I:236:MET:CG	2.59	0.85
1:M:119:LEU:HD21	1:M:149:THR:HG21	1.58	0.85
2:B:70:GLU:CG	2:B:197:MET:HE1	2.04	0.85
1:A:301:LYS:HE2	1:E:58:GLN:NE2	1.91	0.85
1:I:234:MET:HA	1:I:234:MET:CE	2.04	0.85
1:E:137:VAL:CG1	1:E:139:PHE:CZ	2.59	0.85
2:B:250:PRO:N	2:B:295:HIS:HE1	1.75	0.85
1:M:148:GLU:CG	1:M:161:VAL:HG11	2.06	0.85
1:M:51:LEU:HD12	1:M:51:LEU:O	1.76	0.84
1:I:238:ARG:HH12	1:I:271:TYR:HB3	1.02	0.84
2:N:63:LYS:HB3	2:N:188:LEU:CD2	2.07	0.84
2:N:87:TYR:HE2	2:N:197:MET:CB	1.88	0.84
1:M:14:LEU:HD12	1:M:14:LEU:O	1.77	0.84
1:A:125:VAL:CG2	1:A:295:TRP:CB	2.55	0.84
1:E:44:LEU:HD21	1:E:107:TYR:CE2	2.12	0.84
1:E:148:GLU:OE2	1:E:161:VAL:HG12	1.77	0.84
1:E:165:GLU:CG	1:E:191:TYR:CG	2.59	0.84
2:F:149:TYR:CE2	2:F:188:LEU:HD12	2.12	0.84
1:A:125:VAL:HG21	1:A:295:TRP:CB	2.08	0.84
1:E:221:LEU:C	1:E:251:LEU:HD12	1.98	0.84
2:J:184:ASN:O	2:J:188:LEU:CD2	2.25	0.84
1:M:163:HIS:CG	1:M:191:TYR:CE2	2.59	0.84
2:B:46:LEU:HD21	2:F:176:LEU:HD11	1.57	0.84
1:E:56:ASP:OD1	1:E:58:GLN:NE2	2.10	0.84
2:B:40:TYR:OH	2:B:253:THR:HB	1.77	0.84
2:B:246:GLN:CG	2:B:287:SER:OG	2.26	0.84
1:E:122:GLY:O	1:E:291:LEU:CD1	2.25	0.84
2:B:250:PRO:HB3	2:B:294:SER:OG	1.77	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PRO:N	2:B:295:HIS:CE1	2.46	0.83
1:M:148:GLU:OE2	1:M:161:VAL:HG11	1.77	0.83
2:B:246:GLN:CD	2:B:287:SER:HG	1.82	0.83
2:N:67:ILE:HD12	2:N:187:ALA:CB	2.07	0.83
1:A:144:ASP:OD1	1:A:146:VAL:CG2	2.25	0.83
1:I:330:ALA:HB2	1:I:581:LEU:CA	2.07	0.83
1:M:24:LEU:CB	1:M:140:THR:HG21	2.04	0.83
1:A:22:TRP:CD1	1:A:135:THR:OG1	2.28	0.83
1:A:175:ASN:ND2	1:M:245:ASN:HD22	1.75	0.82
1:M:131:GLU:HB2	1:M:151:PHE:HE2	1.42	0.82
1:A:301:LYS:HE2	1:E:58:GLN:OE1	1.77	0.82
2:N:190:ARG:NE	2:N:190:ARG:HA	1.95	0.82
2:J:41:SER:OG	2:J:211:ILE:N	2.10	0.82
1:M:105:ARG:NE	1:M:192:GLN:HE22	1.75	0.82
2:F:140:LYS:HZ3	2:F:140:LYS:HB2	1.43	0.82
1:A:213:LEU:HD13	1:A:240:ALA:HA	1.61	0.82
1:I:238:ARG:HH12	1:I:271:TYR:CB	1.76	0.82
1:A:136:LYS:HG2	1:A:179:PHE:CD2	2.14	0.82
1:E:148:GLU:CD	1:E:182:TYR:CE2	2.51	0.82
1:E:171:LEU:O	1:E:171:LEU:HD12	1.80	0.82
1:E:226:TYR:HD2	1:E:253:TRP:HZ2	1.21	0.82
1:I:21:MET:HG2	1:I:139:PHE:CE1	2.13	0.82
2:N:221:ASP:HB3	2:N:301:ARG:HG2	1.58	0.82
2:B:258:VAL:HG21	2:B:290:LEU:CD1	2.10	0.82
1:E:165:GLU:CG	1:E:191:TYR:HB3	2.10	0.82
2:J:304:PHE:CE1	2:J:421:THR:HG22	2.14	0.82
1:A:161:VAL:HG12	1:A:182:TYR:HD2	1.43	0.82
2:J:302:LYS:HZ1	2:J:330:GLU:CD	1.83	0.82
2:J:185:ASP:HA	2:J:188:LEU:CD2	2.09	0.81
2:N:277:TYR:HE1	2:N:318:GLY:CA	1.93	0.81
1:E:148:GLU:HG2	1:E:182:TYR:CD2	2.14	0.81
1:E:190:ARG:NH1	1:E:191:TYR:CE2	2.48	0.81
1:M:137:VAL:HG11	1:M:139:PHE:CZ	2.14	0.81
2:J:44:PHE:CZ	2:J:253:THR:OG1	2.31	0.81
2:J:250:PRO:HD2	2:J:255:PHE:HA	1.62	0.81
1:E:146:VAL:O	1:E:148:GLU:N	2.13	0.81
2:F:136:LEU:CA	2:F:143:PHE:HE2	1.93	0.81
2:F:140:LYS:HB2	2:F:140:LYS:NZ	1.95	0.81
1:M:127:ALA:O	1:M:151:PHE:HD2	1.63	0.81
2:N:263:ARG:NH1	2:N:268:ASP:O	2.12	0.81
1:A:12:HIS:CE1	1:A:20:MET:HE1	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:GLN:HB3	2:F:142:ALA:HB3	1.63	0.81
2:N:93:VAL:HG21	2:N:198:TRP:HH2	1.44	0.81
1:E:175:ASN:HD21	1:I:245:ASN:HD21	1.28	0.81
1:A:137:VAL:HG22	1:A:181:ILE:CG1	2.10	0.81
1:E:13:TYR:CE1	1:E:294:ILE:HG23	2.15	0.81
1:E:156:GLY:HA2	1:M:153:ASP:HA	1.61	0.81
1:E:221:LEU:CG	1:E:251:LEU:CD1	2.58	0.81
1:I:214:ALA:O	1:I:217:ILE:HG22	1.81	0.81
1:A:12:HIS:CE1	1:A:20:MET:CE	2.64	0.81
1:M:32:ALA:CB	1:M:146:VAL:HG21	2.10	0.81
1:M:148:GLU:HG2	1:M:161:VAL:CG1	2.11	0.81
2:B:70:GLU:HG3	2:B:197:MET:HE3	0.81	0.80
1:I:24:LEU:HG	1:I:140:THR:HG23	1.62	0.80
1:M:143:PHE:HE2	1:M:194:ILE:HG21	1.45	0.80
1:E:21:MET:CE	1:E:139:PHE:CE1	2.65	0.80
1:A:221:LEU:HD23	1:A:221:LEU:O	1.81	0.80
2:B:144:ASP:O	2:B:179:PRO:CG	2.29	0.80
2:B:46:LEU:HD22	2:F:137:PHE:CZ	2.15	0.80
1:I:137:VAL:HG11	1:I:139:PHE:HZ	1.37	0.80
1:E:154:ILE:HD11	1:E:309:VAL:HG22	1.63	0.80
1:E:221:LEU:O	1:E:251:LEU:CD1	2.25	0.80
1:M:24:LEU:HB2	1:M:140:THR:HG22	1.57	0.80
1:M:24:LEU:HD11	1:M:126:LEU:HD22	1.63	0.80
1:M:131:GLU:CB	1:M:155:SER:OG	2.30	0.80
2:B:190:ARG:HD3	3:C:2:U:O4	1.82	0.80
1:E:10:TYR:HE1	1:E:294:ILE:HG13	1.47	0.80
1:M:126:LEU:CD2	1:M:147:ILE:HD12	2.12	0.80
1:E:154:ILE:CD1	1:E:309:VAL:HG22	2.12	0.79
1:I:240:ALA:O	1:I:243:GLN:HG3	1.83	0.79
2:B:259:ALA:HB2	2:B:448:TYR:CZ	2.17	0.79
1:E:440:ARG:HB3	1:E:445:TYR:HE2	1.44	0.79
2:N:67:ILE:CD1	2:N:187:ALA:CB	2.61	0.79
4:H:8:DC:H2'	4:H:9:DA:H8	1.48	0.79
1:I:238:ARG:CZ	1:I:271:TYR:HB3	2.10	0.79
2:J:44:PHE:HZ	2:J:253:THR:HG1	1.24	0.79
1:I:241:ILE:HG23	1:I:277:VAL:HG21	1.63	0.79
1:A:237:LEU:HD22	1:A:268:LEU:HD11	1.63	0.79
2:B:61:MET:HE3	2:B:108:LEU:HD23	1.65	0.79
2:B:251:ASP:HB2	2:F:177:ASN:ND2	1.97	0.79
1:E:439:VAL:HG23	1:E:443:THR:O	1.83	0.79
1:A:298:VAL:O	1:E:58:GLN:OE1	2.00	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:8:DC:H2'	4:P:9:DA:H8	1.48	0.78
1:A:123:HIS:HE1	1:A:144:ASP:CG	1.86	0.78
2:B:61:MET:CE	2:B:108:LEU:HD22	2.13	0.78
1:E:146:VAL:HG23	1:E:147:ILE:H	1.48	0.78
1:E:258:ILE:HG22	1:E:283:GLU:OE1	1.82	0.78
1:M:212:PHE:CD2	1:M:236:MET:SD	2.77	0.78
2:N:239:GLU:OE1	2:N:269:ARG:HG2	1.83	0.78
1:I:326:LYS:HA	1:I:581:LEU:CB	2.13	0.78
1:E:148:GLU:CD	1:E:182:TYR:HE2	1.87	0.78
1:E:148:GLU:OE2	1:E:182:TYR:CE2	2.37	0.78
1:M:143:PHE:CZ	1:M:194:ILE:HG22	2.18	0.78
1:E:13:TYR:HE1	1:E:294:ILE:HG23	1.47	0.78
2:J:40:TYR:CE2	2:J:214:LYS:HD3	2.13	0.78
2:J:185:ASP:O	2:J:189:THR:CG2	2.32	0.78
2:J:190:ARG:NH1	2:J:191:GLN:H	1.82	0.78
1:I:266:GLN:HA	1:I:266:GLN:NE2	1.97	0.77
2:J:186:THR:C	2:J:189:THR:OG1	2.22	0.77
1:M:154:ILE:CD1	1:M:309:VAL:HG22	2.13	0.77
1:M:163:HIS:NE2	1:M:191:TYR:CE2	2.52	0.77
1:A:125:VAL:HG21	1:A:295:TRP:HB3	1.65	0.77
2:J:330:GLU:CD	2:J:414:GLY:CA	2.52	0.77
1:M:192:GLN:NE2	1:M:192:GLN:HA	1.99	0.77
1:E:5:THR:N	1:E:8:GLU:OE1	2.17	0.77
1:I:331:LEU:HD23	1:I:331:LEU:O	1.85	0.77
1:E:226:TYR:CD2	1:E:253:TRP:HZ2	2.03	0.77
2:F:139:GLN:HB3	2:F:142:ALA:CB	2.15	0.77
1:I:212:PHE:CD2	1:I:236:MET:HG2	2.19	0.77
2:J:341:TYR:CE2	2:J:403:LEU:CD2	2.68	0.77
1:A:144:ASP:C	1:A:146:VAL:H	1.87	0.77
1:A:175:ASN:OD1	1:M:245:ASN:ND2	2.18	0.77
1:E:106:LYS:HE3	1:M:176:THR:CG2	2.15	0.77
2:B:177:ASN:ND2	2:F:139:GLN:OE1	2.18	0.77
1:E:10:TYR:CZ	1:E:293:LYS:HB3	2.20	0.77
1:I:217:ILE:HB	1:I:243:GLN:NE2	2.00	0.77
1:M:195:LYS:HZ3	1:M:195:LYS:HB2	1.50	0.77
1:A:381:LEU:HD11	1:A:569:ALA:HB2	1.68	0.76
1:E:164:LEU:HD22	1:E:187:GLY:HA3	1.67	0.76
1:E:122:GLY:CA	1:E:291:LEU:HD12	2.14	0.76
2:F:135:GLY:O	2:F:139:GLN:NE2	2.15	0.76
2:J:190:ARG:HH11	2:J:191:GLN:H	1.30	0.76
2:B:248:PHE:CE1	2:B:290:LEU:HD22	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLU:OE1	1:E:161:VAL:HG11	1.85	0.76
2:J:184:ASN:O	2:J:188:LEU:HD21	1.86	0.76
2:J:51:ARG:NH2	2:J:141:HIS:O	2.19	0.76
2:J:190:ARG:HH11	2:J:190:ARG:CB	1.98	0.76
1:M:195:LYS:HB2	1:M:195:LYS:NZ	2.00	0.76
1:E:42:TRP:HB3	1:E:62:ILE:CD1	2.15	0.76
1:E:148:GLU:OE2	1:E:184:LYS:HE2	1.86	0.76
1:I:217:ILE:HD12	1:I:245:ASN:HB3	1.68	0.76
2:N:93:VAL:HG13	2:N:94:PHE:HD1	1.51	0.76
2:B:246:GLN:CD	2:B:287:SER:OG	2.21	0.76
1:E:10:TYR:CE1	1:E:294:ILE:HG13	2.19	0.76
2:B:251:ASP:OD2	2:B:295:HIS:HA	1.86	0.75
2:J:40:TYR:HE2	2:J:214:LYS:CD	1.99	0.75
1:M:213:LEU:N	1:M:213:LEU:HD23	2.01	0.75
1:A:221:LEU:CD2	1:A:251:LEU:HD12	2.15	0.75
1:E:117:VAL:CG2	1:E:146:VAL:HG11	2.15	0.75
1:I:217:ILE:HD11	1:I:245:ASN:CB	2.16	0.75
1:M:24:LEU:CA	1:M:140:THR:HG22	2.16	0.75
1:A:213:LEU:HD11	1:A:240:ALA:HA	1.66	0.75
2:B:51:ARG:NH2	2:B:141:HIS:O	2.19	0.75
1:I:144:ASP:O	1:I:145:ASP:HB3	1.85	0.75
1:E:210:LYS:HD3	1:I:244:ASN:HD21	0.94	0.75
1:M:123:HIS:ND1	1:M:146:VAL:HG11	2.00	0.75
1:A:217:ILE:HD13	1:A:245:ASN:C	2.06	0.75
1:E:124:ARG:NH2	2:F:321:ASP:OD1	2.19	0.75
2:F:93:VAL:HG13	2:F:94:PHE:HD1	1.51	0.75
2:N:192:CYS:O	2:N:195:ASN:HB2	1.87	0.75
1:A:16:ASN:HD21	1:A:20:MET:HE3	1.52	0.74
1:E:222:VAL:CG2	1:E:252:TYR:HD2	1.98	0.74
2:N:396:LYS:HD3	2:N:397:GLU:HG3	1.69	0.74
1:A:297:GLN:NE2	1:E:50:CYS:O	2.19	0.74
1:E:166:GLY:HA2	1:M:165:GLU:HG3	1.68	0.74
1:I:381:LEU:HD11	1:I:569:ALA:HB2	1.68	0.74
2:F:136:LEU:CB	2:F:143:PHE:HE2	1.94	0.74
1:M:126:LEU:CD2	1:M:147:ILE:CD1	2.65	0.74
1:M:216:ALA:O	1:M:246:ALA:O	2.05	0.74
1:A:410:SER:HB2	1:A:417:LEU:HD23	1.70	0.74
1:E:192:GLN:HB3	1:M:168:TYR:OH	1.83	0.74
2:B:67:ILE:CD1	2:B:193:ARG:NH2	2.50	0.74
1:E:26:ALA:HA	1:E:142:ASN:OD1	1.88	0.74
1:M:24:LEU:CG	1:M:140:THR:HG21	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ASP:OD1	3:C:1:A:N6	2.21	0.74
1:E:122:GLY:HA3	1:E:291:LEU:HD12	1.69	0.74
1:A:217:ILE:HG13	1:M:217:ILE:CD1	2.16	0.74
1:I:143:PHE:HD1	1:I:143:PHE:H	1.36	0.74
2:J:164:ASP:OD1	3:K:1:A:N6	2.21	0.74
1:E:13:TYR:HH	1:E:129:LEU:HD13	1.51	0.73
1:E:239:ALA:O	1:E:242:ASP:HB2	1.88	0.73
1:E:164:LEU:HD12	1:E:208:ILE:CD1	2.17	0.73
1:I:344:ARG:HH21	1:I:567:PHE:HA	1.53	0.73
2:J:40:TYR:CD2	2:J:214:LYS:HB2	2.23	0.73
1:E:443:THR:OG1	1:E:493:ARG:NH1	2.22	0.73
1:M:24:LEU:O	1:M:140:THR:HA	1.88	0.73
1:A:344:ARG:HH21	1:A:567:PHE:HA	1.53	0.73
1:I:410:SER:HB2	1:I:417:LEU:HD23	1.70	0.73
1:E:192:GLN:CA	1:M:168:TYR:OH	2.37	0.73
1:I:330:ALA:HB2	1:I:581:LEU:HG	1.71	0.73
1:E:165:GLU:CG	1:E:191:TYR:CB	2.67	0.73
1:M:44:LEU:HA	1:M:47:ARG:HG3	1.71	0.73
1:E:9:PHE:CZ	1:E:290:MET:CE	2.72	0.73
2:J:188:LEU:HD23	2:J:188:LEU:N	2.03	0.73
2:F:396:LYS:HD3	2:F:397:GLU:HG3	1.69	0.73
2:N:41:SER:HB3	2:N:211:ILE:HB	1.71	0.72
1:E:221:LEU:C	1:E:251:LEU:CD1	2.58	0.72
1:E:222:VAL:CG2	1:E:252:TYR:CD2	2.70	0.72
1:A:15:GLN:NE2	1:E:97:PHE:HE1	1.87	0.72
2:J:304:PHE:CE1	2:J:330:GLU:HB2	2.23	0.72
1:M:9:PHE:CE1	1:M:252:TYR:HD2	1.88	0.72
1:M:56:ASP:HB3	1:M:59:LYS:HB2	1.72	0.72
4:P:8:DC:H2'	4:P:9:DA:C8	2.25	0.72
2:J:341:TYR:HE2	2:J:403:LEU:HD21	1.55	0.72
2:B:190:ARG:HB3	2:B:190:ARG:CZ	2.19	0.72
2:B:299:MET:HG3	2:B:300:PRO:CD	2.19	0.72
1:E:60:HIS:HB2	1:E:67:ILE:HG21	1.70	0.72
1:E:221:LEU:CG	1:E:251:LEU:HD13	2.19	0.72
1:A:15:GLN:HE22	1:E:97:PHE:HE1	1.38	0.72
1:A:217:ILE:CG1	1:M:217:ILE:HD13	2.17	0.72
2:N:280:MET:CE	2:N:315:GLU:CD	2.57	0.72
1:E:509:ILE:HD11	1:E:531:ARG:HH22	1.55	0.72
1:M:216:ALA:HB3	1:M:243:GLN:HE21	1.54	0.72
1:M:226:TYR:CD2	1:M:253:TRP:HH2	2.07	0.72
2:N:263:ARG:HH11	2:N:268:ASP:C	1.92	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:SER:HB3	2:F:211:ILE:HB	1.71	0.72
1:M:252:TYR:CA	1:M:280:TYR:O	2.36	0.72
2:B:363:ARG:NH2	2:B:429:THR:OG1	2.23	0.72
2:J:363:ARG:NH2	2:J:429:THR:OG1	2.23	0.72
1:E:13:TYR:OH	1:E:129:LEU:HD11	1.89	0.72
1:M:154:ILE:HD12	1:M:309:VAL:CG2	2.20	0.72
2:J:104:HIS:NE2	2:J:139:GLN:OE1	2.23	0.71
1:M:21:MET:HG3	1:M:219:PHE:HB2	1.71	0.71
1:A:430:LEU:HD23	1:A:435:ILE:HG13	1.71	0.71
1:M:164:LEU:CD1	1:M:208:ILE:HD12	2.20	0.71
1:E:249:HIS:O	1:E:250:GLY:O	2.08	0.71
2:J:186:THR:O	2:J:189:THR:OG1	2.07	0.71
1:M:49:TYR:OH	1:M:70:LYS:HE3	1.91	0.71
1:A:10:TYR:CE1	1:A:294:ILE:HG13	2.25	0.71
1:E:143:PHE:O	1:E:189:PHE:CE2	2.42	0.71
2:F:63:LYS:HB3	2:F:188:LEU:CD1	2.20	0.71
4:H:8:DC:H2'	4:H:9:DA:C8	2.25	0.71
1:I:24:LEU:CD2	1:I:140:THR:HG21	2.15	0.71
2:J:330:GLU:CD	2:J:414:GLY:HA2	2.10	0.71
4:L:8:DC:H2'	4:L:9:DA:H8	1.55	0.71
4:D:8:DC:H2'	4:D:9:DA:H8	1.55	0.71
4:D:8:DC:H2'	4:D:9:DA:C8	2.25	0.71
1:I:330:ALA:CB	1:I:581:LEU:HG	2.20	0.71
1:I:430:LEU:HD23	1:I:435:ILE:HG13	1.71	0.71
1:I:269:ILE:HD13	1:I:279:ALA:HB1	1.72	0.71
2:B:290:LEU:HD23	2:B:290:LEU:O	1.91	0.71
4:L:8:DC:H2'	4:L:9:DA:C8	2.25	0.71
2:J:186:THR:C	2:J:189:THR:HG1	1.93	0.70
2:J:341:TYR:CE2	2:J:403:LEU:HD21	2.26	0.70
1:E:164:LEU:HD12	1:E:208:ILE:HD12	1.73	0.70
1:I:231:GLU:O	1:I:235:THR:HG23	1.90	0.70
2:N:262:THR:HB	2:N:283:VAL:HG21	1.64	0.70
1:A:217:ILE:HD11	1:A:243:GLN:HG3	1.73	0.70
1:E:21:MET:HG3	1:E:219:PHE:HB2	1.71	0.70
2:J:242:THR:OG1	2:J:270:LYS:NZ	2.23	0.70
1:M:234:MET:SD	1:M:268:LEU:CD1	2.75	0.70
2:N:87:TYR:HD2	2:N:197:MET:HB3	1.50	0.70
2:B:104:HIS:NE2	2:B:139:GLN:OE1	2.23	0.70
1:E:221:LEU:O	1:E:251:LEU:HA	1.91	0.70
1:I:217:ILE:HD12	1:I:245:ASN:C	2.12	0.70
1:I:240:ALA:O	1:I:243:GLN:CG	2.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HG22	1:A:513:PRO:HD2	1.74	0.70
2:B:242:THR:OG1	2:B:270:LYS:NZ	2.23	0.70
1:I:217:ILE:CD1	1:I:245:ASN:CB	2.69	0.70
1:E:165:GLU:HG3	1:E:191:TYR:CB	2.22	0.70
1:E:165:GLU:HG3	1:E:191:TYR:HD1	1.51	0.70
2:J:223:ALA:O	2:J:303:ILE:HD13	1.89	0.70
1:A:10:TYR:HE1	1:A:294:ILE:HG13	1.57	0.70
1:A:175:ASN:HD21	1:M:245:ASN:ND2	1.87	0.70
1:E:165:GLU:HG2	1:E:191:TYR:HB3	1.72	0.70
2:B:62:ARG:HG2	2:B:62:ARG:NH1	2.01	0.69
2:F:82:ASN:OD1	2:F:386:ASN:ND2	2.25	0.69
1:M:509:ILE:HD11	1:M:531:ARG:HH22	1.55	0.69
3:K:11:G:H2'	3:K:12:A:C8	2.28	0.69
1:M:24:LEU:HB2	1:M:140:THR:CB	2.22	0.69
1:M:128:ALA:HB2	1:M:154:ILE:CD1	2.20	0.69
1:E:10:TYR:OH	1:E:290:MET:HA	1.92	0.69
2:F:425:ILE:HG23	2:F:443:PRO:HG3	1.74	0.69
2:B:248:PHE:HE2	2:B:294:SER:HB3	1.58	0.69
1:I:24:LEU:C	1:I:140:THR:HB	2.06	0.69
1:M:24:LEU:CG	1:M:140:THR:CG2	2.71	0.69
1:A:19:HIS:O	1:A:219:PHE:CB	2.41	0.69
1:A:19:HIS:O	1:A:219:PHE:HB2	1.93	0.69
2:B:291:TYR:CD2	2:B:300:PRO:HG3	2.28	0.69
2:F:261:ASP:OD2	2:F:463:VAL:CB	2.39	0.69
1:M:23:PHE:CE1	1:M:141:THR:CG2	2.76	0.69
2:F:137:PHE:HA	2:F:140:LYS:NZ	2.08	0.69
2:J:44:PHE:HZ	2:J:253:THR:CB	2.06	0.69
2:N:197:MET:N	2:N:197:MET:SD	2.65	0.69
1:E:319:ILE:HD12	1:E:320:PRO:HD2	1.75	0.68
1:I:21:MET:SD	1:I:139:PHE:CE1	2.86	0.68
1:M:131:GLU:CB	1:M:151:PHE:HE2	2.06	0.68
2:N:425:ILE:HG23	2:N:443:PRO:HG3	1.74	0.68
1:A:16:ASN:HD21	1:A:20:MET:HE2	1.59	0.68
1:E:19:HIS:HB2	1:E:249:HIS:HD2	1.57	0.68
1:E:164:LEU:HD13	1:E:164:LEU:N	2.07	0.68
2:N:63:LYS:HB3	2:N:188:LEU:HD22	1.75	0.68
2:N:239:GLU:OE2	2:N:269:ARG:HA	1.93	0.68
1:M:21:MET:HE3	1:M:139:PHE:CZ	2.24	0.68
1:I:511:ILE:HG22	1:I:513:PRO:HD2	1.74	0.68
1:E:140:THR:HG21	1:E:182:TYR:CZ	2.28	0.68
1:M:123:HIS:CG	1:M:146:VAL:CG1	2.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:82:ASN:OD1	2:N:386:ASN:ND2	2.24	0.68
1:E:4:LEU:CD1	1:E:8:GLU:OE1	2.30	0.68
2:N:91:GLU:HG3	2:N:97:PRO:HA	1.76	0.68
3:C:11:G:H2'	3:C:12:A:C8	2.28	0.68
1:E:23:PHE:HB2	1:E:221:LEU:HD11	1.76	0.68
1:E:497:ARG:NH1	2:F:373:GLU:OE2	2.27	0.68
2:B:46:LEU:HD21	2:F:176:LEU:CD1	2.23	0.68
1:E:190:ARG:NH1	1:E:191:TYR:HE2	1.91	0.68
1:I:124:ARG:HG2	1:I:309:VAL:HG12	1.76	0.67
1:M:154:ILE:HD13	1:M:309:VAL:HG22	1.75	0.67
2:N:71:LEU:HA	2:N:197:MET:HG3	1.75	0.67
1:M:23:PHE:HA	1:M:139:PHE:O	1.94	0.67
1:M:147:ILE:O	1:M:148:GLU:C	2.31	0.67
2:N:434:ASN:HB2	2:N:473:MET:HB2	1.76	0.67
1:E:106:LYS:HE3	1:M:176:THR:HG22	1.75	0.67
1:E:119:LEU:H	1:E:119:LEU:CD2	2.02	0.67
1:E:122:GLY:C	1:E:291:LEU:HD13	2.14	0.67
1:I:238:ARG:HH11	1:I:271:TYR:CB	2.04	0.67
1:A:22:TRP:HD1	1:A:135:THR:HG1	0.74	0.67
1:A:209:HIS:HA	1:A:236:MET:HE2	1.76	0.67
1:A:221:LEU:HD23	1:A:251:LEU:HD12	1.77	0.67
2:B:259:ALA:CB	2:B:448:TYR:CZ	2.77	0.67
2:B:44:PHE:CE2	2:B:253:THR:OG1	2.45	0.67
1:E:210:LYS:HG3	1:I:244:ASN:HD21	1.59	0.67
2:F:434:ASN:HB2	2:F:473:MET:HB2	1.76	0.67
1:E:165:GLU:OE2	1:M:168:TYR:OH	2.12	0.67
2:F:91:GLU:HG3	2:F:97:PRO:HA	1.76	0.67
2:F:105:LEU:HD22	2:F:143:PHE:HB3	1.74	0.67
1:E:26:ALA:H	1:E:142:ASN:ND2	1.93	0.67
1:I:326:LYS:HA	1:I:581:LEU:HB2	1.77	0.67
1:M:123:HIS:ND1	1:M:146:VAL:CG1	2.58	0.67
1:M:497:ARG:NH1	2:N:373:GLU:OE2	2.27	0.67
1:I:326:LYS:C	1:I:581:LEU:HB3	2.14	0.67
2:N:67:ILE:HD11	2:N:187:ALA:HB1	1.74	0.67
2:B:79:GLU:OE1	2:B:190:ARG:NH2	2.21	0.67
2:B:196:VAL:O	2:B:200:VAL:HG23	1.95	0.67
1:E:119:LEU:HD22	1:E:119:LEU:N	2.05	0.67
1:M:319:ILE:HD12	1:M:320:PRO:HD2	1.75	0.67
1:A:207:GLU:OE1	1:A:207:GLU:N	2.25	0.66
2:B:70:GLU:HG2	2:B:197:MET:HE2	1.68	0.66
1:E:9:PHE:CZ	1:E:290:MET:HE3	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:ARG:HB3	1:E:445:TYR:CE2	2.29	0.66
1:A:330:ALA:HB2	1:A:581:LEU:HG	1.77	0.66
2:F:301:ARG:HH12	2:F:302:LYS:HD2	1.60	0.66
1:I:21:MET:HG3	1:I:139:PHE:HE1	1.56	0.66
1:A:137:VAL:HG22	1:A:181:ILE:CD1	2.24	0.66
1:E:348:VAL:HG12	1:E:399:ILE:HG12	1.77	0.66
2:F:137:PHE:HD1	2:F:140:LYS:HZ1	1.42	0.66
1:I:23:PHE:HD1	1:I:139:PHE:O	1.77	0.66
1:I:326:LYS:HA	1:I:581:LEU:HB3	1.77	0.66
2:J:196:VAL:O	2:J:200:VAL:HG23	1.96	0.66
2:B:259:ALA:CB	2:B:448:TYR:CE2	2.77	0.66
1:E:122:GLY:C	1:E:291:LEU:CD1	2.64	0.66
1:M:9:PHE:HD1	1:M:252:TYR:CD2	2.12	0.66
2:N:301:ARG:HH12	2:N:302:LYS:HD2	1.60	0.66
2:B:143:PHE:CE2	2:B:178:LEU:CD1	2.73	0.66
1:E:170:ALA:CB	1:E:211:CYS:SG	2.82	0.66
2:B:203:ALA:C	2:B:207:LYS:HG3	2.13	0.66
2:B:299:MET:HG3	2:B:300:PRO:HD2	1.78	0.66
1:E:122:GLY:HA2	1:E:291:LEU:HB2	1.76	0.66
1:E:192:GLN:HB2	1:M:168:TYR:CE1	2.29	0.66
1:I:296:ARG:NH2	2:J:328:GLU:OE2	2.27	0.66
1:M:14:LEU:HD22	1:M:297:GLN:HB3	1.78	0.66
1:M:119:LEU:HD21	1:M:149:THR:HG22	1.78	0.66
1:E:117:VAL:HG23	1:E:146:VAL:HG11	1.78	0.66
2:B:248:PHE:CZ	2:B:290:LEU:HD22	2.31	0.66
1:I:268:LEU:HD23	1:I:268:LEU:O	1.95	0.66
1:A:209:HIS:HA	1:A:236:MET:CE	2.26	0.65
1:M:237:LEU:O	1:M:241:ILE:N	2.28	0.65
1:M:238:ARG:HA	1:M:241:ILE:HG13	1.77	0.65
2:N:16:GLU:OE2	2:N:363:ARG:NH1	2.29	0.65
2:N:87:TYR:HD2	2:N:197:MET:CB	2.05	0.65
1:M:268:LEU:C	1:M:268:LEU:HD23	2.16	0.65
2:N:186:THR:O	2:N:190:ARG:HB2	1.95	0.65
2:N:261:ASP:H	2:N:452:PHE:HE2	1.42	0.65
1:M:46:HIS:HB2	1:M:62:ILE:HD13	1.77	0.65
1:M:348:VAL:HG12	1:M:399:ILE:HG12	1.77	0.65
1:E:165:GLU:HG2	1:E:191:TYR:CB	2.27	0.65
2:J:330:GLU:OE1	2:J:414:GLY:HA2	1.93	0.65
1:A:221:LEU:HD21	1:A:251:LEU:CD1	2.26	0.65
1:E:156:GLY:O	1:M:153:ASP:N	2.30	0.65
1:I:13:TYR:HH	1:I:22:TRP:HE1	1.43	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:528:ARG:HA	1:I:531:ARG:HG3	1.78	0.65
1:A:243:GLN:HG2	1:A:246:ALA:HB2	1.79	0.65
2:B:243:CYS:HB3	2:B:260:TYR:O	1.95	0.65
1:E:192:GLN:CB	1:M:168:TYR:CZ	2.55	0.65
2:F:136:LEU:O	2:F:143:PHE:CE2	2.49	0.65
2:J:190:ARG:HH12	2:J:192:CYS:H	1.44	0.65
1:M:127:ALA:CA	1:M:151:PHE:HB2	2.27	0.65
1:E:164:LEU:CD1	1:E:208:ILE:CD1	2.74	0.65
1:M:511:ILE:HG22	1:M:513:PRO:HD2	1.79	0.65
1:A:130:LEU:O	1:A:133:ASN:N	2.28	0.65
1:E:13:TYR:CE1	1:E:294:ILE:CG2	2.79	0.65
1:E:145:ASP:O	1:E:149:THR:OG1	2.10	0.65
1:M:154:ILE:HD12	1:M:309:VAL:HG23	1.79	0.65
2:B:190:ARG:HD2	4:D:21:DA:N6	2.11	0.65
1:E:348:VAL:HG11	1:E:387:ILE:HG21	1.79	0.65
2:F:16:GLU:OE2	2:F:363:ARG:NH1	2.29	0.65
1:I:326:LYS:CA	1:I:581:LEU:HB3	2.27	0.65
2:J:432:ASP:OD1	2:J:469:TYR:OH	2.12	0.65
1:E:148:GLU:OE2	1:E:182:TYR:HD2	1.75	0.64
1:M:137:VAL:CG1	1:M:139:PHE:CZ	2.80	0.64
1:I:21:MET:HG2	1:I:139:PHE:HE1	1.56	0.64
1:M:24:LEU:HG	1:M:140:THR:CG2	2.28	0.64
1:M:154:ILE:CD1	1:M:309:VAL:CG2	2.74	0.64
1:E:163:HIS:HB3	1:E:188:ASP:H	1.63	0.64
2:N:149:TYR:OH	2:N:188:LEU:HD11	1.97	0.64
1:A:161:VAL:HG12	1:A:182:TYR:CD2	2.29	0.64
2:B:304:PHE:HE1	2:B:421:THR:HG22	1.63	0.64
1:E:210:LYS:HD3	1:I:244:ASN:HD22	0.83	0.64
1:E:213:LEU:HD21	1:E:240:ALA:HB2	1.80	0.64
2:N:63:LYS:HB3	2:N:188:LEU:HD21	1.79	0.64
1:A:296:ARG:NH1	1:E:54:ASN:OD1	2.31	0.64
1:M:348:VAL:HG11	1:M:387:ILE:HG21	1.79	0.64
1:A:528:ARG:HA	1:A:531:ARG:HG3	1.78	0.64
2:J:304:PHE:HE1	2:J:421:THR:HG22	1.59	0.64
2:N:263:ARG:CZ	2:N:268:ASP:O	2.45	0.64
2:B:260:TYR:HH	2:B:287:SER:CB	1.99	0.64
4:P:9:DA:H2'	4:P:10:DG:C8	2.33	0.64
1:I:217:ILE:HB	1:I:243:GLN:HE22	1.62	0.64
2:J:326:SER:O	1:M:59:LYS:NZ	2.24	0.64
1:M:132:MET:O	1:M:134:GLN:NE2	2.29	0.64
1:M:219:PHE:O	1:M:248:PRO:HD2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:238:ARG:HA	1:M:241:ILE:CG1	2.28	0.64
2:B:67:ILE:HD11	2:B:193:ARG:HH21	1.61	0.63
1:M:34:LEU:HD11	1:M:144:ASP:OD2	1.98	0.63
1:E:117:VAL:HG23	1:E:146:VAL:CG1	2.27	0.63
1:E:210:LYS:CG	1:I:244:ASN:ND2	2.51	0.63
1:A:296:ARG:NH2	2:B:328:GLU:OE2	2.27	0.63
2:B:68:VAL:O	2:B:71:LEU:HB2	1.97	0.63
1:E:366:LYS:NZ	1:E:389:LYS:O	2.32	0.63
1:M:31:SER:O	1:M:33:GLY:N	2.30	0.63
4:H:9:DA:H2'	4:H:10:DG:C8	2.33	0.63
2:J:425:ILE:O	2:J:429:THR:HG23	1.99	0.63
1:M:128:ALA:CB	1:M:154:ILE:HD11	2.27	0.63
1:A:533:ASN:ND2	2:B:357:ALA:O	2.32	0.63
2:B:425:ILE:O	2:B:429:THR:HG23	1.99	0.63
1:M:216:ALA:HB3	1:M:243:GLN:NE2	2.13	0.63
1:E:511:ILE:HG22	1:E:513:PRO:HD2	1.79	0.63
1:M:226:TYR:O	1:M:253:TRP:HZ2	1.82	0.63
1:E:114:SER:HB2	1:E:145:ASP:OD2	1.94	0.63
1:E:137:VAL:HG12	1:E:139:PHE:CE1	2.32	0.63
2:F:443:PRO:HD2	2:F:446:LEU:HD12	1.80	0.63
2:J:341:TYR:CE2	2:J:403:LEU:HD23	2.33	0.63
1:M:237:LEU:HA	1:M:240:ALA:HB3	1.79	0.63
2:N:443:PRO:HD2	2:N:446:LEU:HD12	1.80	0.63
2:B:396:LYS:HD2	2:B:437:THR:HB	1.80	0.63
2:F:20:LEU:N	2:F:214:LYS:O	2.30	0.63
1:I:241:ILE:CG2	1:I:277:VAL:HG21	2.28	0.62
2:J:396:LYS:HD2	2:J:437:THR:HB	1.80	0.62
1:M:11:GLN:O	1:M:15:GLN:HB2	1.99	0.62
1:A:124:ARG:HG2	1:A:309:VAL:CG1	2.26	0.62
1:A:513:PRO:HB2	1:A:516:ARG:HB2	1.81	0.62
1:E:132:MET:O	1:E:134:GLN:NE2	2.29	0.62
1:M:387:ILE:HA	1:M:390:ILE:HD12	1.80	0.62
1:E:121:ILE:HD11	2:F:317:GLN:NE2	2.14	0.62
2:F:224:TYR:HB2	2:F:247:VAL:HG22	1.81	0.62
2:J:341:TYR:CD2	2:J:403:LEU:CD2	2.82	0.62
2:N:20:LEU:N	2:N:214:LYS:O	2.30	0.62
2:F:51:ARG:NH2	2:F:144:ASP:OD1	2.33	0.62
2:B:471:PHE:HE1	2:F:138:ARG:HD2	1.65	0.62
3:C:12:A:H2'	3:C:13:G:C8	2.34	0.62
2:J:302:LYS:HB2	2:J:328:GLU:HB2	1.80	0.62
1:M:428:ALA:HB2	1:M:561:CYS:HB3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:277:TYR:OH	2:F:321:ASP:OD2	2.18	0.62
2:J:79:GLU:HB2	2:J:192:CYS:HB2	1.82	0.62
3:K:12:A:H2'	3:K:13:G:C8	2.34	0.62
2:N:145:VAL:HG11	2:N:204:LEU:HD22	1.80	0.62
2:B:255:PHE:HD2	2:B:433:TRP:CH2	2.16	0.62
1:I:513:PRO:HB2	1:I:516:ARG:HB2	1.81	0.62
1:M:123:HIS:CG	1:M:146:VAL:HG11	2.34	0.62
1:E:428:ALA:HB2	1:E:561:CYS:HB3	1.80	0.62
1:I:533:ASN:ND2	2:J:357:ALA:O	2.32	0.62
2:J:304:PHE:CE1	2:J:330:GLU:CB	2.82	0.62
1:A:175:ASN:ND2	1:M:245:ASN:ND2	2.46	0.61
1:A:123:HIS:CE1	1:A:144:ASP:CG	2.68	0.61
1:E:174:LEU:O	1:E:174:LEU:HD23	1.99	0.61
2:J:304:PHE:CD1	2:J:330:GLU:HB2	2.35	0.61
1:M:30:ARG:HE	1:M:36:THR:HG21	1.65	0.61
1:M:44:LEU:CA	1:M:47:ARG:HG3	2.29	0.61
1:E:286:THR:HG23	1:E:289:GLU:HB3	1.81	0.61
2:F:82:ASN:ND2	4:H:23:DT:OP2	2.33	0.61
2:F:107:CYS:SG	2:F:108:LEU:N	2.73	0.61
1:I:296:ARG:NH1	1:M:54:ASN:OD1	2.31	0.61
1:M:23:PHE:CE1	1:M:141:THR:HG23	2.35	0.61
2:B:184:ASN:ND2	3:C:1:A:N3	2.42	0.61
1:E:387:ILE:HA	1:E:390:ILE:HD12	1.80	0.61
2:J:64:LEU:HD11	2:J:149:TYR:HB2	1.81	0.61
2:F:71:LEU:HD21	2:F:200:VAL:HG12	1.82	0.61
1:M:237:LEU:O	1:M:241:ILE:CD1	2.48	0.61
2:B:248:PHE:CE2	2:B:294:SER:HB3	2.35	0.61
2:N:191:GLN:O	2:N:192:CYS:C	2.34	0.61
2:N:224:TYR:HB2	2:N:247:VAL:HG22	1.81	0.61
2:B:432:ASP:OD1	2:B:469:TYR:OH	2.13	0.61
2:N:82:ASN:ND2	4:P:23:DT:OP2	2.33	0.61
2:N:186:THR:HB	3:O:2:U:OP2	1.99	0.61
1:A:4:LEU:HB3	1:A:282:VAL:HG12	1.81	0.61
1:E:192:GLN:OE1	1:E:192:GLN:HA	2.00	0.61
2:N:71:LEU:HD21	2:N:200:VAL:HG12	1.82	0.61
2:N:263:ARG:NH1	2:N:268:ASP:C	2.53	0.61
1:A:4:LEU:O	1:A:282:VAL:CG1	2.46	0.61
2:B:79:GLU:HB2	2:B:192:CYS:HB2	1.82	0.61
2:B:190:ARG:CG	2:B:190:ARG:HH11	2.14	0.61
1:E:156:GLY:O	1:M:153:ASP:HA	2.01	0.61
2:F:190:ARG:NH1	4:H:21:DA:C6	2.69	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:366:LYS:NZ	1:M:389:LYS:O	2.32	0.61
2:N:280:MET:HE3	2:N:315:GLU:CD	2.21	0.61
2:F:187:ALA:HB1	3:G:2:U:C6	2.36	0.60
1:I:213:LEU:N	1:I:213:LEU:HD23	2.15	0.60
4:L:9:DA:H2'	4:L:10:DG:C8	2.36	0.60
2:F:145:VAL:CG2	2:F:208:ALA:HB2	2.32	0.60
2:J:250:PRO:HA	2:J:295:HIS:CE1	2.34	0.60
2:N:269:ARG:HB3	2:N:269:ARG:CZ	2.31	0.60
1:A:124:ARG:HG3	1:A:309:VAL:HG12	1.83	0.60
1:E:241:ILE:O	1:E:242:ASP:C	2.39	0.60
1:E:153:ASP:CA	1:M:156:GLY:O	2.49	0.60
1:I:171:LEU:CD1	1:I:211:CYS:HA	2.30	0.60
1:M:212:PHE:HD2	1:M:236:MET:SD	2.23	0.60
1:M:226:TYR:O	1:M:253:TRP:CZ2	2.54	0.60
2:N:335:ILE:HB	2:N:408:MET:HB3	1.84	0.60
1:A:405:ASP:OD1	1:A:405:ASP:N	2.35	0.60
1:M:213:LEU:HD22	1:M:240:ALA:HA	1.83	0.60
1:M:362:ARG:NH2	1:M:390:ILE:O	2.33	0.60
2:B:67:ILE:HD11	2:B:193:ARG:HH22	1.66	0.60
2:F:262:THR:O	2:F:262:THR:HG22	2.02	0.60
1:I:241:ILE:HA	1:I:246:ALA:CB	2.32	0.60
2:J:281:GLN:OE1	2:J:321:ASP:CB	2.50	0.60
1:M:204:ASN:OD1	1:M:232:ASN:ND2	2.35	0.60
2:B:258:VAL:HG21	2:B:290:LEU:HD12	1.82	0.60
1:E:148:GLU:CD	1:E:182:TYR:CD2	2.71	0.60
1:E:153:ASP:HA	1:M:156:GLY:O	2.02	0.60
1:E:288:ASP:OD2	2:F:277:TYR:HE2	1.85	0.60
2:F:250:PRO:HA	2:F:295:HIS:CE1	2.37	0.60
1:A:121:ILE:HD12	1:A:121:ILE:N	2.09	0.60
2:J:184:ASN:ND2	3:K:1:A:N3	2.42	0.60
1:M:131:GLU:HB2	1:M:155:SER:OG	2.02	0.60
2:N:107:CYS:SG	2:N:108:LEU:N	2.74	0.60
2:B:261:ASP:OD1	2:B:262:THR:N	2.35	0.59
2:B:301:ARG:NH1	1:E:59:LYS:O	2.35	0.59
4:D:9:DA:H2'	4:D:10:DG:C8	2.36	0.59
1:E:30:ARG:O	1:E:30:ARG:HD3	2.02	0.59
1:E:204:ASN:OD1	1:E:232:ASN:ND2	2.35	0.59
1:M:23:PHE:HB2	1:M:221:LEU:HD11	1.84	0.59
2:N:262:THR:CB	2:N:283:VAL:HG22	2.20	0.59
1:E:106:LYS:HE3	1:M:176:THR:HG21	1.84	0.59
2:F:335:ILE:HB	2:F:408:MET:HB3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:44:PHE:HZ	2:J:253:THR:HB	1.65	0.59
1:E:213:LEU:HB3	1:E:243:GLN:HE22	1.67	0.59
1:E:241:ILE:N	1:E:241:ILE:HD12	2.16	0.59
2:J:261:ASP:OD1	2:J:262:THR:N	2.35	0.59
1:M:24:LEU:O	1:M:140:THR:CA	2.50	0.59
1:E:164:LEU:HD22	1:E:187:GLY:CA	2.32	0.59
1:E:362:ARG:NH2	1:E:390:ILE:O	2.33	0.59
3:K:10:A:H2'	3:K:11:G:C8	2.38	0.59
4:L:9:DA:H2'	4:L:10:DG:H8	1.67	0.59
1:M:41:ILE:HD11	1:M:89:TYR:HB2	1.83	0.59
2:J:223:ALA:C	2:J:303:ILE:CD1	2.71	0.59
2:J:281:GLN:OE1	2:J:321:ASP:HB3	2.01	0.59
1:M:161:VAL:HG12	1:M:182:TYR:HD2	1.66	0.59
2:B:44:PHE:HB2	2:B:46:LEU:HG	1.84	0.59
2:B:190:ARG:HH11	2:B:190:ARG:HG2	1.68	0.59
3:C:10:A:H2'	3:C:11:G:C8	2.38	0.59
1:M:148:GLU:OE2	1:M:161:VAL:CG1	2.49	0.59
2:J:400:LEU:N	2:J:400:LEU:HD23	2.16	0.59
1:M:268:LEU:HD22	1:M:269:ILE:HD13	1.85	0.59
1:A:151:PHE:HD2	1:A:159:LEU:HB2	1.67	0.59
1:A:338:VAL:HG22	1:A:573:ILE:HG13	1.85	0.59
2:B:251:ASP:OD2	2:B:295:HIS:C	2.41	0.59
1:E:30:ARG:NH1	1:E:36:THR:OG1	2.34	0.59
1:I:319:ILE:HD11	2:J:418:TRP:CE2	2.38	0.59
1:M:552:GLY:HA2	1:M:575:THR:HG23	1.83	0.59
1:A:124:ARG:NH1	1:A:308:LYS:O	2.36	0.59
2:F:136:LEU:CA	2:F:143:PHE:CE2	2.75	0.59
2:N:75:ALA:H	2:N:87:TYR:HB3	1.68	0.59
2:N:250:PRO:HA	2:N:295:HIS:CE1	2.37	0.59
1:A:245:ASN:HB3	1:M:214:ALA:HB2	1.85	0.58
2:B:231:ILE:HB	4:D:15:DA:H5"	1.85	0.58
2:J:185:ASP:O	2:J:189:THR:OG1	2.21	0.58
2:N:51:ARG:NH1	2:N:142:ALA:O	2.35	0.58
1:E:136:LYS:HB3	1:E:179:PHE:CD1	2.39	0.58
2:F:75:ALA:H	2:F:87:TYR:HB3	1.68	0.58
1:M:131:GLU:CA	1:M:151:PHE:HE2	2.15	0.58
1:I:151:PHE:HD2	1:I:159:LEU:HB2	1.67	0.58
1:E:22:TRP:HE3	1:E:24:LEU:HD21	1.67	0.58
1:E:44:LEU:HD21	1:E:107:TYR:CZ	2.37	0.58
1:E:241:ILE:O	1:E:243:GLN:N	2.36	0.58
1:I:257:SER:HB3	1:I:260:LYS:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:11:G:H2'	3:O:12:A:C8	2.39	0.58
1:A:301:LYS:CE	1:E:58:GLN:NE2	2.63	0.58
2:B:177:ASN:OD1	2:B:471:PHE:HZ	1.86	0.58
4:D:9:DA:H2'	4:D:10:DG:H8	1.66	0.58
1:M:190:ARG:NH1	1:M:191:TYR:CE1	2.72	0.58
1:A:333:THR:HG21	2:B:340:TRP:HE3	1.69	0.58
1:I:330:ALA:O	2:J:345:VAL:HG22	2.03	0.58
1:M:430:LEU:HD22	1:M:437:HIS:HB2	1.86	0.58
1:A:11:GLN:NE2	1:E:96:VAL:O	2.37	0.58
2:B:177:ASN:CG	2:F:139:GLN:OE1	2.42	0.58
1:E:407:ILE:O	1:E:411:VAL:HG22	2.04	0.58
2:F:105:LEU:CD2	2:F:143:PHE:HD2	2.17	0.58
1:A:20:MET:O	1:A:135:THR:OG1	2.21	0.58
1:M:112:LEU:HB3	1:M:144:ASP:HB2	1.83	0.58
1:M:119:LEU:HG	1:M:150:ALA:CB	2.29	0.58
1:A:244:ASN:HD22	1:M:210:LYS:HA	1.68	0.58
1:E:552:GLY:HA2	1:E:575:THR:HG23	1.84	0.58
2:N:261:ASP:HB2	2:N:456:VAL:HG21	1.85	0.58
2:B:296:ASN:HD22	2:F:470:ARG:CZ	2.14	0.57
2:F:79:GLU:HG3	2:F:192:CYS:HB2	1.86	0.57
1:I:333:THR:HG21	2:J:340:TRP:HE3	1.69	0.57
1:I:338:VAL:HG22	1:I:573:ILE:HG13	1.85	0.57
1:M:12:HIS:HB3	1:M:252:TYR:OH	2.03	0.57
1:M:19:HIS:HB2	1:M:249:HIS:NE2	2.19	0.57
2:N:263:ARG:NE	2:N:268:ASP:O	2.37	0.57
1:M:273:GLN:NE2	1:M:279:ALA:O	2.37	0.57
1:A:257:SER:HB3	1:A:260:LYS:HG2	1.86	0.57
1:A:319:ILE:HD11	2:B:418:TRP:CE2	2.38	0.57
1:A:355:THR:HG23	1:A:358:GLU:H	1.70	0.57
1:A:454:LYS:HZ1	1:A:462:ARG:HH12	1.52	0.57
1:E:62:ILE:O	1:E:62:ILE:HG13	2.03	0.57
2:J:301:ARG:O	2:J:327:THR:HA	2.03	0.57
1:M:162:TYR:CD2	1:M:169:ALA:HB3	2.39	0.57
1:M:533:ASN:ND2	2:N:357:ALA:O	2.36	0.57
1:A:221:LEU:HD23	1:A:221:LEU:C	2.25	0.57
2:B:55:LEU:HD23	2:B:148:VAL:HG22	1.87	0.57
2:B:262:THR:HG22	2:B:283:VAL:HG21	1.86	0.57
1:E:226:TYR:CD2	1:E:253:TRP:CZ2	2.83	0.57
3:G:11:G:H2'	3:G:12:A:C8	2.39	0.57
1:E:41:ILE:HG22	1:E:45:LYS:HE2	1.85	0.57
1:E:273:GLN:NE2	1:E:279:ALA:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:9:DA:H2'	4:H:10:DG:H8	1.69	0.57
1:I:212:PHE:CE2	1:I:236:MET:SD	2.96	0.57
1:I:454:LYS:HZ1	1:I:462:ARG:HH12	1.52	0.57
2:J:40:TYR:OH	2:J:214:LYS:HE2	2.05	0.57
1:E:174:LEU:HD13	1:E:214:ALA:HB3	1.87	0.57
1:I:326:LYS:C	1:I:582:GLY:O	2.43	0.57
1:I:360:LYS:HA	1:I:363:ILE:HD12	1.87	0.57
1:M:407:ILE:O	1:M:411:VAL:HG22	2.04	0.57
1:I:405:ASP:OD1	1:I:405:ASP:N	2.35	0.57
2:B:177:ASN:OD1	2:B:471:PHE:CZ	2.57	0.57
1:E:120:ASN:OD1	1:E:288:ASP:OD2	2.22	0.57
2:J:231:ILE:HB	4:L:15:DA:H5"	1.85	0.57
1:I:300:ASP:OD1	1:M:58:GLN:NE2	2.37	0.57
1:M:9:PHE:CD1	1:M:252:TYR:CE2	2.93	0.57
2:N:262:THR:HB	2:N:283:VAL:HG23	1.81	0.57
1:A:429:LEU:HG	1:A:547:LEU:HD12	1.87	0.57
2:B:257:PHE:CE1	2:B:448:TYR:HD2	2.23	0.57
1:E:5:THR:CG2	1:E:8:GLU:OE1	2.41	0.57
2:J:386:ASN:ND2	2:J:389:ASN:O	2.32	0.57
1:A:248:PRO:HB2	1:M:175:ASN:ND2	2.20	0.56
1:E:254:THR:O	1:E:254:THR:OG1	2.19	0.56
1:E:430:LEU:HD22	1:E:437:HIS:HB2	1.86	0.56
1:M:221:LEU:HB2	1:M:247:PHE:CE1	2.40	0.56
1:M:263:PRO:O	1:M:267:ASP:CG	2.43	0.56
2:N:239:GLU:OE1	2:N:269:ARG:CG	2.53	0.56
1:A:217:ILE:HD12	1:A:245:ASN:O	2.00	0.56
1:I:143:PHE:N	1:I:143:PHE:CD1	2.72	0.56
1:M:119:LEU:CG	1:M:150:ALA:HB2	2.31	0.56
1:E:19:HIS:HB2	1:E:249:HIS:CD2	2.40	0.56
1:E:439:VAL:CG2	1:E:443:THR:O	2.52	0.56
1:I:268:LEU:HD23	1:I:268:LEU:C	2.26	0.56
1:I:330:ALA:CB	1:I:580:SER:O	2.49	0.56
2:J:40:TYR:HB3	2:J:211:ILE:O	2.04	0.56
1:M:23:PHE:HE1	1:M:141:THR:CG2	2.18	0.56
1:M:251:LEU:O	1:M:251:LEU:HG	2.05	0.56
2:B:46:LEU:HD22	2:F:137:PHE:HE2	1.70	0.56
2:F:334:ILE:HG13	2:F:446:LEU:HD11	1.87	0.56
2:J:40:TYR:CE2	2:J:214:LYS:CD	2.82	0.56
2:J:170:LYS:HZ1	3:K:1:A:P	2.29	0.56
1:E:513:PRO:HB2	1:E:516:ARG:HB2	1.88	0.56
1:E:533:ASN:ND2	2:F:357:ALA:O	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:LEU:HD23	2:F:188:LEU:O	2.04	0.56
2:N:334:ILE:HG13	2:N:446:LEU:HD11	1.87	0.56
1:A:16:ASN:ND2	1:A:20:MET:HE2	2.20	0.56
2:B:143:PHE:CZ	2:B:178:LEU:HD13	2.24	0.56
2:B:386:ASN:ND2	2:B:389:ASN:O	2.32	0.56
1:E:154:ILE:CD1	1:E:309:VAL:CG2	2.83	0.56
2:F:187:ALA:CB	3:G:2:U:C6	2.87	0.56
1:I:367:SER:O	1:I:367:SER:OG	2.21	0.56
1:A:4:LEU:HB3	1:A:282:VAL:CG1	2.36	0.56
1:E:165:GLU:OE1	1:E:165:GLU:HA	2.05	0.56
2:F:440:LYS:HD2	2:F:447:VAL:HG11	1.88	0.56
1:I:23:PHE:CD1	1:I:140:THR:HA	2.41	0.56
2:J:262:THR:HG22	2:J:283:VAL:HG21	1.86	0.56
1:E:164:LEU:HA	1:E:167:SER:HB2	1.87	0.56
1:E:221:LEU:HB2	1:E:247:PHE:CE1	2.40	0.56
1:I:139:PHE:O	1:I:140:THR:HG23	2.06	0.56
1:I:212:PHE:CE2	1:I:236:MET:HG2	2.41	0.56
1:A:136:LYS:CG	1:A:179:PHE:CD2	2.87	0.56
2:B:54:TYR:CD1	2:B:64:LEU:HD21	2.41	0.56
2:F:19:LEU:HB3	2:F:21:PHE:HE1	1.71	0.56
1:I:139:PHE:CD1	1:I:139:PHE:N	2.73	0.56
1:M:163:HIS:CE1	1:M:191:TYR:CE2	2.94	0.56
2:N:261:ASP:OD2	2:N:263:ARG:HB2	2.06	0.56
1:A:219:PHE:N	1:A:219:PHE:CD1	2.73	0.55
1:A:360:LYS:HA	1:A:363:ILE:HD12	1.87	0.55
2:B:435:ASN:OD1	2:B:437:THR:OG1	2.18	0.55
2:B:468:ASP:OD1	2:B:469:TYR:N	2.39	0.55
2:J:468:ASP:OD1	2:J:469:TYR:N	2.39	0.55
1:I:429:LEU:HG	1:I:547:LEU:HD12	1.87	0.55
1:M:475:THR:HG23	1:M:487:ALA:HB2	1.89	0.55
1:A:15:GLN:NE2	1:E:97:PHE:CE1	2.70	0.55
2:B:54:TYR:CG	2:B:64:LEU:HD21	2.41	0.55
1:E:122:GLY:CA	1:E:291:LEU:CD1	2.82	0.55
1:I:143:PHE:HD1	1:I:143:PHE:N	2.04	0.55
1:M:18:GLN:O	1:M:134:GLN:O	2.25	0.55
1:A:125:VAL:HG23	1:A:295:TRP:CB	2.34	0.55
1:A:302:PRO:HD2	1:A:305:ILE:HD12	1.88	0.55
2:B:251:ASP:OD2	2:B:295:HIS:CA	2.53	0.55
1:E:137:VAL:CG1	1:E:139:PHE:CE1	2.88	0.55
1:I:22:TRP:HB2	1:I:138:VAL:HG22	1.88	0.55
1:M:174:LEU:HD11	1:M:215:ALA:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:188:LEU:C	2:N:189:THR:O	2.44	0.55
1:A:136:LYS:HB3	1:A:179:PHE:CG	2.42	0.55
1:I:253:TRP:CE2	1:I:265:VAL:HG22	2.42	0.55
1:I:355:THR:HG23	1:I:358:GLU:H	1.70	0.55
2:J:244:CYS:SG	2:J:245:SER:N	2.80	0.55
2:N:440:LYS:HD2	2:N:447:VAL:HG11	1.88	0.55
1:A:11:GLN:OE1	1:E:96:VAL:HG12	2.03	0.55
1:A:121:ILE:HG21	1:A:292:SER:OG	2.07	0.55
1:E:105:ARG:HB2	1:E:194:ILE:HD11	1.88	0.55
1:E:137:VAL:HG12	1:E:139:PHE:CZ	2.40	0.55
1:E:217:ILE:HD13	1:I:217:ILE:CG2	2.28	0.55
4:L:15:DA:H8	4:L:15:DA:H5'	1.72	0.55
2:B:244:CYS:SG	2:B:245:SER:N	2.80	0.55
1:E:140:THR:HG23	1:E:140:THR:O	2.06	0.55
2:J:55:LEU:HD23	2:J:148:VAL:HG22	1.87	0.55
2:J:170:LYS:HA	2:J:173:VAL:HG12	1.88	0.55
1:M:483:GLU:OE2	1:M:516:ARG:NE	2.40	0.55
2:N:32:ARG:NH2	2:N:384:GLY:O	2.40	0.55
1:A:14:LEU:CD1	1:A:297:GLN:HB2	2.33	0.55
1:I:302:PRO:HD2	1:I:305:ILE:HD12	1.89	0.55
2:J:328:GLU:HG3	1:M:59:LYS:HE3	1.89	0.55
1:A:128:ALA:HB1	1:A:305:ILE:CG2	2.37	0.55
1:M:24:LEU:HB2	1:M:140:THR:HB	1.89	0.55
1:M:24:LEU:O	1:M:140:THR:HB	2.07	0.55
1:M:317:VAL:HG21	2:N:411:ARG:HB3	1.89	0.55
1:E:143:PHE:O	1:E:189:PHE:CD2	2.60	0.54
1:E:210:LYS:HD2	1:I:244:ASN:ND2	2.07	0.54
1:E:483:GLU:OE2	1:E:516:ARG:NE	2.40	0.54
3:K:11:G:H2'	3:K:12:A:H8	1.72	0.54
1:M:120:ASN:ND2	1:M:288:ASP:OD2	2.40	0.54
2:N:184:ASN:C	2:N:186:THR:H	2.10	0.54
2:N:188:LEU:O	2:N:189:THR:O	2.24	0.54
2:B:146:LEU:HD22	2:B:178:LEU:HD21	1.90	0.54
2:B:170:LYS:HA	2:B:173:VAL:HG12	1.89	0.54
1:E:133:ASN:OD1	1:E:136:LYS:NZ	2.27	0.54
1:E:475:THR:HG23	1:E:487:ALA:HB2	1.89	0.54
1:E:580:SER:OG	2:F:367:GLN:NE2	2.40	0.54
1:I:429:LEU:HD13	1:I:559:ILE:HD13	1.89	0.54
1:M:24:LEU:O	1:M:140:THR:CB	2.55	0.54
1:M:162:TYR:CE2	1:M:169:ALA:HB1	2.43	0.54
4:P:9:DA:H2'	4:P:10:DG:H8	1.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:ARG:CD	3:C:2:U:O4	2.54	0.54
1:E:106:LYS:CE	1:M:176:THR:HG22	2.37	0.54
2:F:32:ARG:NH2	2:F:384:GLY:O	2.40	0.54
4:H:14:DT:H2"	4:H:15:DA:H8	1.73	0.54
1:I:21:MET:HG2	1:I:139:PHE:CD1	2.42	0.54
1:I:144:ASP:O	1:I:145:ASP:CB	2.54	0.54
1:M:23:PHE:O	1:M:23:PHE:HD1	1.91	0.54
4:D:15:DA:H8	4:D:15:DA:H5'	1.72	0.54
2:F:187:ALA:CB	3:G:2:U:C5	2.90	0.54
1:I:552:GLY:HA2	1:I:575:THR:HG22	1.90	0.54
1:M:580:SER:OG	2:N:367:GLN:NE2	2.40	0.54
1:M:164:LEU:CD1	1:M:208:ILE:CD1	2.86	0.54
2:N:280:MET:HE1	2:N:315:GLU:CD	2.28	0.54
1:A:121:ILE:H	1:A:121:ILE:CD1	1.99	0.54
1:A:125:VAL:HG23	1:A:295:TRP:CG	2.43	0.54
1:A:214:ALA:HA	1:M:217:ILE:HG21	1.90	0.54
2:B:377:TRP:CE2	2:B:406:PRO:HB3	2.43	0.54
1:E:26:ALA:H	1:E:142:ASN:HD21	1.56	0.54
2:N:280:MET:HE3	2:N:315:GLU:CB	2.37	0.54
1:A:552:GLY:HA2	1:A:575:THR:HG22	1.90	0.54
2:B:299:MET:HG3	2:B:300:PRO:HD3	1.89	0.54
1:E:26:ALA:H	1:E:142:ASN:CG	2.10	0.54
1:I:330:ALA:HB1	1:I:580:SER:C	2.27	0.54
1:M:513:PRO:HB2	1:M:516:ARG:HB2	1.88	0.54
2:B:170:LYS:HZ1	3:C:1:A:P	2.31	0.54
1:E:171:LEU:HD12	1:E:171:LEU:C	2.27	0.54
1:A:19:HIS:O	1:A:219:PHE:HB3	2.08	0.54
2:B:229:TYR:HA	2:B:241:THR:O	2.08	0.54
2:F:203:ALA:O	2:F:207:LYS:HG3	2.08	0.54
1:M:51:LEU:HD12	1:M:51:LEU:C	2.27	0.54
1:A:16:ASN:ND2	1:A:20:MET:CE	2.67	0.53
2:B:296:ASN:ND2	2:F:470:ARG:NE	2.56	0.53
1:M:566:GLU:CD	1:M:566:GLU:H	2.12	0.53
2:N:19:LEU:HB3	2:N:21:PHE:HE1	1.71	0.53
2:N:47:PRO:HG3	2:N:209:GLY:HA3	1.90	0.53
2:N:261:ASP:N	2:N:452:PHE:HE2	2.06	0.53
1:A:429:LEU:HD13	1:A:559:ILE:HD13	1.89	0.53
2:B:67:ILE:CD1	2:B:193:ARG:HH22	2.18	0.53
2:B:471:PHE:CE1	2:F:138:ARG:HD2	2.42	0.53
1:E:158:HIS:CG	1:M:148:GLU:HB3	2.42	0.53
1:M:237:LEU:C	1:M:241:ILE:HG12	2.19	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:VAL:HG21	2:F:411:ARG:HB3	1.89	0.53
1:I:269:ILE:HD13	1:I:279:ALA:CB	2.38	0.53
1:M:30:ARG:NE	1:M:36:THR:HG21	2.24	0.53
2:B:190:ARG:CZ	2:B:190:ARG:CB	2.85	0.53
2:J:229:TYR:HA	2:J:241:THR:O	2.08	0.53
2:N:93:VAL:HG13	2:N:94:PHE:CD1	2.38	0.53
4:P:14:DT:H2"	4:P:15:DA:H8	1.73	0.53
1:A:121:ILE:CG2	1:A:292:SER:OG	2.57	0.53
2:B:133:MET:SD	2:B:178:LEU:HD23	2.49	0.53
2:J:377:TRP:CE2	2:J:406:PRO:HB3	2.43	0.53
2:J:401:THR:HG1	2:J:402:PRO:HD2	1.69	0.53
2:N:242:THR:HG22	2:N:270:LYS:HZ2	1.73	0.53
2:N:308:THR:HG23	2:N:446:LEU:HD22	1.90	0.53
1:A:572:GLU:N	1:A:572:GLU:OE1	2.42	0.53
2:B:135:GLY:O	2:B:139:GLN:NE2	2.41	0.53
1:E:140:THR:HG21	1:E:182:TYR:CE1	2.43	0.53
1:E:237:LEU:O	1:E:241:ILE:CD1	2.50	0.53
1:E:241:ILE:N	1:E:241:ILE:CD1	2.72	0.53
1:I:212:PHE:CD1	1:I:236:MET:SD	3.01	0.53
1:I:324:PRO:HB3	2:J:7:GLN:HG2	1.90	0.53
1:I:462:ARG:HD3	1:I:474:ILE:HG23	1.91	0.53
2:J:135:GLY:O	2:J:139:GLN:NE2	2.41	0.53
1:M:34:LEU:HD13	1:M:144:ASP:HB3	1.90	0.53
1:E:156:GLY:C	1:M:153:ASP:HB2	2.26	0.53
1:E:566:GLU:CD	1:E:566:GLU:H	2.12	0.53
2:F:47:PRO:HG3	2:F:209:GLY:HA3	1.90	0.53
2:F:187:ALA:HB1	3:G:2:U:C5	2.44	0.53
1:M:164:LEU:HA	1:M:167:SER:HB2	1.89	0.53
2:B:54:TYR:CG	2:B:64:LEU:CD2	2.92	0.53
2:B:136:LEU:HA	2:B:139:GLN:HE21	1.73	0.53
1:E:121:ILE:HD13	1:E:124:ARG:HH21	1.73	0.53
2:N:203:ALA:O	2:N:207:LYS:HG3	2.08	0.53
1:A:349:THR:HB	1:A:397:ASN:HB2	1.91	0.53
2:B:284:LEU:HD11	2:B:305:ILE:HD11	1.91	0.53
1:E:60:HIS:HB3	1:E:67:ILE:CD1	2.39	0.53
1:E:148:GLU:CD	1:E:161:VAL:HG12	2.15	0.53
1:I:349:THR:HB	1:I:397:ASN:HB2	1.91	0.53
1:I:572:GLU:N	1:I:572:GLU:OE1	2.42	0.53
2:J:136:LEU:HA	2:J:139:GLN:HE21	1.73	0.53
1:M:14:LEU:HD12	1:M:14:LEU:C	2.25	0.53
2:N:277:TYR:CD1	2:N:318:GLY:CA	2.92	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CE1	1:A:13:TYR:HB2	2.44	0.52
1:A:125:VAL:HG21	1:A:295:TRP:HB2	1.76	0.52
2:B:444:VAL:HA	2:B:447:VAL:HG12	1.91	0.52
3:C:13:G:H2'	3:C:14:C:C6	2.44	0.52
1:M:163:HIS:NE2	1:M:191:TYR:CZ	2.77	0.52
1:E:139:PHE:N	1:E:139:PHE:CD1	2.77	0.52
2:J:40:TYR:CE2	2:J:214:LYS:CE	2.92	0.52
1:M:162:TYR:HD2	1:M:169:ALA:HB3	1.74	0.52
1:M:268:LEU:HD23	1:M:268:LEU:O	2.08	0.52
1:E:21:MET:HB3	1:E:139:PHE:HE1	1.73	0.52
1:E:156:GLY:C	1:M:153:ASP:HA	2.28	0.52
2:F:93:VAL:HG13	2:F:94:PHE:CD1	2.38	0.52
3:G:12:A:H2'	3:G:13:G:C8	2.44	0.52
3:O:12:A:H2'	3:O:13:G:C8	2.44	0.52
2:B:259:ALA:HB2	2:B:448:TYR:CD2	2.44	0.52
2:F:137:PHE:HA	2:F:140:LYS:HZ1	1.75	0.52
2:F:308:THR:HG23	2:F:446:LEU:HD22	1.90	0.52
1:I:213:LEU:N	1:I:213:LEU:CD2	2.73	0.52
1:I:213:LEU:HB3	1:I:243:GLN:OE1	2.09	0.52
2:J:435:ASN:OD1	2:J:437:THR:OG1	2.18	0.52
2:J:193:ARG:O	2:J:197:MET:HG2	2.09	0.52
1:M:209:HIS:HD1	1:M:209:HIS:C	2.12	0.52
2:B:143:PHE:HE2	2:B:178:LEU:HD11	1.68	0.52
2:B:250:PRO:CA	2:B:295:HIS:HE1	1.97	0.52
1:M:188:ASP:HB3	1:M:190:ARG:CD	2.39	0.52
1:M:195:LYS:O	1:M:195:LYS:HG2	2.10	0.52
2:N:87:TYR:CB	2:N:198:TRP:HE1	2.22	0.52
2:N:184:ASN:O	2:N:186:THR:N	2.43	0.52
1:A:175:ASN:CG	1:M:245:ASN:ND2	2.63	0.52
2:B:334:ILE:HD11	2:B:425:ILE:HD13	1.91	0.52
3:C:11:G:H2'	3:C:12:A:H8	1.72	0.52
2:F:284:LEU:HD13	2:F:323:PHE:HE1	1.75	0.52
1:I:212:PHE:CB	1:I:236:MET:SD	2.98	0.52
2:J:223:ALA:CB	2:J:303:ILE:CD1	2.67	0.52
2:J:374:CYS:SG	2:J:375:LEU:N	2.82	0.52
3:K:13:G:H2'	3:K:14:C:C6	2.44	0.52
2:B:173:VAL:O	2:B:176:LEU:HB2	2.09	0.52
2:B:190:ARG:CB	2:B:190:ARG:NH1	2.73	0.52
2:B:374:CYS:SG	2:B:375:LEU:N	2.82	0.52
1:I:7:ASN:HD22	1:M:52:HIS:CE1	2.26	0.52
1:I:24:LEU:HG	1:I:140:THR:HG21	0.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:TYR:OH	2:B:321:ASP:OD2	2.27	0.52
1:E:4:LEU:HD11	1:E:8:GLU:HB2	1.92	0.52
1:E:46:HIS:HE1	1:E:57:TYR:CE1	2.13	0.52
2:F:262:THR:HG23	2:F:283:VAL:CG2	2.40	0.52
2:N:269:ARG:CB	2:N:269:ARG:NH1	2.73	0.52
1:A:299:LYS:NZ	1:E:47:ARG:HH22	2.08	0.52
2:J:444:VAL:HA	2:J:447:VAL:HG12	1.91	0.52
1:M:188:ASP:HB3	1:M:190:ARG:HD3	1.92	0.52
1:A:462:ARG:HD3	1:A:474:ILE:HG23	1.91	0.51
1:A:512:LYS:HB3	1:A:513:PRO:HD3	1.93	0.51
2:F:105:LEU:CD2	2:F:143:PHE:HB3	2.39	0.51
2:J:196:VAL:HG12	3:K:2:U:C4	2.44	0.51
2:J:284:LEU:HD11	2:J:305:ILE:HD11	1.91	0.51
1:M:32:ALA:CB	1:M:146:VAL:CG2	2.87	0.51
1:E:146:VAL:HG23	1:E:147:ILE:N	2.22	0.51
2:N:277:TYR:CE1	2:N:318:GLY:N	2.77	0.51
2:N:284:LEU:HD13	2:N:323:PHE:HE1	1.75	0.51
2:B:196:VAL:HG12	3:C:2:U:C4	2.44	0.51
2:F:28:THR:O	2:F:430:LYS:NZ	2.42	0.51
2:F:136:LEU:C	2:F:143:PHE:CE2	2.83	0.51
1:M:440:ARG:HB3	1:M:445:TYR:HE2	1.76	0.51
2:N:184:ASN:C	2:N:186:THR:N	2.61	0.51
2:B:174:ALA:N	2:B:175:PRO:CD	2.72	0.51
1:M:192:GLN:NE2	1:M:192:GLN:CA	2.73	0.51
2:N:89:GLY:O	2:N:93:VAL:HG12	2.11	0.51
1:A:21:MET:HE3	1:A:221:LEU:HB2	1.93	0.51
1:E:442:ARG:HG2	4:H:10:DG:OP2	2.10	0.51
2:F:46:LEU:HB2	2:F:47:PRO:HD3	1.92	0.51
1:I:459:LEU:O	1:I:462:ARG:HB2	2.10	0.51
2:J:149:TYR:OH	2:J:185:ASP:OD1	2.25	0.51
2:N:46:LEU:HB2	2:N:47:PRO:HD3	1.91	0.51
2:N:426:LEU:O	2:N:429:THR:OG1	2.29	0.51
1:E:146:VAL:C	1:E:148:GLU:N	2.63	0.51
1:E:190:ARG:HH12	1:E:191:TYR:HE2	1.57	0.51
2:N:280:MET:HE3	2:N:315:GLU:OE1	2.09	0.51
1:A:459:LEU:O	1:A:462:ARG:HB2	2.10	0.51
1:E:580:SER:HB3	2:F:8:LEU:HB2	1.92	0.51
2:J:105:LEU:HD21	2:J:142:ALA:HB3	1.92	0.51
2:B:193:ARG:O	2:B:197:MET:HG2	2.09	0.51
1:E:208:ILE:O	1:E:209:HIS:C	2.47	0.51
1:E:560:SER:HB2	1:E:568:LYS:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:23:PHE:HE1	1:M:141:THR:HG23	1.76	0.51
1:M:165:GLU:OE1	1:M:165:GLU:HA	2.11	0.51
2:N:28:THR:O	2:N:430:LYS:NZ	2.42	0.51
2:N:242:THR:HG22	2:N:270:LYS:NZ	2.26	0.51
1:E:30:ARG:HB2	1:E:36:THR:CG2	2.41	0.51
1:E:120:ASN:HA	2:F:321:ASP:CG	2.31	0.51
1:E:143:PHE:CD1	1:E:143:PHE:N	2.77	0.51
2:J:100:MET:CE	2:J:101:PRO:HD2	2.41	0.51
1:M:580:SER:HB3	2:N:8:LEU:HB2	1.92	0.51
2:B:100:MET:CE	2:B:101:PRO:HD2	2.41	0.51
2:B:291:TYR:HD2	2:B:300:PRO:HG3	1.76	0.51
1:E:40:ILE:CD1	1:E:107:TYR:OH	2.59	0.51
2:J:55:LEU:HD22	2:J:133:MET:HB3	1.93	0.51
1:M:131:GLU:HG3	1:M:155:SER:CB	2.29	0.51
2:N:190:ARG:HA	2:N:190:ARG:HE	1.74	0.51
1:A:21:MET:HG2	1:A:137:VAL:O	2.11	0.50
2:B:61:MET:HE3	2:B:108:LEU:HD21	1.86	0.50
1:E:43:ASP:O	1:E:47:ARG:HG3	2.11	0.50
1:I:139:PHE:O	1:I:140:THR:CG2	2.59	0.50
2:J:334:ILE:HD11	2:J:425:ILE:HD13	1.91	0.50
1:M:9:PHE:CE1	1:M:252:TYR:CE2	2.98	0.50
1:M:41:ILE:HG22	1:M:45:LYS:HE3	1.92	0.50
2:B:133:MET:SD	2:B:178:LEU:CD2	2.99	0.50
2:B:243:CYS:SG	2:B:453:ALA:HA	2.51	0.50
2:J:379:GLN:NE2	2:J:405:ASN:O	2.44	0.50
1:M:137:VAL:HG11	1:M:139:PHE:CE2	2.46	0.50
2:B:105:LEU:HD21	2:B:142:ALA:HB3	1.93	0.50
2:B:114:HIS:O	2:B:117:ALA:HB3	2.11	0.50
2:B:296:ASN:HD22	2:F:470:ARG:NH2	2.09	0.50
1:E:224:SER:HB2	1:E:254:THR:OG1	2.11	0.50
1:I:313:ARG:HB2	2:J:320:PHE:CE2	2.46	0.50
2:J:243:CYS:SG	2:J:453:ALA:HA	2.51	0.50
1:M:133:ASN:OD1	1:M:136:LYS:NZ	2.27	0.50
1:M:238:ARG:HG3	1:M:271:TYR:CZ	2.45	0.50
2:B:248:PHE:HE1	2:B:290:LEU:HD22	1.70	0.50
1:E:48:TYR:HE1	1:E:52:HIS:NE2	2.08	0.50
1:E:164:LEU:HD12	1:E:208:ILE:HD11	1.92	0.50
2:F:292:GLN:NE2	2:F:299:MET:SD	2.85	0.50
1:I:330:ALA:CB	1:I:581:LEU:CA	2.80	0.50
2:J:196:VAL:HG12	3:K:2:U:C5	2.47	0.50
2:J:302:LYS:NZ	2:J:330:GLU:CD	2.50	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:269:ARG:HB3	2:N:269:ARG:NH1	2.26	0.50
2:N:292:GLN:NE2	2:N:299:MET:SD	2.85	0.50
1:E:213:LEU:HB3	1:E:243:GLN:NE2	2.27	0.50
1:E:283:GLU:HG3	1:E:283:GLU:O	2.12	0.50
1:I:481:ALA:HB1	1:I:484:LEU:HD13	1.92	0.50
1:I:525:ARG:HH12	1:I:529:ARG:HH11	1.60	0.50
1:A:481:ALA:HB1	1:A:484:LEU:HD13	1.92	0.50
2:B:55:LEU:HD11	2:B:132:SER:HB3	1.92	0.50
2:B:186:THR:O	2:B:187:ALA:C	2.49	0.50
1:I:21:MET:SD	1:I:221:LEU:HD12	2.52	0.50
1:M:163:HIS:NE2	1:M:191:TYR:OH	2.38	0.50
1:A:144:ASP:C	1:A:146:VAL:N	2.50	0.50
1:A:176:THR:O	1:M:19:HIS:CE1	2.65	0.50
1:E:165:GLU:OE2	1:M:168:TYR:CZ	2.65	0.50
1:E:500:LYS:HE2	1:E:502:TRP:HZ2	1.77	0.50
1:M:252:TYR:HD1	1:M:280:TYR:HB2	1.76	0.50
1:A:13:TYR:C	1:A:13:TYR:CD1	2.85	0.50
1:A:212:PHE:CD1	1:A:212:PHE:C	2.85	0.50
2:F:89:GLY:O	2:F:93:VAL:HG12	2.11	0.50
1:I:232:ASN:ND2	1:I:233:VAL:HG13	2.27	0.50
1:I:416:PHE:HE2	3:K:17:U:H1'	1.77	0.50
1:M:244:ASN:N	1:M:244:ASN:ND2	2.60	0.50
1:M:500:LYS:HE2	1:M:502:TRP:HZ2	1.77	0.50
2:N:432:ASP:OD1	2:N:469:TYR:OH	2.23	0.50
1:A:313:ARG:HB2	2:B:320:PHE:CE2	2.46	0.50
2:B:70:GLU:HG2	2:B:197:MET:HE1	1.83	0.50
2:F:426:LEU:O	2:F:429:THR:OG1	2.29	0.50
1:I:238:ARG:NH1	1:I:271:TYR:HB2	2.14	0.50
1:I:324:PRO:HB3	2:J:7:GLN:CG	2.42	0.50
1:A:416:PHE:HE2	3:C:17:U:H1'	1.77	0.49
2:B:196:VAL:HG12	3:C:2:U:C5	2.47	0.49
2:B:323:PHE:CD2	2:B:327:THR:HG21	2.47	0.49
1:E:478:VAL:HG13	1:E:523:PHE:CD2	2.47	0.49
1:M:269:ILE:HD13	1:M:269:ILE:N	2.27	0.49
2:N:56:ALA:HB2	2:N:149:TYR:HB3	1.94	0.49
3:O:11:G:H2'	3:O:12:A:H8	1.77	0.49
1:A:130:LEU:O	1:A:131:GLU:C	2.48	0.49
1:A:232:ASN:ND2	1:A:233:VAL:HG13	2.27	0.49
1:A:244:ASN:ND2	1:M:210:LYS:O	2.45	0.49
2:B:222:GLU:HG2	2:B:302:LYS:HB3	1.94	0.49
2:B:301:ARG:CZ	1:E:59:LYS:O	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HD12	1:E:8:GLU:CD	2.26	0.49
1:I:253:TRP:CZ3	1:I:268:LEU:HD13	2.46	0.49
2:J:167:ASP:OD2	2:J:455:VAL:HA	2.13	0.49
2:J:323:PHE:CD2	2:J:327:THR:HG21	2.47	0.49
1:M:478:VAL:HG13	1:M:523:PHE:CD2	2.47	0.49
2:N:415:ASN:OD1	2:N:416:GLY:N	2.45	0.49
1:E:148:GLU:OE2	1:E:184:LYS:CE	2.60	0.49
1:E:384:GLU:O	1:E:388:ARG:HG2	2.12	0.49
3:G:11:G:H2'	3:G:12:A:H8	1.77	0.49
2:J:55:LEU:HD11	2:J:132:SER:HB3	1.93	0.49
1:M:49:TYR:CD1	1:M:49:TYR:C	2.85	0.49
2:B:250:PRO:CD	2:B:254:GLY:O	2.54	0.49
2:F:415:ASN:OD1	2:F:416:GLY:N	2.45	0.49
1:I:512:LYS:HB3	1:I:513:PRO:HD3	1.92	0.49
2:F:56:ALA:HB2	2:F:149:TYR:HB3	1.94	0.49
2:J:100:MET:HE3	2:J:101:PRO:HD2	1.93	0.49
1:M:440:ARG:HB3	1:M:445:TYR:CE2	2.47	0.49
2:N:335:ILE:HD12	4:P:12:DT:H5"	1.94	0.49
1:A:125:VAL:HG13	1:A:291:LEU:HB3	1.93	0.49
2:B:55:LEU:HD22	2:B:133:MET:HB3	1.94	0.49
2:B:167:ASP:OD2	2:B:455:VAL:HA	2.13	0.49
2:F:134:SER:O	2:F:137:PHE:HB2	2.11	0.49
1:I:16:ASN:HD22	1:I:16:ASN:C	2.06	0.49
2:J:114:HIS:O	2:J:117:ALA:HB3	2.11	0.49
1:M:168:TYR:CD1	1:M:168:TYR:C	2.86	0.49
1:M:271:TYR:CD1	1:M:271:TYR:C	2.85	0.49
2:F:335:ILE:HD12	4:H:12:DT:H5"	1.94	0.49
1:M:428:ALA:HB1	1:M:559:ILE:HG13	1.94	0.49
3:O:10:A:H2'	3:O:11:G:C8	2.48	0.49
1:E:210:LYS:CA	1:E:210:LYS:CE	2.89	0.49
4:P:7:DA:H2'	4:P:8:DC:C6	2.48	0.49
1:A:561:CYS:SG	1:A:569:ALA:HB3	2.53	0.49
2:B:260:TYR:HA	2:B:452:PHE:CE2	2.48	0.49
1:I:209:HIS:O	1:I:213:LEU:HD23	2.12	0.49
2:N:181:GLN:NE2	2:N:182:ILE:O	2.45	0.49
1:A:525:ARG:HH12	1:A:529:ARG:HH11	1.60	0.49
1:A:536:SER:HB3	2:B:343:LEU:HD21	1.94	0.49
2:B:117:ALA:O	2:B:156:LYS:NZ	2.39	0.49
2:B:190:ARG:CG	2:B:190:ARG:NH1	2.73	0.49
2:F:139:GLN:HB3	2:F:142:ALA:HB2	1.95	0.49
2:F:181:GLN:NE2	2:F:182:ILE:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:LEU:HB2	1:I:140:THR:OG1	2.09	0.49
1:I:331:LEU:HD13	2:J:365:LEU:HD21	1.93	0.49
2:N:344:LYS:HB2	2:N:361:VAL:HA	1.94	0.49
1:E:122:GLY:C	1:E:291:LEU:HD12	2.31	0.48
1:E:217:ILE:HG21	1:I:217:ILE:HG23	1.89	0.48
1:E:288:ASP:CG	2:F:277:TYR:HE2	2.16	0.48
1:I:536:SER:HB3	2:J:343:LEU:HD21	1.94	0.48
2:J:277:TYR:OH	2:J:321:ASP:OD2	2.27	0.48
1:M:248:PRO:C	1:M:278:ARG:NH1	2.66	0.48
1:M:509:ILE:HD11	1:M:531:ARG:NH2	2.27	0.48
1:E:164:LEU:HD21	1:E:186:HIS:C	2.33	0.48
1:E:428:ALA:HB1	1:E:559:ILE:HG13	1.94	0.48
1:I:322:PRO:HD2	2:J:9:ALA:HB1	1.94	0.48
1:A:245:ASN:HD22	1:M:214:ALA:HB1	1.77	0.48
2:B:257:PHE:CE1	2:B:448:TYR:CD2	3.01	0.48
2:B:257:PHE:CE2	2:B:444:VAL:HB	2.48	0.48
1:M:32:ALA:HB1	1:M:146:VAL:CG2	2.43	0.48
1:M:236:MET:O	1:M:240:ALA:N	2.43	0.48
1:M:560:SER:HB2	1:M:568:LYS:HD3	1.93	0.48
2:N:284:LEU:HD13	2:N:323:PHE:CE1	2.48	0.48
1:A:18:GLN:H	1:A:18:GLN:NE2	2.11	0.48
1:E:121:ILE:CD1	2:F:317:GLN:NE2	2.76	0.48
1:E:248:PRO:O	1:E:278:ARG:NH1	2.47	0.48
4:H:6:DA:H2'	4:H:7:DA:C8	2.49	0.48
1:I:234:MET:HA	1:I:234:MET:HE1	1.89	0.48
1:I:407:ILE:O	1:I:411:VAL:HG13	2.13	0.48
2:J:49:GLN:NE2	2:J:49:GLN:H	2.11	0.48
1:M:41:ILE:O	1:M:45:LYS:HG3	2.13	0.48
1:M:226:TYR:CD2	1:M:253:TRP:CZ2	3.00	0.48
1:M:463:LYS:HD2	1:M:463:LYS:O	2.13	0.48
2:B:137:PHE:CZ	2:B:176:LEU:CD1	2.96	0.48
1:E:163:HIS:ND1	1:E:163:HIS:N	2.60	0.48
1:E:423:GLU:OE1	1:E:444:HIS:NE2	2.33	0.48
4:H:7:DA:H2'	4:H:8:DC:C6	2.48	0.48
1:M:221:LEU:O	1:M:251:LEU:HA	2.13	0.48
1:M:384:GLU:O	1:M:388:ARG:HG2	2.12	0.48
1:E:154:ILE:HD11	1:E:309:VAL:CG2	2.40	0.48
1:I:309:VAL:HG23	1:I:310:ARG:H	1.79	0.48
1:I:561:CYS:SG	1:I:569:ALA:HB3	2.53	0.48
2:N:285:SER:HA	2:N:288:LEU:CD2	2.44	0.48
4:P:6:DA:H2'	4:P:7:DA:H8	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:OE2	1:A:218:ARG:NH2	2.47	0.48
2:B:29:HIS:HD2	2:B:30:PRO:HD2	1.79	0.48
1:E:26:ALA:CA	1:E:142:ASN:OD1	2.60	0.48
2:F:100:MET:HG2	2:F:101:PRO:HD2	1.96	0.48
3:G:10:A:H2'	3:G:11:G:C8	2.48	0.48
1:I:269:ILE:CD1	1:I:279:ALA:HB1	2.39	0.48
2:J:70:GLU:HB3	2:J:197:MET:HE1	1.95	0.48
1:M:423:GLU:OE1	1:M:444:HIS:NE2	2.33	0.48
1:M:460:ASP:N	1:M:460:ASP:OD1	2.47	0.48
1:A:407:ILE:O	1:A:411:VAL:HG13	2.13	0.48
4:D:16:DA:H2"	4:D:17:DC:H5"	1.96	0.48
1:E:190:ARG:NH1	1:E:191:TYR:CZ	2.82	0.48
1:E:240:ALA:O	1:E:243:GLN:HG3	2.13	0.48
1:E:460:ASP:N	1:E:460:ASP:OD1	2.47	0.48
1:A:245:ASN:HD22	1:M:214:ALA:CB	2.27	0.48
2:B:49:GLN:NE2	2:B:49:GLN:H	2.11	0.48
1:E:9:PHE:CE2	1:E:290:MET:CE	2.97	0.48
1:E:164:LEU:CD1	1:E:208:ILE:HD11	2.43	0.48
1:E:463:LYS:HD2	1:E:463:LYS:O	2.14	0.48
2:F:284:LEU:HD13	2:F:323:PHE:CE1	2.48	0.48
1:I:213:LEU:HD13	1:I:240:ALA:HA	1.95	0.48
1:M:32:ALA:HB2	1:M:146:VAL:HG21	1.91	0.48
1:A:508:GLU:OE2	1:A:517:ARG:NH1	2.43	0.48
2:B:251:ASP:HB2	2:F:177:ASN:HD22	1.77	0.48
2:B:332:VAL:HG11	2:B:409:LEU:HD23	1.96	0.48
4:D:18:DA:H4'	4:D:19:DG:OP1	2.14	0.48
2:J:386:ASN:ND2	2:J:388:GLN:O	2.47	0.48
1:M:484:LEU:HD21	1:M:519:GLU:HB2	1.96	0.48
2:N:242:THR:CG2	2:N:270:LYS:NZ	2.77	0.48
1:A:419:SER:HA	1:A:422:GLU:HG2	1.96	0.47
2:B:149:TYR:OH	2:B:185:ASP:OD1	2.25	0.47
2:B:409:LEU:HD21	2:B:425:ILE:HD12	1.97	0.47
2:B:465:GLU:OE1	2:B:465:GLU:N	2.47	0.47
2:F:285:SER:HA	2:F:288:LEU:CD2	2.44	0.47
2:F:327:THR:O	2:F:327:THR:OG1	2.31	0.47
4:H:18:DA:H2"	4:H:19:DG:O5'	2.14	0.47
1:I:295:TRP:O	1:I:298:VAL:HG12	2.15	0.47
1:M:44:LEU:HD23	1:M:47:ARG:HD3	1.96	0.47
1:A:254:THR:HB	1:A:290:MET:HE2	1.96	0.47
1:A:374:TYR:HD1	1:A:375:THR:N	2.13	0.47
2:B:190:ARG:NH1	2:B:190:ARG:HA	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:THR:O	1:E:141:THR:OG1	2.29	0.47
1:E:209:HIS:CE1	1:E:213:LEU:HD11	2.49	0.47
1:E:288:ASP:OD1	2:F:277:TYR:CE2	2.67	0.47
2:F:344:LYS:HB2	2:F:361:VAL:HA	1.95	0.47
4:H:23:DT:H2"	4:H:24:DA:OP2	2.15	0.47
1:I:419:SER:HA	1:I:422:GLU:HG2	1.96	0.47
2:J:56:ALA:HB2	2:J:149:TYR:HB3	1.96	0.47
4:P:6:DA:H2'	4:P:7:DA:C8	2.49	0.47
1:A:367:SER:O	1:A:367:SER:OG	2.21	0.47
1:E:163:HIS:CD2	1:E:191:TYR:HE2	2.06	0.47
4:L:16:DA:H2"	4:L:17:DC:H5"	1.96	0.47
2:F:134:SER:HA	2:F:137:PHE:CD2	2.49	0.47
1:M:522:ASP:O	1:M:526:SER:N	2.38	0.47
1:A:22:TRP:HB2	1:A:138:VAL:HG22	1.96	0.47
1:A:381:LEU:HB2	1:A:420:PHE:HZ	1.80	0.47
2:B:386:ASN:ND2	2:B:388:GLN:O	2.47	0.47
4:H:6:DA:H2'	4:H:7:DA:H8	1.79	0.47
1:I:240:ALA:O	1:I:243:GLN:HG2	2.15	0.47
1:I:325:GLY:HA3	2:J:10:ALA:HB2	1.95	0.47
1:I:483:GLU:OE2	1:I:516:ARG:NE	2.47	0.47
1:M:244:ASN:N	1:M:244:ASN:HD22	2.10	0.47
1:M:253:TRP:C	1:M:253:TRP:CD1	2.88	0.47
2:N:195:ASN:HD22	2:N:195:ASN:HA	1.56	0.47
2:N:401:THR:HB	3:O:6:U:H5"	1.96	0.47
1:A:483:GLU:OE2	1:A:516:ARG:NE	2.47	0.47
2:B:401:THR:HB	3:C:6:U:H4'	1.95	0.47
1:E:4:LEU:HD11	1:E:8:GLU:CB	2.44	0.47
1:I:141:THR:HG21	1:I:226:TYR:CE1	2.49	0.47
1:I:217:ILE:CD1	1:I:245:ASN:CA	2.93	0.47
1:I:253:TRP:HZ3	1:I:268:LEU:HD13	1.79	0.47
1:I:508:GLU:OE2	1:I:517:ARG:NH1	2.43	0.47
1:M:81:PRO:HD2	1:M:91:PHE:CE2	2.49	0.47
1:A:309:VAL:HG23	1:A:310:ARG:H	1.79	0.47
1:E:60:HIS:HB3	1:E:67:ILE:HD12	1.96	0.47
1:E:445:TYR:CE1	1:E:491:SER:HB3	2.49	0.47
1:I:267:ASP:C	1:I:271:TYR:CD2	2.84	0.47
1:I:305:ILE:O	1:I:309:VAL:HG22	2.15	0.47
1:I:374:TYR:HD1	1:I:375:THR:N	2.13	0.47
2:J:29:HIS:HD2	2:J:30:PRO:HD2	1.79	0.47
1:M:127:ALA:O	1:M:151:PHE:CD2	2.54	0.47
4:P:18:DA:H2"	4:P:19:DG:O5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:PRO:HD2	1:E:91:PHE:CE2	2.49	0.47
1:E:217:ILE:CG2	1:I:217:ILE:HG21	2.26	0.47
1:E:484:LEU:HD21	1:E:519:GLU:HB2	1.96	0.47
2:F:87:TYR:CE2	2:F:197:MET:HB3	2.49	0.47
2:F:171:ALA:HB2	2:F:455:VAL:HG13	1.97	0.47
2:F:219:ASP:HB3	2:F:222:GLU:HG3	1.97	0.47
2:F:401:THR:HB	3:G:6:U:H5"	1.96	0.47
1:M:26:ALA:HA	1:M:142:ASN:OD1	2.15	0.47
1:M:445:TYR:CE1	1:M:491:SER:HB3	2.49	0.47
2:N:219:ASP:HB3	2:N:222:GLU:HG3	1.97	0.47
2:N:277:TYR:HE1	2:N:318:GLY:N	2.12	0.47
1:A:141:THR:HG21	1:A:226:TYR:CE1	2.50	0.47
1:E:62:ILE:O	1:E:68:LYS:HG3	2.15	0.47
2:F:444:VAL:HA	2:F:447:VAL:HG22	1.96	0.47
1:M:221:LEU:CB	1:M:247:PHE:CE1	2.98	0.47
1:A:440:ARG:HG2	1:A:441:HIS:ND1	2.30	0.47
1:A:580:SER:HB3	2:B:8:LEU:HB2	1.97	0.47
1:E:83:GLN:O	1:E:85:SER:N	2.48	0.47
1:E:140:THR:CG2	1:E:182:TYR:CE1	2.97	0.47
1:I:580:SER:HB3	2:J:8:LEU:HB2	1.97	0.47
1:M:61:ASP:OD1	1:M:64:ASN:N	2.46	0.47
1:M:502:TRP:HH2	2:N:8:LEU:HD21	1.80	0.47
1:A:305:ILE:O	1:A:309:VAL:HG22	2.15	0.46
2:B:12:SER:HB2	2:B:366:TYR:CE2	2.50	0.46
2:B:379:GLN:NE2	2:B:405:ASN:O	2.48	0.46
1:E:223:VAL:HG11	1:E:253:TRP:CD2	2.50	0.46
2:B:56:ALA:HB2	2:B:149:TYR:HB3	1.96	0.46
1:I:121:ILE:H	1:I:121:ILE:HD12	1.81	0.46
1:I:217:ILE:HD12	1:I:245:ASN:CB	2.40	0.46
1:I:495:GLU:OE2	2:J:340:TRP:NE1	2.32	0.46
2:J:155:LYS:HA	2:J:158:PHE:CG	2.50	0.46
2:J:185:ASP:O	2:J:189:THR:CB	2.63	0.46
1:M:8:GLU:O	1:M:12:HIS:ND1	2.47	0.46
1:M:247:PHE:O	1:M:278:ARG:NH1	2.48	0.46
2:B:100:MET:HE3	2:B:101:PRO:HD2	1.96	0.46
1:E:139:PHE:HZ	1:E:215:ALA:CB	2.27	0.46
2:F:229:TYR:O	2:F:450:GLN:NE2	2.40	0.46
3:K:8:U:H2'	3:K:9:U:C6	2.51	0.46
1:M:83:GLN:O	1:M:85:SER:N	2.48	0.46
2:N:444:VAL:HA	2:N:447:VAL:HG22	1.96	0.46
4:P:23:DT:H2"	4:P:24:DA:OP2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TRP:O	1:A:298:VAL:HG12	2.15	0.46
2:B:330:GLU:N	2:B:330:GLU:OE1	2.48	0.46
1:E:9:PHE:CE2	1:E:290:MET:HE3	2.50	0.46
1:E:509:ILE:HD11	1:E:531:ARG:NH2	2.27	0.46
1:M:125:VAL:HG12	1:M:291:LEU:HD12	1.98	0.46
3:C:11:G:N2	4:D:14:DT:O2	2.49	0.46
1:E:468:LYS:HA	1:E:468:LYS:HD2	1.73	0.46
2:F:136:LEU:HA	2:F:143:PHE:HE2	1.78	0.46
2:F:225:ILE:HG23	2:F:244:CYS:SG	2.56	0.46
1:I:238:ARG:HH11	1:I:271:TYR:HB2	1.78	0.46
1:I:440:ARG:HG2	1:I:441:HIS:ND1	2.30	0.46
1:M:83:GLN:HG3	1:M:84:TRP:H	1.81	0.46
1:M:286:THR:HG23	1:M:289:GLU:H	1.80	0.46
2:B:296:ASN:ND2	2:F:470:ARG:NH2	2.64	0.46
2:F:44:PHE:HD2	2:F:46:LEU:HG	1.80	0.46
1:I:267:ASP:C	1:I:271:TYR:HD2	2.15	0.46
2:J:224:TYR:HB2	2:J:247:VAL:HG12	1.97	0.46
2:J:277:TYR:CE1	2:J:281:GLN:HG3	2.50	0.46
2:J:332:VAL:HG11	2:J:409:LEU:HD23	1.96	0.46
1:M:162:TYR:CD2	1:M:169:ALA:CB	2.98	0.46
3:O:18:U:H2'	3:O:19:A:C8	2.51	0.46
1:A:384:GLU:O	1:A:388:ARG:HG2	2.16	0.46
1:E:10:TYR:HB3	1:E:297:GLN:OE1	2.15	0.46
1:E:148:GLU:OE2	1:E:161:VAL:CB	2.64	0.46
2:F:143:PHE:O	2:F:143:PHE:CD1	2.69	0.46
1:I:381:LEU:HB2	1:I:420:PHE:HZ	1.80	0.46
2:J:173:VAL:HG21	2:J:180:ILE:HD11	1.97	0.46
2:J:190:ARG:HH11	2:J:191:GLN:N	2.07	0.46
1:M:339:VAL:HG12	1:M:572:GLU:HG3	1.97	0.46
2:N:225:ILE:HG23	2:N:244:CYS:SG	2.56	0.46
2:B:224:TYR:HB2	2:B:247:VAL:HG12	1.97	0.46
1:E:174:LEU:HD13	1:E:214:ALA:CB	2.46	0.46
2:F:316:ILE:HD11	2:F:412:PHE:HD2	1.81	0.46
1:I:384:GLU:O	1:I:388:ARG:HG2	2.16	0.46
2:J:12:SER:HB2	2:J:366:TYR:CE2	2.50	0.46
2:J:246:GLN:O	2:J:257:PHE:HA	2.16	0.46
2:J:409:LEU:HD21	2:J:425:ILE:HD12	1.97	0.46
4:L:15:DA:H5'	4:L:15:DA:C8	2.51	0.46
1:M:31:SER:C	1:M:33:GLY:N	2.69	0.46
1:M:50:CYS:O	1:M:53:GLU:O	2.33	0.46
1:M:213:LEU:HA	1:M:243:GLN:HE22	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:PHE:HD2	2:N:46:LEU:HG	1.79	0.46
2:N:100:MET:HG2	2:N:101:PRO:HD2	1.96	0.46
2:B:155:LYS:HA	2:B:158:PHE:CG	2.50	0.46
2:B:379:GLN:NE2	2:B:441:LYS:HD2	2.31	0.46
2:B:430:LYS:HE2	2:B:430:LYS:HB3	1.78	0.46
1:E:58:GLN:HE21	1:E:58:GLN:HB2	1.62	0.46
1:E:502:TRP:HH2	2:F:8:LEU:HD21	1.81	0.46
1:I:497:ARG:HD3	1:I:497:ARG:HA	1.62	0.46
4:L:18:DA:H4'	4:L:19:DG:OP1	2.14	0.46
1:A:213:LEU:HD13	1:A:243:GLN:HE22	1.80	0.46
2:B:248:PHE:HE2	2:B:294:SER:CB	2.25	0.46
3:C:8:U:H2'	3:C:9:U:C6	2.51	0.46
1:E:10:TYR:CE1	1:E:293:LYS:HB3	2.50	0.46
1:E:213:LEU:HA	1:E:213:LEU:HD23	1.48	0.46
1:E:284:THR:O	1:E:284:THR:OG1	2.29	0.46
1:E:339:VAL:HG12	1:E:572:GLU:HG3	1.97	0.46
2:F:432:ASP:OD1	2:F:469:TYR:OH	2.23	0.46
1:M:91:PHE:CZ	1:M:95:LEU:HD12	2.51	0.46
1:M:492:ILE:HA	1:M:504:MET:O	2.16	0.46
2:N:270:LYS:HE3	2:N:279:GLU:OE1	2.15	0.46
1:A:9:PHE:O	1:A:9:PHE:CD1	2.70	0.45
1:E:23:PHE:HB3	1:E:223:VAL:HG23	1.98	0.45
1:E:223:VAL:HG11	1:E:253:TRP:CE3	2.50	0.45
1:I:291:LEU:HD23	1:I:291:LEU:HA	1.79	0.45
2:J:302:LYS:HE3	2:J:328:GLU:HB3	1.97	0.45
3:K:11:G:N2	4:L:14:DT:O2	2.49	0.45
2:B:173:VAL:HG21	2:B:180:ILE:HD11	1.97	0.45
2:B:173:VAL:HG22	2:B:178:LEU:HB3	1.96	0.45
2:B:255:PHE:HD2	2:B:433:TRP:CZ2	2.33	0.45
1:E:83:GLN:HG3	1:E:84:TRP:H	1.81	0.45
1:E:91:PHE:CZ	1:E:95:LEU:HD12	2.51	0.45
1:E:287:PHE:CE2	1:E:291:LEU:CD1	2.94	0.45
2:F:262:THR:HG23	2:F:283:VAL:HG23	1.98	0.45
4:H:16:DA:H2"	4:H:17:DC:H5"	1.97	0.45
2:N:171:ALA:HB2	2:N:455:VAL:HG13	1.97	0.45
1:A:298:VAL:HG13	1:A:301:LYS:HD3	1.99	0.45
2:N:316:ILE:HD11	2:N:412:PHE:HD2	1.81	0.45
1:E:49:TYR:HE2	1:E:60:HIS:NE2	2.15	0.45
1:E:159:LEU:CD1	1:E:180:PRO:HG2	2.47	0.45
1:E:220:GLY:HA2	1:E:247:PHE:HB3	1.98	0.45
2:F:136:LEU:C	2:F:143:PHE:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:379:GLN:NE2	2:J:441:LYS:HD2	2.31	0.45
1:M:24:LEU:CG	1:M:140:THR:HG22	2.45	0.45
1:M:46:HIS:HD2	1:M:71:ILE:HD11	1.82	0.45
1:M:174:LEU:HD21	1:M:218:ARG:HD3	1.99	0.45
1:E:213:LEU:HD21	1:E:240:ALA:CB	2.45	0.45
1:I:531:ARG:O	2:J:402:PRO:HB3	2.16	0.45
1:M:140:THR:C	1:M:142:ASN:H	2.20	0.45
2:N:158:PHE:O	3:O:1:A:N6	2.35	0.45
2:N:239:GLU:OE1	2:N:269:ARG:CD	2.64	0.45
4:P:16:DA:H2"	4:P:17:DC:H5"	1.97	0.45
1:E:385:PRO:O	1:E:389:LYS:HG3	2.17	0.45
2:F:187:ALA:HB2	3:G:2:U:C5	2.51	0.45
1:I:268:LEU:C	1:I:268:LEU:CD2	2.84	0.45
2:J:113:CYS:O	2:J:116:VAL:HG12	2.16	0.45
1:A:387:ILE:HA	1:A:390:ILE:HG22	1.99	0.45
1:E:219:PHE:O	1:E:248:PRO:HD2	2.17	0.45
1:E:492:ILE:HA	1:E:504:MET:O	2.16	0.45
1:I:267:ASP:HB3	1:I:271:TYR:HE2	1.82	0.45
1:I:326:LYS:CA	1:I:581:LEU:CB	2.87	0.45
2:J:40:TYR:O	2:J:40:TYR:CD1	2.70	0.45
2:J:281:GLN:OE1	2:J:321:ASP:HB2	2.14	0.45
1:M:195:LYS:NZ	1:M:195:LYS:CB	2.72	0.45
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.79	0.45
1:A:463:LYS:HD2	1:A:463:LYS:HA	1.73	0.45
2:B:52:LEU:O	2:B:101:PRO:HB3	2.17	0.45
1:E:305:ILE:O	1:E:309:VAL:HG23	2.17	0.45
1:E:360:LYS:HD3	1:E:360:LYS:HA	1.77	0.45
2:F:247:VAL:HG12	2:F:257:PHE:CD1	2.51	0.45
2:F:301:ARG:NH1	2:F:302:LYS:HD2	2.29	0.45
2:J:277:TYR:CD1	2:J:281:GLN:HG3	2.52	0.45
1:A:333:THR:HG22	1:A:334:ASN:H	1.81	0.45
2:B:290:LEU:HD23	2:B:290:LEU:C	2.36	0.45
1:E:174:LEU:C	1:E:174:LEU:CD2	2.85	0.45
2:F:191:GLN:OE1	2:F:191:GLN:N	2.50	0.45
2:F:310:HIS:HB2	2:F:412:PHE:CZ	2.51	0.45
3:G:18:U:H2'	3:G:19:A:C8	2.51	0.45
1:I:463:LYS:HD2	1:I:463:LYS:HA	1.73	0.45
1:I:468:LYS:HB3	1:I:468:LYS:HE3	1.74	0.45
2:J:185:ASP:CA	2:J:188:LEU:CD2	2.80	0.45
2:J:330:GLU:OE2	2:J:414:GLY:HA2	2.16	0.45
1:M:6:ASP:OD1	1:M:7:ASN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:O	1:A:182:TYR:HB3	2.17	0.45
1:E:13:TYR:CG	1:E:13:TYR:O	2.70	0.45
1:E:106:LYS:NZ	1:M:176:THR:HG22	2.32	0.45
1:E:122:GLY:HA2	1:E:291:LEU:CB	2.45	0.45
1:E:256:PRO:HA	1:E:285:GLY:O	2.17	0.45
1:I:238:ARG:HH12	1:I:271:TYR:CA	2.29	0.45
2:J:281:GLN:HG2	2:J:318:GLY:O	2.17	0.45
1:E:13:TYR:O	1:E:13:TYR:CD1	2.70	0.44
1:E:30:ARG:HH11	1:E:36:THR:HG1	1.60	0.44
1:E:60:HIS:ND1	1:E:60:HIS:N	2.66	0.44
1:E:252:TYR:HA	1:E:280:TYR:O	2.17	0.44
1:E:342:SER:HA	1:E:404:ILE:O	2.17	0.44
1:E:381:LEU:HB2	1:E:420:PHE:HZ	1.82	0.44
1:I:387:ILE:HA	1:I:390:ILE:HG22	1.99	0.44
1:I:418:LYS:NZ	4:L:11:DC:OP1	2.50	0.44
2:J:377:TRP:CD2	2:J:406:PRO:HB3	2.53	0.44
1:M:23:PHE:O	1:M:23:PHE:CD1	2.70	0.44
1:M:119:LEU:HD12	1:M:146:VAL:HG13	1.98	0.44
1:A:19:HIS:HB2	1:A:219:PHE:HB3	1.98	0.44
2:B:113:CYS:O	2:B:116:VAL:HG12	2.16	0.44
2:B:234:ASN:OD1	2:B:235:ALA:N	2.50	0.44
1:E:9:PHE:CZ	1:E:290:MET:HE2	2.51	0.44
1:E:152:SER:OG	1:M:158:HIS:HA	2.17	0.44
2:F:35:SER:HA	2:F:93:VAL:HG23	1.98	0.44
1:I:331:LEU:HD13	2:J:365:LEU:CD2	2.47	0.44
2:J:465:GLU:N	2:J:465:GLU:OE1	2.47	0.44
1:M:34:LEU:CD1	1:M:144:ASP:HB3	2.48	0.44
2:N:247:VAL:HG12	2:N:257:PHE:CD1	2.51	0.44
2:N:260:TYR:O	2:N:260:TYR:CD1	2.70	0.44
2:N:275:LEU:HB2	2:N:280:MET:CE	2.48	0.44
1:A:131:GLU:HB2	1:A:151:PHE:HE1	1.83	0.44
1:A:418:LYS:NZ	4:D:11:DC:OP1	2.50	0.44
2:B:377:TRP:CD2	2:B:406:PRO:HB3	2.53	0.44
1:E:21:MET:HE1	1:E:139:PHE:CZ	2.52	0.44
2:F:55:LEU:HB3	2:F:148:VAL:HG22	2.00	0.44
2:J:52:LEU:O	2:J:101:PRO:HB3	2.17	0.44
1:M:61:ASP:OD2	1:M:64:ASN:HB2	2.17	0.44
1:M:371:LEU:HD21	1:M:423:GLU:HG2	2.00	0.44
2:N:310:HIS:HB2	2:N:412:PHE:CZ	2.51	0.44
1:A:9:PHE:CD1	1:A:9:PHE:C	2.89	0.44
1:E:161:VAL:HG12	1:E:182:TYR:CD2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:HIS:CG	2:F:32:ARG:HB3	2.53	0.44
2:F:44:PHE:CD2	2:F:46:LEU:HG	2.52	0.44
2:F:139:GLN:HE21	2:F:139:GLN:H	1.65	0.44
2:F:376:LEU:HD22	2:F:409:LEU:HD11	2.00	0.44
1:M:385:PRO:O	1:M:389:LYS:HG3	2.17	0.44
2:N:29:HIS:CG	2:N:32:ARG:HB3	2.53	0.44
1:E:121:ILE:HD12	1:E:121:ILE:HA	1.78	0.44
1:E:130:LEU:HD21	1:E:138:VAL:HG23	2.00	0.44
1:E:512:LYS:HB3	1:E:513:PRO:HD3	1.99	0.44
2:J:234:ASN:OD1	2:J:235:ALA:N	2.50	0.44
1:M:305:ILE:O	1:M:309:VAL:HG23	2.17	0.44
2:N:284:LEU:HD23	2:N:284:LEU:HA	1.74	0.44
2:N:376:LEU:HD22	2:N:409:LEU:HD11	1.99	0.44
2:B:248:PHE:CZ	2:B:290:LEU:CD2	2.99	0.44
1:E:60:HIS:CB	1:E:67:ILE:HD12	2.48	0.44
1:E:163:HIS:CD2	1:E:165:GLU:HB2	2.53	0.44
1:I:241:ILE:HA	1:I:246:ALA:HB1	2.00	0.44
1:M:44:LEU:HA	1:M:47:ARG:CG	2.46	0.44
1:M:137:VAL:CG1	1:M:139:PHE:CE2	3.00	0.44
2:N:35:SER:HA	2:N:93:VAL:HG23	1.98	0.44
2:N:87:TYR:HD1	2:N:88:GLY:N	2.16	0.44
2:N:105:LEU:HD23	2:N:105:LEU:HA	1.82	0.44
2:N:280:MET:HE3	2:N:315:GLU:HB3	1.99	0.44
2:N:284:LEU:HD12	2:N:319:ALA:HA	2.00	0.44
2:B:232:LYS:HB3	2:B:239:GLU:HB3	1.99	0.44
4:D:6:DA:H2'	4:D:7:DA:H8	1.82	0.44
2:F:379:GLN:HE21	2:F:441:LYS:HG3	1.83	0.44
3:G:11:G:N2	4:H:14:DT:O2	2.51	0.44
1:I:330:ALA:HB2	1:I:581:LEU:CG	2.44	0.44
1:I:333:THR:HG22	1:I:334:ASN:H	1.81	0.44
2:J:185:ASP:OD1	2:J:188:LEU:HD11	2.18	0.44
2:J:232:LYS:HB3	2:J:239:GLU:HB3	1.99	0.44
2:J:341:TYR:HD2	2:J:403:LEU:HD23	1.69	0.44
2:J:410:ARG:HG2	2:J:412:PHE:CE2	2.53	0.44
1:M:269:ILE:HG13	1:M:281:LEU:HB2	2.00	0.44
2:N:196:VAL:HG12	2:N:197:MET:SD	2.57	0.44
4:P:18:DA:H4'	4:P:19:DG:OP1	2.18	0.44
2:B:258:VAL:CG1	2:B:290:LEU:HD11	2.37	0.44
1:E:148:GLU:CG	1:E:161:VAL:CG1	2.95	0.44
1:E:168:TYR:CE1	1:M:192:GLN:N	2.85	0.44
1:E:371:LEU:HD21	1:E:423:GLU:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:270:LYS:HA	2:F:270:LYS:HD2	1.84	0.44
2:J:225:ILE:N	2:J:304:PHE:O	2.48	0.44
1:A:394:ASP:OD1	1:A:395:GLU:N	2.51	0.44
4:D:15:DA:H5'	4:D:15:DA:C8	2.51	0.44
1:E:61:ASP:OD1	1:E:61:ASP:N	2.50	0.44
1:E:148:GLU:HG2	1:E:182:TYR:HD2	1.78	0.44
1:E:223:VAL:CG1	1:E:253:TRP:CD2	3.01	0.44
2:F:55:LEU:HD23	2:F:148:VAL:HG22	1.99	0.44
2:F:87:TYR:HD1	2:F:88:GLY:N	2.16	0.44
2:F:149:TYR:CE2	2:F:188:LEU:CD1	2.95	0.44
2:F:220:LYS:O	2:F:291:TYR:OH	2.36	0.44
1:M:23:PHE:CD1	1:M:23:PHE:C	2.92	0.44
1:M:342:SER:HA	1:M:404:ILE:O	2.17	0.44
1:M:502:TRP:CH2	2:N:8:LEU:HD21	2.53	0.44
2:N:44:PHE:CD2	2:N:46:LEU:HG	2.52	0.44
1:A:218:ARG:HB3	1:A:218:ARG:HH11	1.83	0.43
2:B:410:ARG:HG2	2:B:412:PHE:CE2	2.53	0.43
1:E:482:LYS:HB3	1:E:482:LYS:HE2	1.77	0.43
1:I:131:GLU:HB2	1:I:151:PHE:HE1	1.83	0.43
1:I:310:ARG:HB2	2:J:325:SER:HB2	2.00	0.43
2:J:40:TYR:CE2	2:J:214:LYS:HB2	2.52	0.43
1:M:24:LEU:H	1:M:140:THR:CG2	2.13	0.43
1:M:136:LYS:HB3	1:M:179:PHE:CG	2.53	0.43
1:M:381:LEU:HB2	1:M:420:PHE:HZ	1.82	0.43
1:M:415:THR:OG1	4:P:9:DA:N3	2.44	0.43
2:N:229:TYR:O	2:N:450:GLN:NE2	2.40	0.43
2:N:327:THR:O	2:N:327:THR:OG1	2.31	0.43
1:A:309:VAL:HG23	1:A:310:ARG:N	2.33	0.43
2:F:187:ALA:CB	3:G:2:U:H6	2.30	0.43
2:F:331:LEU:HB2	2:F:413:SER:HB3	2.00	0.43
3:G:7:G:H2'	3:G:8:U:C6	2.54	0.43
1:I:214:ALA:O	1:I:217:ILE:CG2	2.59	0.43
1:M:426:LEU:HG	1:M:444:HIS:CD2	2.53	0.43
1:M:497:ARG:HD3	1:M:497:ARG:HA	1.70	0.43
1:M:512:LYS:HB3	1:M:513:PRO:HD3	1.99	0.43
3:O:17:U:H2'	3:O:18:U:C6	2.54	0.43
1:A:130:LEU:O	1:A:132:MET:N	2.51	0.43
1:E:9:PHE:HZ	1:E:290:MET:CE	2.29	0.43
1:E:247:PHE:HA	1:E:248:PRO:HD2	1.73	0.43
4:H:18:DA:H4'	4:H:19:DG:OP1	2.18	0.43
2:J:195:ASN:OD1	3:K:2:U:N3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:223:ALA:CA	2:J:303:ILE:CD1	2.96	0.43
1:M:151:PHE:CD1	1:M:151:PHE:C	2.91	0.43
1:M:164:LEU:CD2	1:M:186:HIS:C	2.87	0.43
2:N:79:GLU:HG3	2:N:192:CYS:HB2	1.99	0.43
1:A:221:LEU:HG	1:A:222:VAL:N	2.32	0.43
2:B:18:LEU:HD23	2:B:28:THR:HG22	2.00	0.43
2:B:259:ALA:HB3	2:B:448:TYR:CZ	2.54	0.43
1:E:272:ALA:O	1:E:277:VAL:HG12	2.19	0.43
1:E:426:LEU:HG	1:E:444:HIS:CD2	2.53	0.43
2:F:136:LEU:O	2:F:143:PHE:HE2	2.00	0.43
1:I:285:GLY:HA3	1:I:289:GLU:OE1	2.18	0.43
1:I:298:VAL:HG13	1:I:301:LYS:HD3	1.99	0.43
2:J:304:PHE:CZ	2:J:421:THR:HG22	2.54	0.43
4:L:6:DA:H2'	4:L:7:DA:H8	1.83	0.43
1:A:217:ILE:HG23	1:A:245:ASN:HD22	1.83	0.43
1:A:576:ARG:HA	1:A:576:ARG:HD3	1.92	0.43
1:I:482:LYS:HA	1:I:482:LYS:HD3	1.90	0.43
2:J:446:LEU:HD23	2:J:446:LEU:HA	1.84	0.43
1:M:330:ALA:HB2	1:M:581:LEU:HA	2.01	0.43
2:N:135:GLY:O	2:N:139:GLN:NE2	2.52	0.43
2:N:191:GLN:CD	2:N:191:GLN:N	2.71	0.43
2:N:269:ARG:HH11	2:N:269:ARG:HB2	1.83	0.43
3:O:11:G:N2	4:P:14:DT:O2	2.51	0.43
2:B:290:LEU:C	2:B:290:LEU:CD2	2.87	0.43
1:E:217:ILE:HA	1:E:245:ASN:O	2.19	0.43
1:E:502:TRP:CH2	2:F:8:LEU:HD21	2.53	0.43
3:G:17:U:H2'	3:G:18:U:C6	2.53	0.43
1:I:309:VAL:HG23	1:I:310:ARG:N	2.33	0.43
2:J:320:PHE:HE1	2:J:413:SER:HG	1.63	0.43
1:M:130:LEU:HD21	1:M:138:VAL:HG23	2.00	0.43
1:A:249:HIS:CE1	1:M:175:ASN:O	2.71	0.43
1:A:362:ARG:HD2	1:A:391:PHE:HE1	1.83	0.43
1:E:234:MET:SD	1:E:268:LEU:HD13	2.58	0.43
2:F:63:LYS:CB	2:F:188:LEU:HD11	2.28	0.43
2:F:262:THR:OG1	2:F:283:VAL:HG21	2.17	0.43
2:J:117:ALA:O	2:J:156:LYS:NZ	2.39	0.43
2:J:188:LEU:CD2	2:J:188:LEU:N	2.73	0.43
1:M:209:HIS:HE1	1:M:213:LEU:HD11	1.84	0.43
1:M:238:ARG:HA	1:M:241:ILE:HG12	1.99	0.43
2:N:55:LEU:HD23	2:N:148:VAL:HG22	1.99	0.43
2:N:238:GLN:OE1	3:O:12:A:H4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG23	1:A:295:TRP:HB2	1.91	0.43
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.92	0.43
1:A:310:ARG:HB2	2:B:325:SER:HB2	2.00	0.43
2:N:379:GLN:HE21	2:N:441:LYS:HG3	1.83	0.43
1:E:137:VAL:HA	1:E:181:ILE:HG12	2.01	0.43
1:E:165:GLU:HG3	1:E:191:TYR:HB3	1.86	0.43
2:J:21:PHE:HZ	2:J:30:PRO:HA	1.84	0.43
2:J:46:LEU:HD11	2:N:137:PHE:CD2	2.53	0.43
1:M:22:TRP:CE3	1:M:24:LEU:HD21	2.54	0.43
1:M:22:TRP:HE3	1:M:24:LEU:HD21	1.83	0.43
1:M:31:SER:C	1:M:33:GLY:H	2.22	0.43
1:M:164:LEU:HD11	1:M:208:ILE:HD12	2.00	0.43
1:M:310:ARG:HE	1:M:310:ARG:HB2	1.67	0.43
2:N:242:THR:HG21	2:N:270:LYS:HZ1	1.84	0.43
1:E:21:MET:CE	1:E:139:PHE:CZ	3.01	0.43
2:J:20:LEU:HD12	2:J:20:LEU:HA	1.83	0.43
1:M:468:LYS:HA	1:M:468:LYS:HD2	1.73	0.43
2:N:377:TRP:CD2	2:N:406:PRO:HB3	2.54	0.43
3:O:8:U:H2'	3:O:9:U:C6	2.54	0.43
1:A:12:HIS:ND1	1:A:12:HIS:C	2.72	0.42
1:A:125:VAL:HG13	1:A:291:LEU:HD13	2.00	0.42
1:A:128:ALA:HB1	1:A:305:ILE:HG21	2.00	0.42
1:A:242:ASP:OD2	1:A:275:LYS:NZ	2.51	0.42
1:A:322:PRO:HD2	2:B:9:ALA:HB1	2.01	0.42
2:B:229:TYR:HB3	2:B:242:THR:HG22	2.01	0.42
1:E:44:LEU:CD2	1:E:107:TYR:CZ	3.02	0.42
2:F:377:TRP:CD2	2:F:406:PRO:HB3	2.54	0.42
3:G:8:U:H2'	3:G:9:U:C6	2.54	0.42
1:I:265:VAL:CG1	1:I:281:LEU:CD1	2.97	0.42
2:J:18:LEU:HD23	2:J:28:THR:HG22	2.00	0.42
2:J:184:ASN:C	2:J:188:LEU:HD21	2.40	0.42
1:M:218:ARG:HE	1:M:218:ARG:HB3	1.57	0.42
1:M:360:LYS:HD3	1:M:360:LYS:HA	1.77	0.42
1:M:465:VAL:HG11	1:M:527:ARG:NH2	2.34	0.42
2:N:55:LEU:HB3	2:N:148:VAL:HG22	2.00	0.42
1:E:154:ILE:HD13	1:E:309:VAL:CG2	2.48	0.42
1:E:525:ARG:O	1:E:529:ARG:HG3	2.19	0.42
2:F:19:LEU:HB3	2:F:21:PHE:CE1	2.52	0.42
2:F:382:VAL:HG11	2:F:438:LEU:HD21	2.01	0.42
2:J:301:ARG:O	2:J:328:GLU:N	2.49	0.42
1:M:525:ARG:O	1:M:529:ARG:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:19:LEU:HB3	2:N:21:PHE:CE1	2.52	0.42
3:O:7:G:H2'	3:O:8:U:C6	2.54	0.42
1:A:237:LEU:O	1:A:241:ILE:HG13	2.20	0.42
1:A:343:ILE:HD12	1:A:343:ILE:HA	1.86	0.42
1:I:394:ASP:OD1	1:I:395:GLU:N	2.51	0.42
2:J:229:TYR:HB3	2:J:242:THR:HG22	2.01	0.42
1:M:31:SER:O	1:M:32:ALA:C	2.56	0.42
1:M:432:GLU:OE1	1:M:432:GLU:N	2.52	0.42
2:N:280:MET:CE	2:N:315:GLU:OE1	2.66	0.42
1:A:176:THR:O	1:M:19:HIS:HE1	2.02	0.42
1:A:285:GLY:HA3	1:A:289:GLU:OE1	2.18	0.42
2:B:72:GLN:HG3	2:B:98:LEU:HD23	2.01	0.42
2:B:195:ASN:OD1	3:C:2:U:N3	2.49	0.42
1:E:137:VAL:HA	1:E:181:ILE:CG1	2.49	0.42
1:E:168:TYR:HE2	1:M:165:GLU:OE2	2.03	0.42
1:E:522:ASP:O	1:E:526:SER:N	2.38	0.42
2:F:284:LEU:HD12	2:F:319:ALA:HA	2.00	0.42
1:I:362:ARG:HD2	1:I:391:PHE:HE1	1.83	0.42
2:J:72:GLN:HG3	2:J:98:LEU:HD23	2.01	0.42
2:J:461:GLU:O	2:J:461:GLU:HG2	2.19	0.42
1:M:209:HIS:C	1:M:209:HIS:ND1	2.72	0.42
2:N:301:ARG:NH1	2:N:302:LYS:HD2	2.29	0.42
1:A:241:ILE:HG23	1:A:277:VAL:HG21	2.02	0.42
2:B:188:LEU:H	2:B:188:LEU:HG	1.40	0.42
1:E:213:LEU:CD2	1:E:240:ALA:CB	2.98	0.42
2:F:238:GLN:OE1	3:G:12:A:H4'	2.19	0.42
2:N:213:TRP:CE2	2:N:433:TRP:HD1	2.38	0.42
2:N:331:LEU:HB2	2:N:413:SER:HB3	2.00	0.42
2:N:382:VAL:HG11	2:N:438:LEU:HD21	2.02	0.42
1:A:124:ARG:HD3	1:A:309:VAL:HA	2.02	0.42
1:A:209:HIS:ND1	1:A:209:HIS:C	2.73	0.42
1:E:245:ASN:HD22	1:E:245:ASN:HA	1.57	0.42
1:I:139:PHE:C	1:I:140:THR:HG23	2.40	0.42
1:M:241:ILE:HG12	1:M:241:ILE:H	1.48	0.42
2:N:168:ARG:HE	2:N:172:LYS:HE2	1.85	0.42
1:I:21:MET:HE2	1:I:215:ALA:HB1	2.01	0.42
1:I:321:LEU:O	1:I:322:PRO:O	2.36	0.42
1:M:291:LEU:HD13	1:M:291:LEU:HA	1.81	0.42
1:A:304:ALA:O	1:A:308:LYS:HG2	2.20	0.42
1:E:32:ALA:HB2	1:E:123:HIS:NE2	2.34	0.42
1:E:155:SER:HB3	1:E:157:LYS:HE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:VAL:HG11	1:E:527:ARG:NH2	2.34	0.42
2:F:168:ARG:HE	2:F:172:LYS:HE2	1.85	0.42
1:I:223:VAL:HG13	1:I:253:TRP:HA	2.02	0.42
2:J:177:ASN:O	2:J:177:ASN:ND2	2.52	0.42
1:M:237:LEU:HB3	1:M:241:ILE:HD11	2.02	0.42
1:A:332:ARG:HD3	1:A:537:TYR:HE1	1.85	0.42
1:A:366:LYS:HA	1:A:366:LYS:HD2	1.86	0.42
1:A:468:LYS:HB3	1:A:468:LYS:HE3	1.74	0.42
1:A:495:GLU:OE2	2:B:340:TRP:NE1	2.32	0.42
2:B:146:LEU:CD2	2:B:178:LEU:HD21	2.49	0.42
1:E:330:ALA:HB2	1:E:581:LEU:HA	2.01	0.42
2:F:130:VAL:O	2:F:133:MET:HB2	2.20	0.42
2:F:139:GLN:NE2	2:F:139:GLN:H	2.18	0.42
1:M:151:PHE:CD1	1:M:159:LEU:HD22	2.55	0.42
1:M:395:GLU:H	1:M:395:GLU:HG2	1.66	0.42
2:B:47:PRO:HG3	2:B:205:TYR:CZ	2.55	0.42
2:B:151:PRO:HD2	2:B:154:TRP:CE3	2.55	0.42
2:B:461:GLU:HG2	2:B:461:GLU:O	2.19	0.42
1:E:137:VAL:HG13	1:E:181:ILE:HD11	2.01	0.42
2:F:105:LEU:HD23	2:F:105:LEU:HA	1.82	0.42
1:I:22:TRP:HD1	1:I:135:THR:OG1	2.03	0.42
1:M:122:GLY:N	1:M:288:ASP:OD1	2.53	0.42
1:M:154:ILE:HB	1:M:308:LYS:HB2	2.02	0.42
2:N:151:PRO:HD2	2:N:154:TRP:CE3	2.55	0.42
2:N:220:LYS:O	2:N:291:TYR:OH	2.36	0.42
2:B:21:PHE:HZ	2:B:30:PRO:HA	1.84	0.41
2:B:190:ARG:C	2:B:192:CYS:N	2.72	0.41
2:B:221:ASP:HA	2:B:291:TYR:OH	2.19	0.41
1:E:136:LYS:HB3	1:E:179:PHE:CG	2.55	0.41
1:E:140:THR:HG21	1:E:182:TYR:OH	2.19	0.41
2:F:196:VAL:HG22	3:G:2:U:C4	2.55	0.41
1:I:430:LEU:HD22	1:I:437:HIS:HB2	2.01	0.41
1:I:484:LEU:HD23	1:I:511:ILE:HG21	2.02	0.41
2:B:227:LEU:HD23	2:B:244:CYS:HB2	2.02	0.41
4:D:20:DG:H2"	4:D:21:DA:H8	1.85	0.41
1:E:153:ASP:N	1:M:156:GLY:O	2.53	0.41
1:I:177:GLU:OE2	1:I:218:ARG:NH2	2.53	0.41
2:J:224:TYR:CE2	2:J:424:SER:HB2	2.55	0.41
4:L:20:DG:H2"	4:L:21:DA:H8	1.85	0.41
1:M:162:TYR:CE2	1:M:169:ALA:CB	3.02	0.41
2:N:110:LEU:HD12	2:N:110:LEU:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASN:HB2	1:A:19:HIS:CE1	2.55	0.41
1:A:241:ILE:HG22	1:A:275:LYS:HD2	2.01	0.41
1:A:484:LEU:HD23	1:A:511:ILE:HG21	2.02	0.41
2:B:110:LEU:HD12	2:B:112:GLU:H	1.85	0.41
2:B:137:PHE:CE1	2:B:176:LEU:CD1	3.03	0.41
2:B:248:PHE:CE2	2:B:294:SER:CB	3.03	0.41
1:E:526:SER:HA	1:E:529:ARG:HG3	2.02	0.41
2:F:145:VAL:HG22	2:F:208:ALA:HB2	2.01	0.41
2:F:213:TRP:CE2	2:F:433:TRP:HD1	2.38	0.41
1:I:217:ILE:HA	1:I:245:ASN:O	2.20	0.41
1:I:552:GLY:O	1:I:576:ARG:NE	2.53	0.41
2:J:47:PRO:HG3	2:J:205:TYR:CZ	2.55	0.41
1:M:411:VAL:HG21	1:M:501:LEU:HD21	2.01	0.41
2:N:262:THR:HG21	2:N:283:VAL:CG2	2.12	0.41
2:N:285:SER:O	2:N:288:LEU:HD23	2.20	0.41
1:A:478:VAL:HG13	1:A:481:ALA:HB3	2.02	0.41
2:B:61:MET:HE1	2:B:108:LEU:HD22	1.96	0.41
2:B:303:ILE:HG13	2:B:323:PHE:CE2	2.56	0.41
1:E:120:ASN:HA	2:F:321:ASP:HB3	2.02	0.41
1:E:340:THR:OG1	1:E:572:GLU:HG2	2.20	0.41
1:E:493:ARG:NH2	2:F:339:ASN:OD1	2.51	0.41
2:F:261:ASP:HB2	2:F:463:VAL:HA	2.02	0.41
1:I:440:ARG:HD3	1:I:510:TRP:CZ3	2.56	0.41
1:I:478:VAL:HG13	1:I:481:ALA:HB3	2.02	0.41
1:E:497:ARG:HD3	1:E:497:ARG:HA	1.70	0.41
1:E:561:CYS:SG	1:E:569:ALA:HB3	2.60	0.41
2:F:285:SER:O	2:F:288:LEU:HD23	2.20	0.41
1:I:212:PHE:CZ	1:I:237:LEU:HG	2.55	0.41
1:I:238:ARG:HH12	1:I:271:TYR:C	2.24	0.41
2:J:44:PHE:CD2	2:N:176:LEU:HD21	2.56	0.41
1:M:23:PHE:O	1:M:223:VAL:HG23	2.21	0.41
2:N:130:VAL:O	2:N:133:MET:HB2	2.20	0.41
2:B:179:PRO:HG2	2:B:179:PRO:O	2.21	0.41
2:B:257:PHE:HE2	2:B:444:VAL:HB	1.83	0.41
1:E:268:LEU:HD23	1:E:269:ILE:HD13	2.02	0.41
2:F:140:LYS:NZ	2:F:140:LYS:CB	2.73	0.41
1:I:362:ARG:O	1:I:365:GLN:HG2	2.21	0.41
2:J:151:PRO:HD2	2:J:154:TRP:CE3	2.55	0.41
2:J:335:ILE:HA	4:L:13:DC:OP1	2.21	0.41
1:M:436:LEU:HD12	1:M:436:LEU:HA	1.90	0.41
2:N:269:ARG:CB	2:N:269:ARG:HH11	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:C	1:A:212:PHE:HD1	2.24	0.41
1:A:482:LYS:HA	1:A:482:LYS:HD3	1.90	0.41
1:A:497:ARG:HD3	1:A:497:ARG:HA	1.62	0.41
2:B:224:TYR:CE2	2:B:424:SER:HB2	2.55	0.41
1:E:22:TRP:CE3	1:E:24:LEU:HD21	2.53	0.41
2:F:151:PRO:HD2	2:F:154:TRP:CE3	2.55	0.41
2:N:64:LEU:HD21	2:N:149:TYR:HB2	2.03	0.41
2:B:61:MET:CE	2:B:108:LEU:HD23	2.34	0.41
1:E:213:LEU:HD22	1:E:243:GLN:NE2	2.36	0.41
1:E:411:VAL:HG21	1:E:501:LEU:HD21	2.01	0.41
2:F:64:LEU:HD21	2:F:149:TYR:HB2	2.03	0.41
2:F:196:VAL:HG22	3:G:2:U:C5	2.55	0.41
2:F:243:CYS:SG	2:F:453:ALA:HA	2.61	0.41
2:F:332:VAL:HG22	2:F:411:ARG:HG2	2.02	0.41
3:G:7:G:H2'	3:G:8:U:H6	1.86	0.41
1:I:135:THR:HG23	1:I:135:THR:O	2.21	0.41
1:I:171:LEU:HD13	1:I:211:CYS:CA	2.50	0.41
1:I:241:ILE:CG1	1:I:247:PHE:HE2	2.34	0.41
1:M:268:LEU:C	1:M:268:LEU:CD2	2.85	0.41
1:M:340:THR:OG1	1:M:572:GLU:HG2	2.20	0.41
1:M:561:CYS:SG	1:M:569:ALA:HB3	2.60	0.41
2:N:75:ALA:HB1	2:N:194:ALA:HB2	2.02	0.41
1:A:123:HIS:CE1	1:A:144:ASP:OD1	2.74	0.41
1:A:343:ILE:HG22	1:A:404:ILE:HD11	2.03	0.41
1:A:362:ARG:O	1:A:365:GLN:HG2	2.20	0.41
1:A:552:GLY:O	1:A:576:ARG:NE	2.53	0.41
2:B:70:GLU:OE1	2:B:70:GLU:HA	2.21	0.41
2:B:258:VAL:C	2:B:448:TYR:HE2	2.24	0.41
1:E:29:SER:O	1:E:34:LEU:HB2	2.20	0.41
1:E:168:TYR:OH	1:M:191:TYR:C	2.48	0.41
1:E:418:LYS:NZ	4:H:11:DC:OP1	2.54	0.41
2:F:62:ARG:HA	2:F:65:ASP:OD2	2.21	0.41
1:I:4:LEU:HD12	1:I:4:LEU:HA	1.93	0.41
1:I:304:ALA:O	1:I:308:LYS:HG2	2.20	0.41
1:I:386:GLU:H	1:I:386:GLU:HG2	1.61	0.41
1:I:425:ILE:HG21	1:I:503:ILE:HD11	2.03	0.41
2:J:64:LEU:HD11	2:J:149:TYR:CB	2.48	0.41
2:J:110:LEU:HD12	2:J:112:GLU:H	1.85	0.41
1:M:24:LEU:CD1	1:M:140:THR:HG21	2.51	0.41
1:M:24:LEU:HD12	1:M:140:THR:HG21	2.03	0.41
1:M:164:LEU:HD21	1:M:186:HIS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:ILE:HG23	1:M:245:ASN:OD1	2.21	0.41
1:E:49:TYR:CZ	1:E:55:GLN:HG3	2.56	0.41
1:E:174:LEU:HD23	1:E:174:LEU:C	2.41	0.41
2:F:110:LEU:HD12	2:F:110:LEU:H	1.85	0.41
1:I:332:ARG:HD3	1:I:537:TYR:HE1	1.85	0.41
1:M:363:ILE:HD11	1:M:372:LEU:HD13	2.03	0.41
1:M:462:ARG:HG2	1:M:471:LEU:HG	2.03	0.41
1:A:440:ARG:HD3	1:A:510:TRP:CZ3	2.56	0.40
2:B:223:ALA:HB3	2:B:303:ILE:HD13	2.01	0.40
1:E:288:ASP:CG	2:F:277:TYR:CE2	2.94	0.40
1:E:432:GLU:OE1	1:E:432:GLU:N	2.52	0.40
1:E:462:ARG:HG2	1:E:471:LEU:HG	2.03	0.40
2:F:18:LEU:HD12	2:F:18:LEU:H	1.87	0.40
3:G:19:A:H2'	3:G:20:A:O4'	2.21	0.40
1:I:9:PHE:HB2	1:I:282:VAL:HG11	2.03	0.40
1:I:23:PHE:CD1	1:I:139:PHE:O	2.66	0.40
2:J:227:LEU:HD23	2:J:244:CYS:HB2	2.02	0.40
1:M:62:ILE:O	1:M:68:LYS:HG3	2.21	0.40
1:M:123:HIS:CD2	1:M:146:VAL:HG11	2.56	0.40
1:M:149:THR:HG22	1:M:150:ALA:N	2.35	0.40
2:N:243:CYS:SG	2:N:453:ALA:HA	2.61	0.40
3:O:19:A:H2'	3:O:20:A:O4'	2.21	0.40
1:A:147:ILE:HG21	1:A:182:TYR:CE1	2.57	0.40
1:A:430:LEU:HD22	1:A:437:HIS:HB2	2.01	0.40
2:B:32:ARG:O	2:B:36:GLN:HG2	2.21	0.40
3:C:13:G:H2'	3:C:14:C:H6	1.84	0.40
1:E:363:ILE:HD11	1:E:372:LEU:HD13	2.03	0.40
2:F:262:THR:O	2:F:262:THR:CG2	2.69	0.40
1:I:366:LYS:HA	1:I:366:LYS:HD2	1.86	0.40
2:J:32:ARG:O	2:J:36:GLN:HG2	2.21	0.40
1:M:35:PRO:HG2	1:M:112:LEU:CD2	2.51	0.40
1:M:49:TYR:O	1:M:49:TYR:HD1	2.04	0.40
1:M:90:SER:CB	1:M:198:THR:H	2.34	0.40
1:M:188:ASP:HB3	1:M:190:ARG:HD2	2.03	0.40
1:M:266:GLN:HE21	1:M:270:THR:HG23	1.86	0.40
1:A:177:GLU:HB2	1:M:19:HIS:NE2	2.36	0.40
2:B:255:PHE:CD2	2:B:433:TRP:CZ2	3.09	0.40
2:B:335:ILE:HA	4:D:13:DC:OP1	2.21	0.40
1:E:134:GLN:N	1:E:134:GLN:CD	2.75	0.40
1:E:436:LEU:HD12	1:E:436:LEU:HA	1.90	0.40
1:M:21:MET:CE	1:M:139:PHE:CZ	2.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:ILE:CG2	1:M:45:LYS:HE3	2.51	0.40
1:M:143:PHE:CE2	1:M:194:ILE:HG21	2.33	0.40
2:N:332:VAL:HG22	2:N:411:ARG:HG2	2.02	0.40
1:A:135:THR:HG23	1:A:135:THR:O	2.21	0.40
1:A:248:PRO:CB	1:M:175:ASN:ND2	2.84	0.40
2:B:363:ARG:NH2	2:B:429:THR:HG1	2.17	0.40
1:E:30:ARG:HD3	1:E:30:ARG:C	2.41	0.40
1:E:90:SER:CB	1:E:198:THR:H	2.34	0.40
1:E:210:LYS:HB2	1:E:210:LYS:HE3	1.51	0.40
1:E:435:ILE:H	1:E:435:ILE:HG12	1.71	0.40
2:F:51:ARG:CZ	2:F:144:ASP:OD1	2.69	0.40
2:F:379:GLN:NE2	2:F:441:LYS:HG3	2.37	0.40
1:I:343:ILE:HG22	1:I:404:ILE:HD11	2.03	0.40
1:I:437:HIS:O	1:I:438:ARG:HD2	2.22	0.40
1:M:24:LEU:HG	1:M:140:THR:HG21	1.93	0.40
1:M:35:PRO:HG2	1:M:112:LEU:HD21	2.01	0.40
1:M:134:GLN:CD	1:M:134:GLN:N	2.75	0.40
2:N:197:MET:O	2:N:201:SER:CB	2.57	0.40
1:A:8:GLU:OE2	1:E:98:ARG:HD2	2.22	0.40
1:A:139:PHE:CD2	1:A:212:PHE:CD2	3.09	0.40
1:A:335:ALA:HB1	1:A:502:TRP:HB3	2.03	0.40
2:B:44:PHE:HE2	2:B:253:THR:OG1	2.00	0.40
2:B:190:ARG:NH1	2:B:190:ARG:CA	2.84	0.40
1:E:53:GLU:O	1:E:55:GLN:HG2	2.22	0.40
1:E:137:VAL:CG1	1:E:181:ILE:HD11	2.52	0.40
1:E:264:ALA:HA	1:E:267:ASP:OD2	2.20	0.40
1:E:371:LEU:HD23	1:E:371:LEU:HA	1.87	0.40
2:J:430:LYS:HE2	2:J:430:LYS:HB3	1.78	0.40
2:N:239:GLU:OE1	2:N:269:ARG:HD2	2.21	0.40
2:N:242:THR:HG21	2:N:275:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/587 (77%)	428 (95%)	20 (4%)	2 (0%)	30	60
1	E	570/587 (97%)	531 (93%)	36 (6%)	3 (0%)	25	54
1	I	451/587 (77%)	430 (95%)	18 (4%)	3 (1%)	19	47
1	M	570/587 (97%)	536 (94%)	33 (6%)	1 (0%)	44	72
2	B	450/473 (95%)	426 (95%)	22 (5%)	2 (0%)	30	60
2	F	450/473 (95%)	432 (96%)	17 (4%)	1 (0%)	44	72
2	J	450/473 (95%)	427 (95%)	22 (5%)	1 (0%)	44	72
2	N	450/473 (95%)	427 (95%)	20 (4%)	3 (1%)	19	47
All	All	3841/4240 (91%)	3637 (95%)	188 (5%)	16 (0%)	32	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
2	B	190	ARG
2	B	191	GLN
1	I	145	ASP
2	N	189	THR
1	E	242	ASP
1	I	141	THR
2	N	192	CYS
1	E	147	ILE
1	M	141	THR
1	I	322	PRO
1	A	131	GLU
2	F	261	ASP
2	N	185	ASP
1	E	250	GLY
2	J	404	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	389/502 (78%)	363 (93%)	26 (7%)	13 39
1	E	493/502 (98%)	447 (91%)	46 (9%)	7 26
1	I	390/502 (78%)	360 (92%)	30 (8%)	10 34
1	M	493/502 (98%)	450 (91%)	43 (9%)	8 28
2	B	394/407 (97%)	375 (95%)	19 (5%)	21 48
2	F	394/407 (97%)	369 (94%)	25 (6%)	15 40
2	J	394/407 (97%)	373 (95%)	21 (5%)	19 45
2	N	394/407 (97%)	369 (94%)	25 (6%)	15 40
All	All	3341/3636 (92%)	3106 (93%)	235 (7%)	15 37

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	16	ASN
1	A	18	GLN
1	A	19	HIS
1	A	21	MET
1	A	121	ILE
1	A	136	LYS
1	A	141	THR
1	A	142	ASN
1	A	143	PHE
1	A	181	ILE
1	A	212	PHE
1	A	218	ARG
1	A	219	PHE
1	A	221	LEU
1	A	229	ARG
1	A	253	TRP
1	A	297	GLN
1	A	299	LYS
1	A	313	ARG
1	A	374	TYR
1	A	402	TYR
1	A	405	ASP
1	A	459	LEU
1	A	467	PHE
1	A	541	ASP
2	B	49	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	60	HIS
2	B	62	ARG
2	B	64	LEU
2	B	67	ILE
2	B	90	PHE
2	B	128	LYS
2	B	166	HIS
2	B	188	LEU
2	B	190	ARG
2	B	244	CYS
2	B	256	GLU
2	B	257	PHE
2	B	284	LEU
2	B	289	HIS
2	B	293	SER
2	B	362	ASP
2	B	374	CYS
2	B	424	SER
1	E	12	HIS
1	E	16	ASN
1	E	20	MET
1	E	36	THR
1	E	38	SER
1	E	40	ILE
1	E	55	GLN
1	E	58	GLN
1	E	60	HIS
1	E	61	ASP
1	E	62	ILE
1	E	78	LYS
1	E	90	SER
1	E	93	PHE
1	E	98	ARG
1	E	101	TYR
1	E	119	LEU
1	E	120	ASN
1	E	121	ILE
1	E	139	PHE
1	E	141	THR
1	E	143	PHE
1	E	144	ASP
1	E	154	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	163	HIS
1	E	164	LEU
1	E	174	LEU
1	E	180	PRO
1	E	205	ASP
1	E	210	LYS
1	E	217	ILE
1	E	224	SER
1	E	243	GLN
1	E	245	ASN
1	E	259	SER
1	E	284	THR
1	E	286	THR
1	E	287	PHE
1	E	331	LEU
1	E	350	LEU
1	E	352	SER
1	E	365	GLN
1	E	454	LYS
1	E	506	LYS
1	E	541	ASP
1	E	568	LYS
2	F	18	LEU
2	F	32	ARG
2	F	44	PHE
2	F	87	TYR
2	F	132	SER
2	F	139	GLN
2	F	140	LYS
2	F	150	LEU
2	F	185	ASP
2	F	190	ARG
2	F	191	GLN
2	F	201	SER
2	F	215	LEU
2	F	218	TRP
2	F	255	PHE
2	F	257	PHE
2	F	263	ARG
2	F	285	SER
2	F	293	SER
2	F	337	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	346	ASP
2	F	377	TRP
2	F	386	ASN
2	F	454	ASP
2	F	468	ASP
1	I	15	GLN
1	I	16	ASN
1	I	20	MET
1	I	136	LYS
1	I	139	PHE
1	I	141	THR
1	I	143	PHE
1	I	213	LEU
1	I	218	ARG
1	I	219	PHE
1	I	229	ARG
1	I	234	MET
1	I	237	LEU
1	I	242	ASP
1	I	243	GLN
1	I	244	ASN
1	I	267	ASP
1	I	269	ILE
1	I	297	GLN
1	I	299	LYS
1	I	313	ARG
1	I	326	LYS
1	I	329	PRO
1	I	331	LEU
1	I	374	TYR
1	I	402	TYR
1	I	405	ASP
1	I	459	LEU
1	I	467	PHE
1	I	541	ASP
2	J	41	SER
2	J	49	GLN
2	J	60	HIS
2	J	65	ASP
2	J	69	ARG
2	J	90	PHE
2	J	128	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	166	HIS
2	J	190	ARG
2	J	244	CYS
2	J	255	PHE
2	J	257	PHE
2	J	281	GLN
2	J	284	LEU
2	J	301	ARG
2	J	302	LYS
2	J	303	ILE
2	J	362	ASP
2	J	374	CYS
2	J	400	LEU
2	J	424	SER
1	M	14	LEU
1	M	16	ASN
1	M	20	MET
1	M	30	ARG
1	M	47	ARG
1	M	49	TYR
1	M	51	LEU
1	M	55	GLN
1	M	61	ASP
1	M	78	LYS
1	M	90	SER
1	M	93	PHE
1	M	98	ARG
1	M	101	TYR
1	M	139	PHE
1	M	151	PHE
1	M	153	ASP
1	M	154	ILE
1	M	155	SER
1	M	164	LEU
1	M	165	GLU
1	M	190	ARG
1	M	192	GLN
1	M	194	ILE
1	M	195	LYS
1	M	205	ASP
1	M	209	HIS
1	M	211	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	212	PHE
1	M	224	SER
1	M	241	ILE
1	M	245	ASN
1	M	251	LEU
1	M	259	SER
1	M	288	ASP
1	M	331	LEU
1	M	350	LEU
1	M	352	SER
1	M	365	GLN
1	M	454	LYS
1	M	506	LYS
1	M	541	ASP
1	M	568	LYS
2	N	18	LEU
2	N	32	ARG
2	N	44	PHE
2	N	87	TYR
2	N	132	SER
2	N	150	LEU
2	N	185	ASP
2	N	190	ARG
2	N	195	ASN
2	N	197	MET
2	N	201	SER
2	N	215	LEU
2	N	218	TRP
2	N	255	PHE
2	N	257	PHE
2	N	268	ASP
2	N	270	LYS
2	N	285	SER
2	N	293	SER
2	N	337	SER
2	N	346	ASP
2	N	377	TRP
2	N	386	ASN
2	N	454	ASP
2	N	468	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	16	ASN
1	A	18	GLN
1	A	19	HIS
1	A	123	HIS
1	A	243	GLN
1	A	245	ASN
1	A	249	HIS
2	B	29	HIS
2	B	60	HIS
2	B	295	HIS
2	B	296	ASN
2	B	379	GLN
1	E	46	HIS
1	E	55	GLN
1	E	58	GLN
1	E	175	ASN
1	E	243	GLN
2	F	177	ASN
2	F	195	ASN
2	F	367	GLN
2	F	379	GLN
2	F	386	ASN
2	F	436	ASN
1	I	7	ASN
1	I	142	ASN
1	I	175	ASN
1	I	244	ASN
2	J	29	HIS
2	J	379	GLN
1	M	55	GLN
1	M	123	HIS
1	M	192	GLN
1	M	244	ASN
1	M	245	ASN
1	M	266	GLN
2	N	139	GLN
2	N	195	ASN
2	N	281	GLN
2	N	367	GLN
2	N	379	GLN
2	N	386	ASN
2	N	436	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	20/21 (95%)	7 (35%)	0
3	G	20/21 (95%)	7 (35%)	0
3	K	20/21 (95%)	7 (35%)	0
3	O	20/21 (95%)	7 (35%)	0
All	All	80/84 (95%)	28 (35%)	0

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	4	C
3	C	5	C
3	C	12	A
3	C	13	G
3	C	15	U
3	C	16	G
3	C	17	U
3	G	4	C
3	G	5	C
3	G	6	U
3	G	13	G
3	G	15	U
3	G	16	G
3	G	17	U
3	K	4	C
3	K	5	C
3	K	12	A
3	K	13	G
3	K	15	U
3	K	16	G
3	K	17	U
3	O	4	C
3	O	5	C
3	O	6	U
3	O	13	G
3	O	15	U
3	O	16	G
3	O	17	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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.

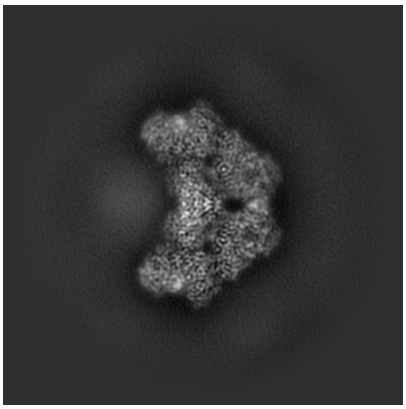
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39028. These allow visual inspection of the internal detail of the map and identification of artifacts.

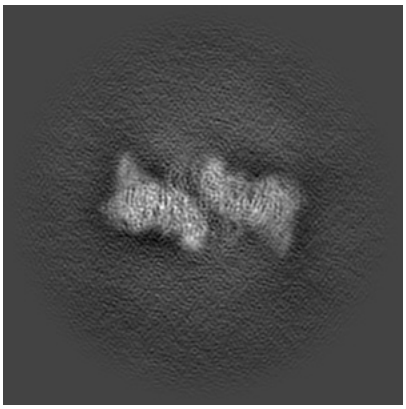
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

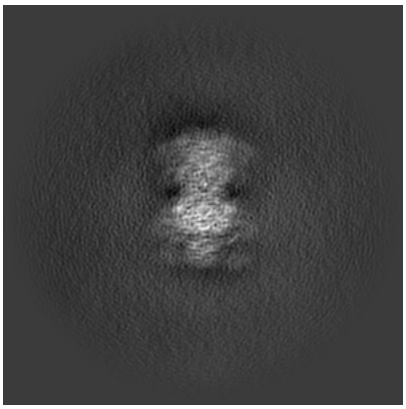
6.1.1 Primary map



X

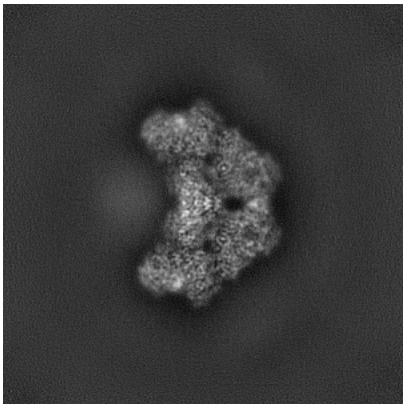


Y

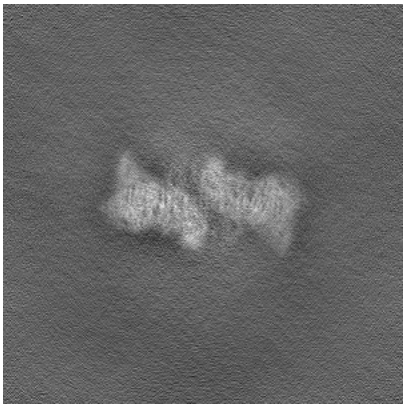


Z

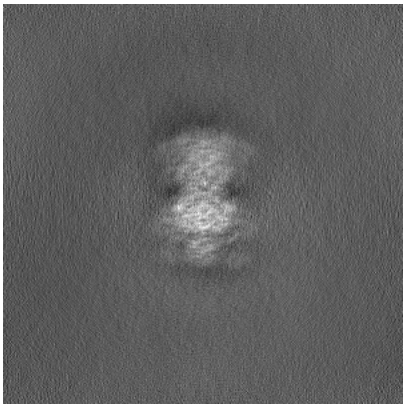
6.1.2 Raw map



X



Y

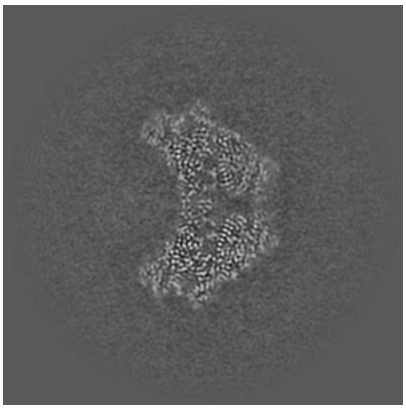


Z

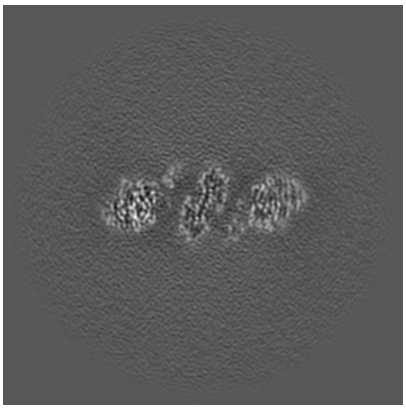
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



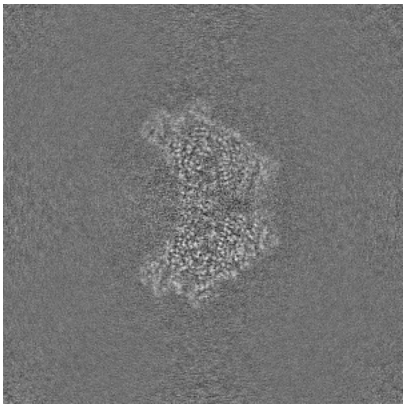
X Index: 230



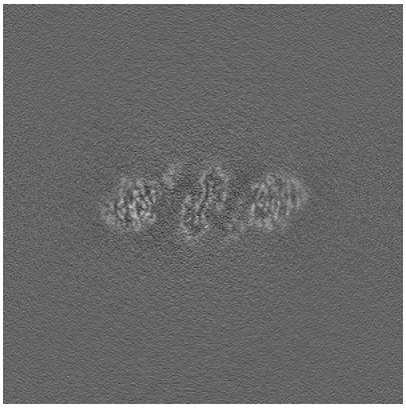
Y Index: 230

Z Index: 230

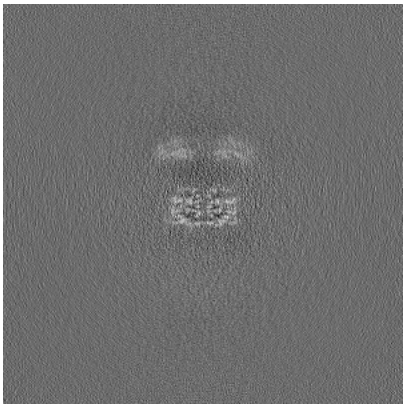
6.2.2 Raw map



X Index: 230



Y Index: 230

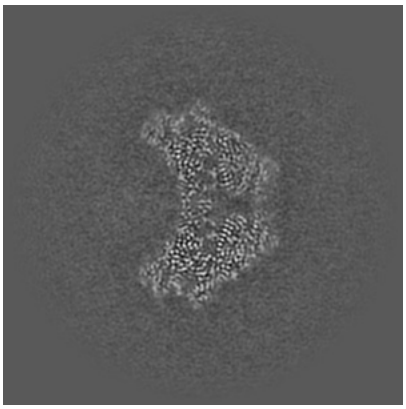


Z Index: 230

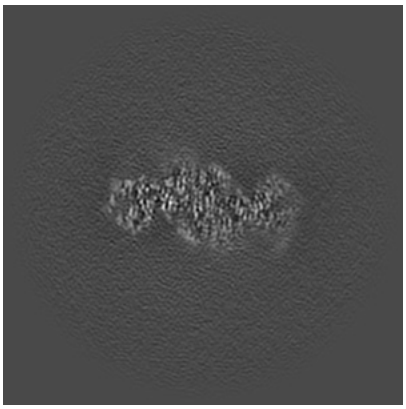
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

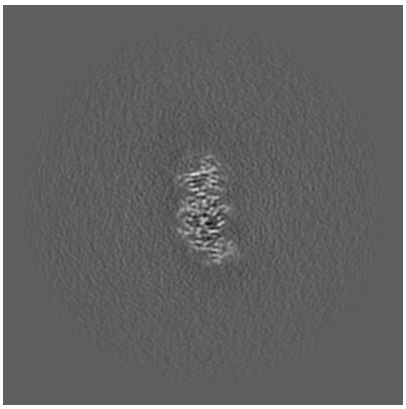
6.3.1 Primary map



X Index: 230

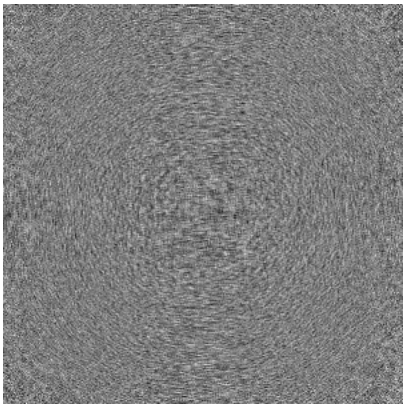


Y Index: 213

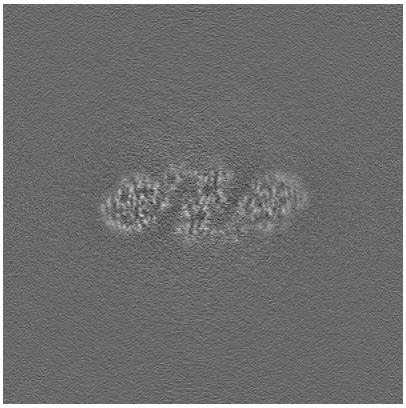


Z Index: 167

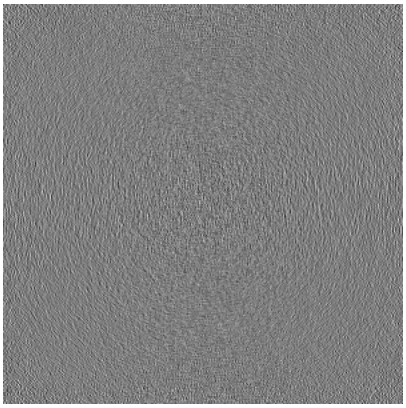
6.3.2 Raw map



X Index: 0



Y Index: 227

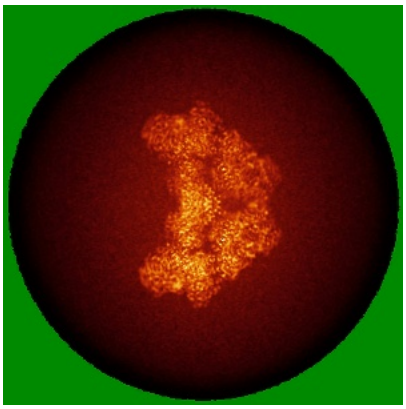


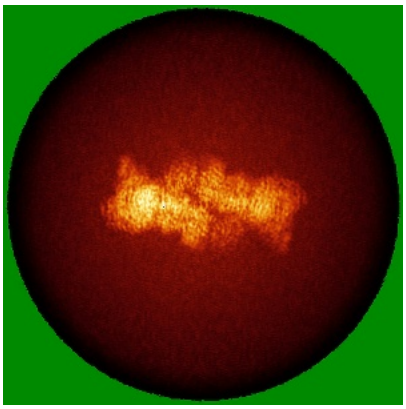
Z Index: 0

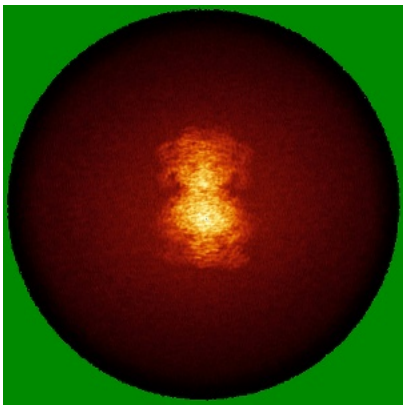
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

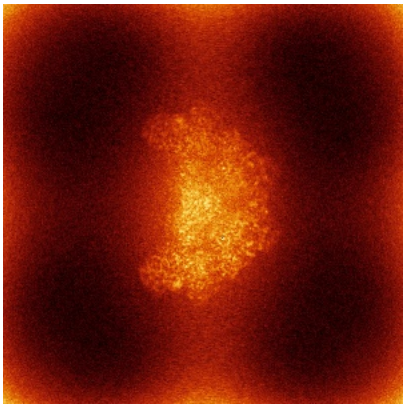
6.4.1 Primary map

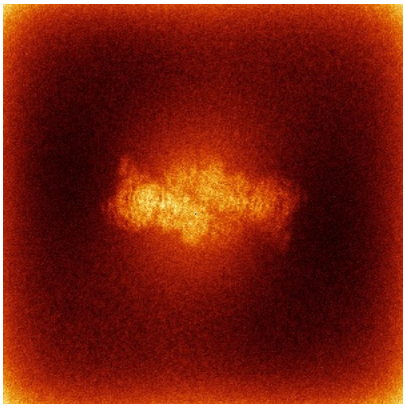

X

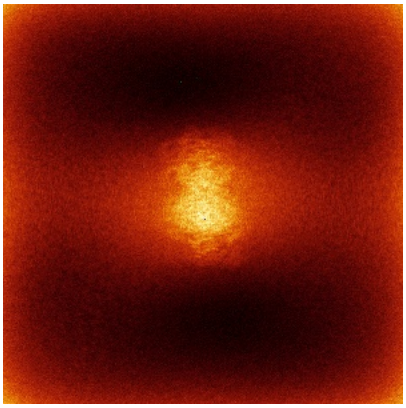

Y


Z

6.4.2 Raw map


X

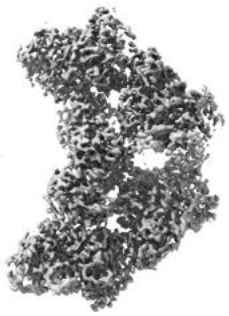

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



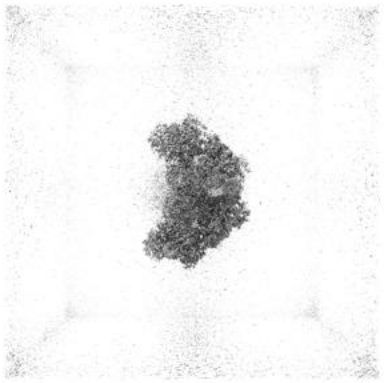
X

Y

Z

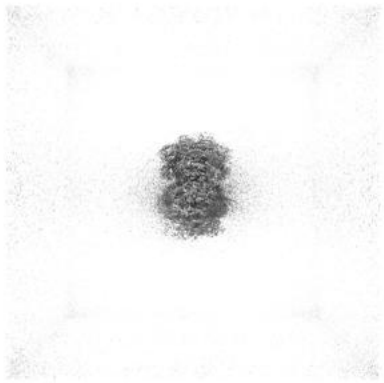
The images above show the 3D surface view of the map at the recommended contour level 0.375. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

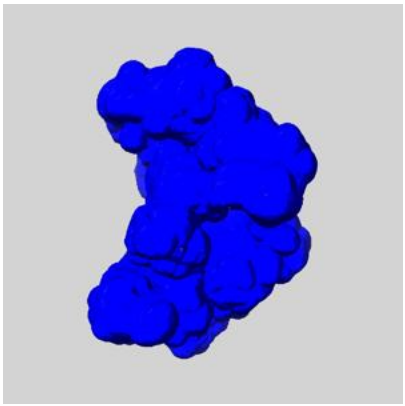
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

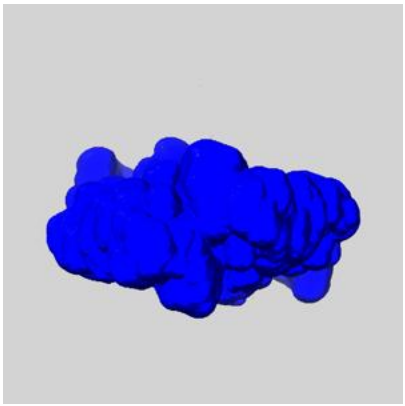
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

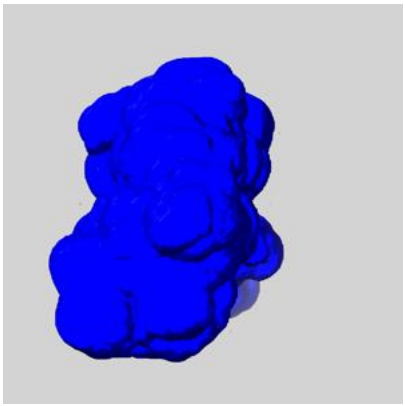
6.6.1 emd_39028_msk_1.map (i)



X



Y

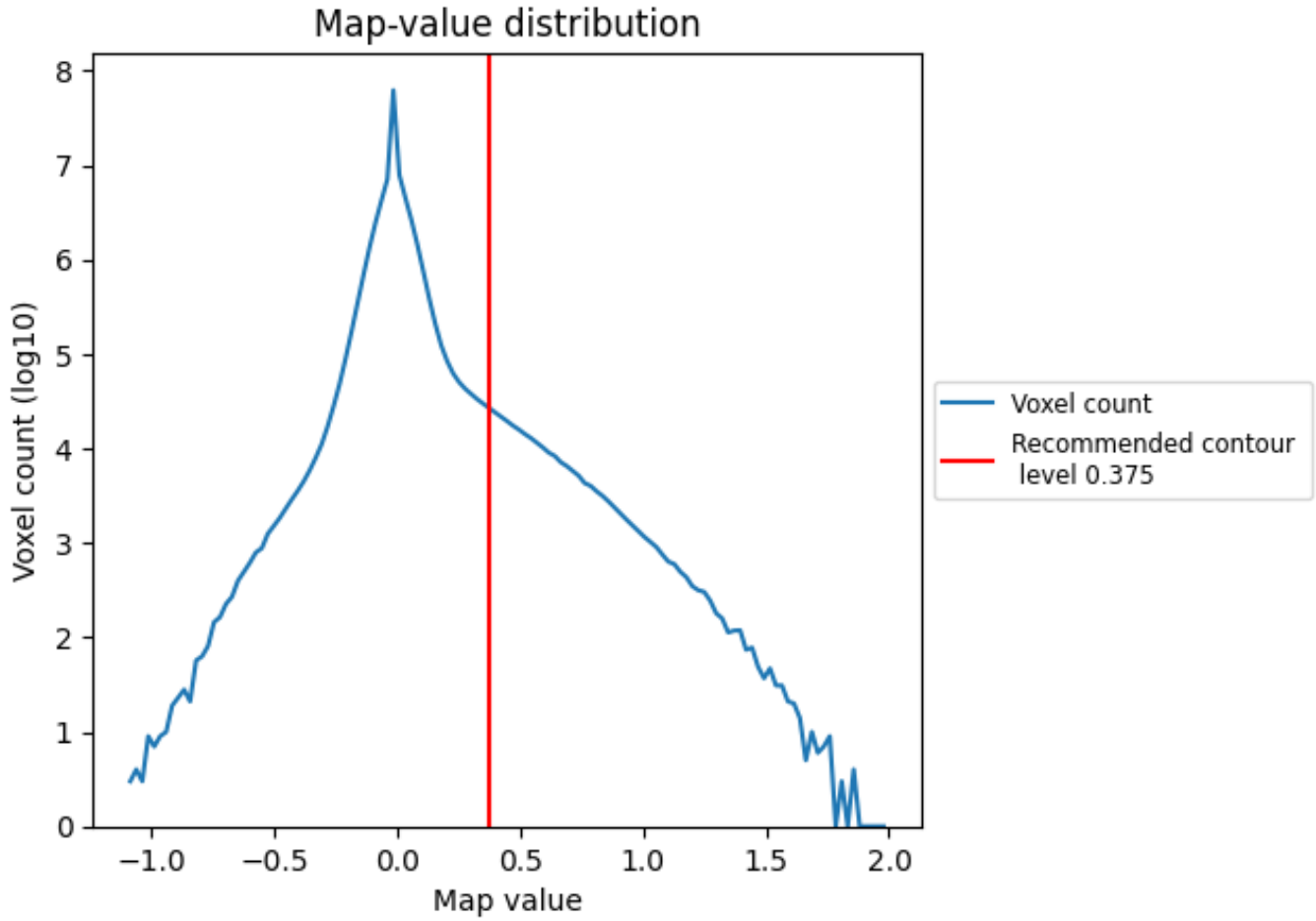


Z

7 Map analysis

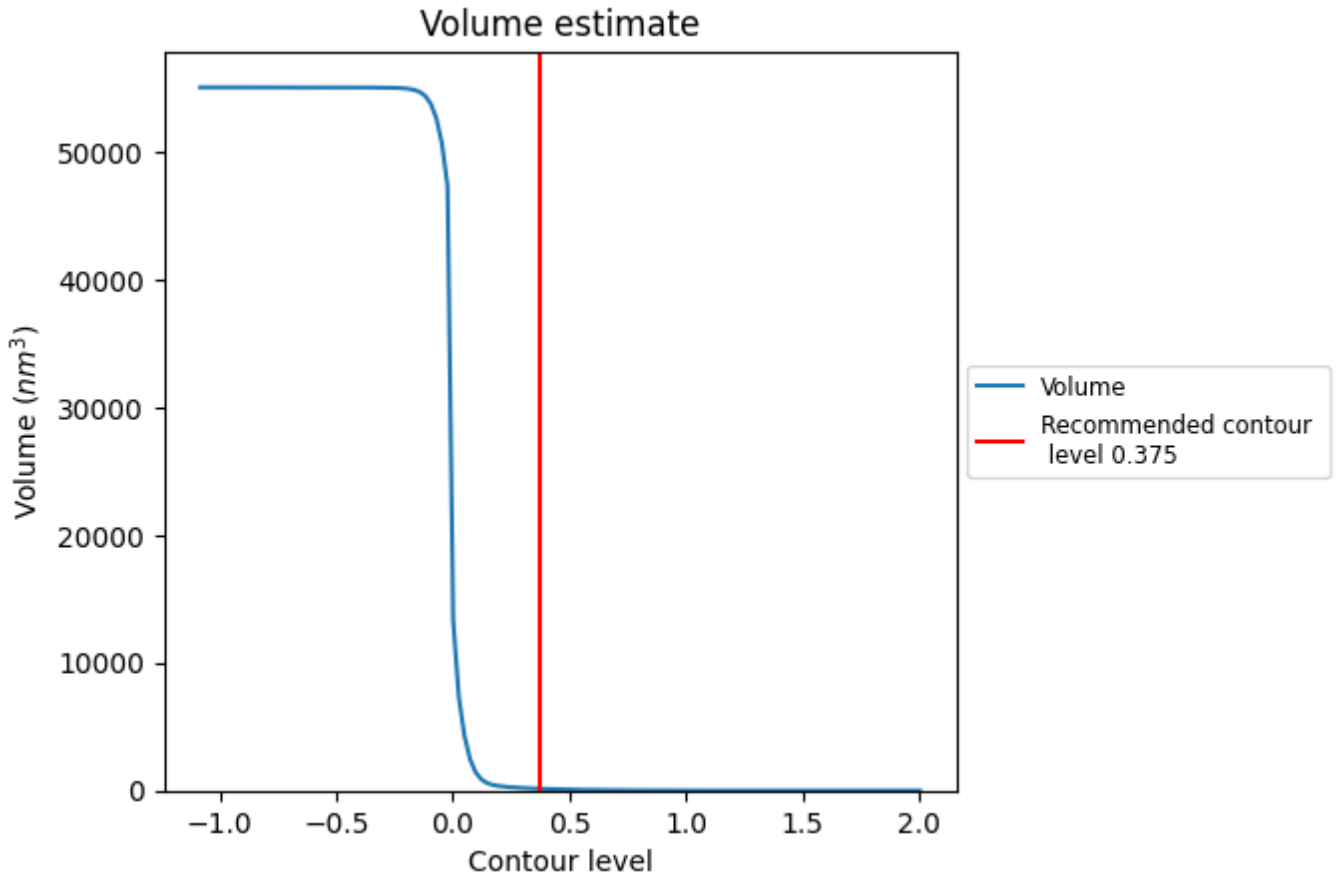
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

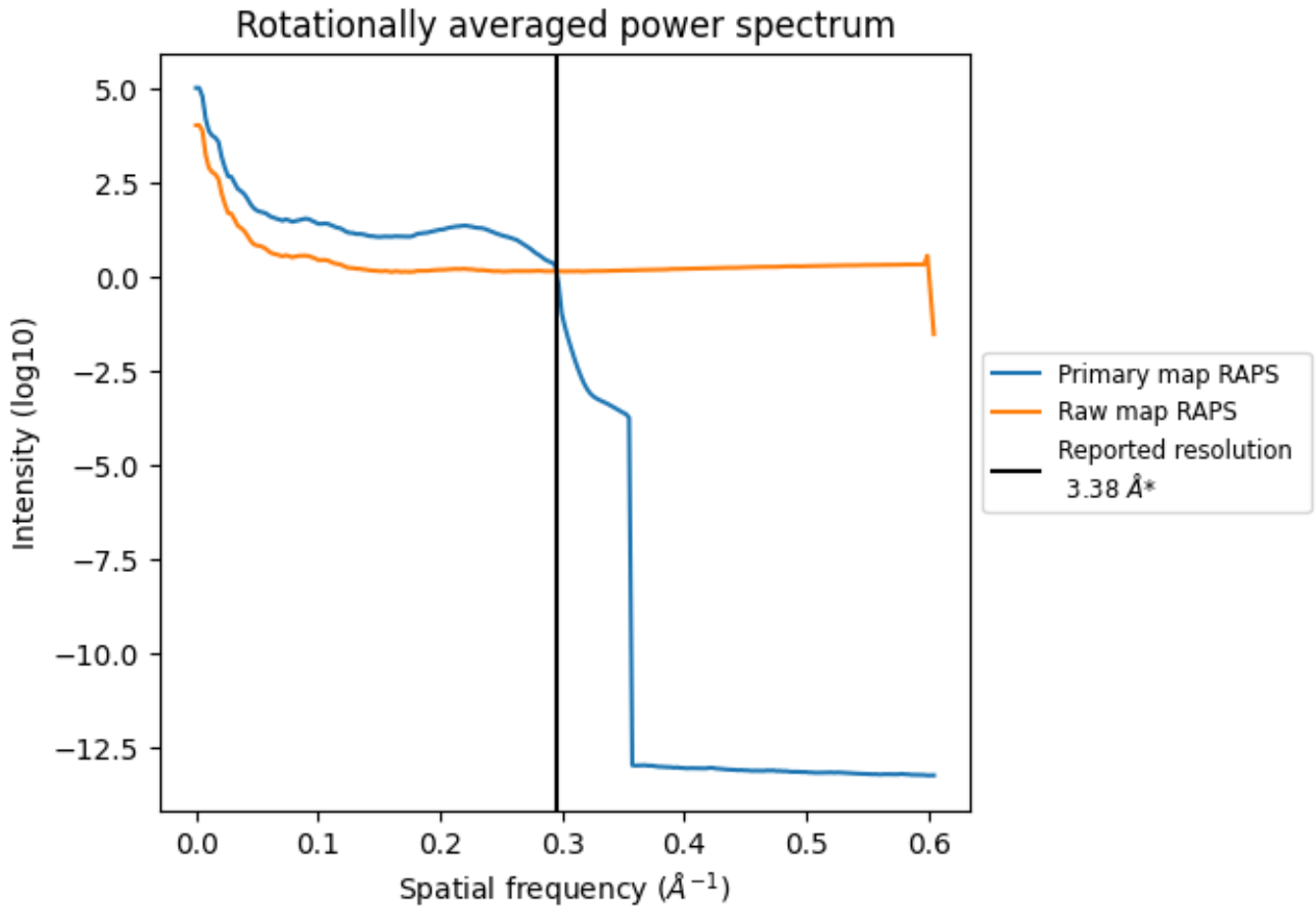
7.2 Volume estimate



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 128 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 (i)

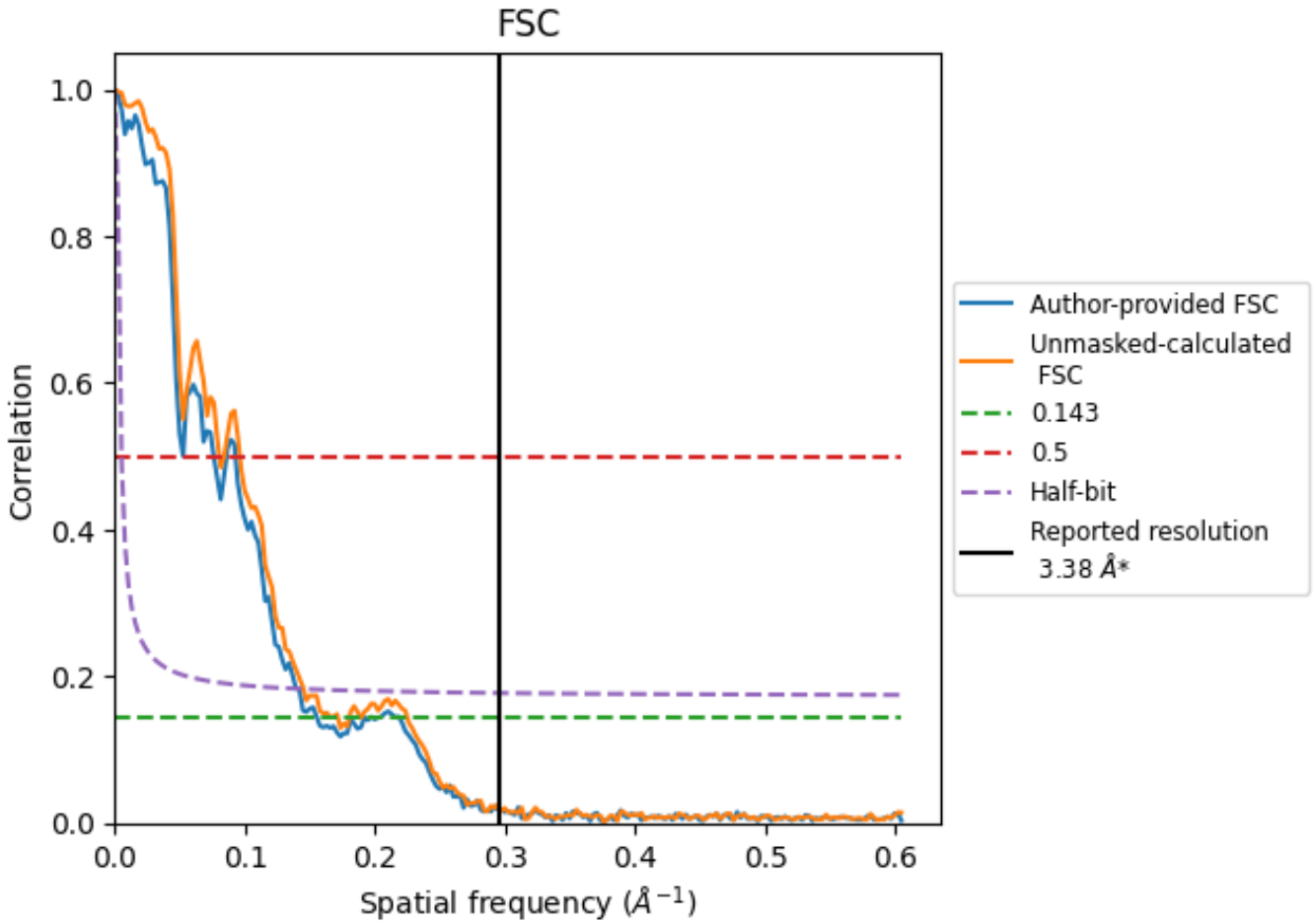


*Reported resolution corresponds to spatial frequency of 0.296 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.296 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	6.44	19.05	7.09
Unmasked-calculated*	5.83	12.44	6.90

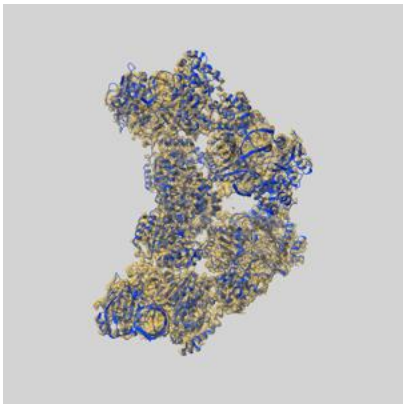
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.44 differs from the reported value 3.38 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.83 differs from the reported value 3.38 by more than 10 %

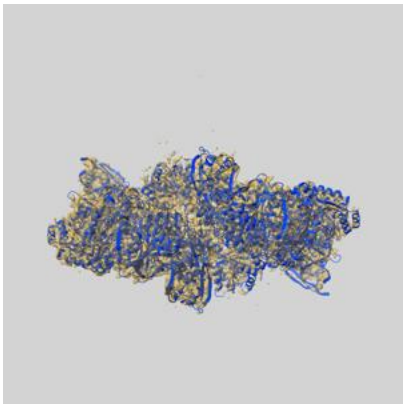
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39028 and PDB model 8Y80. Per-residue inclusion information can be found in section 3 on page 6.

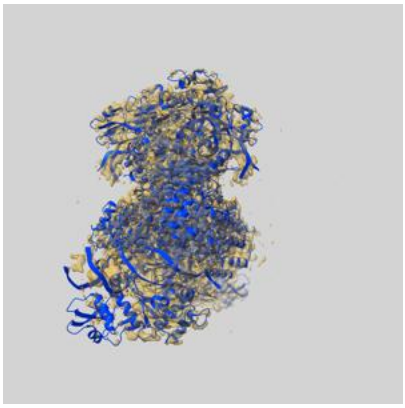
9.1 Map-model overlay



X



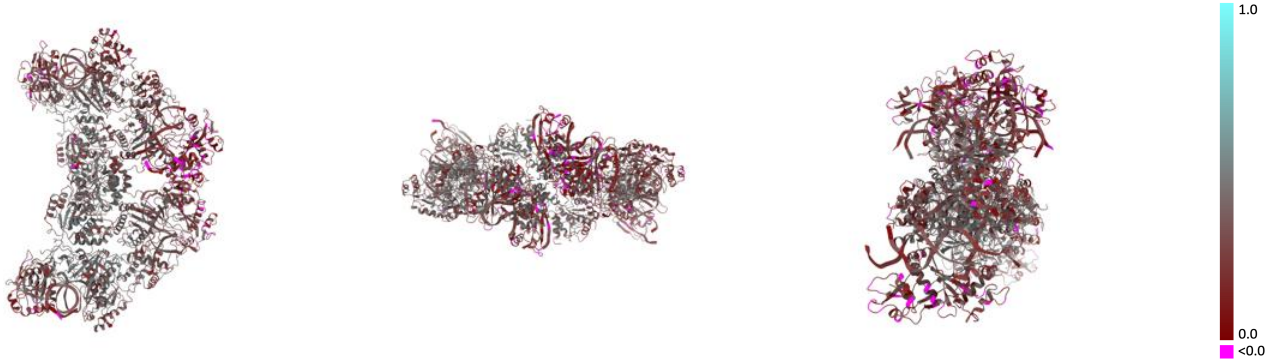
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.375 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.

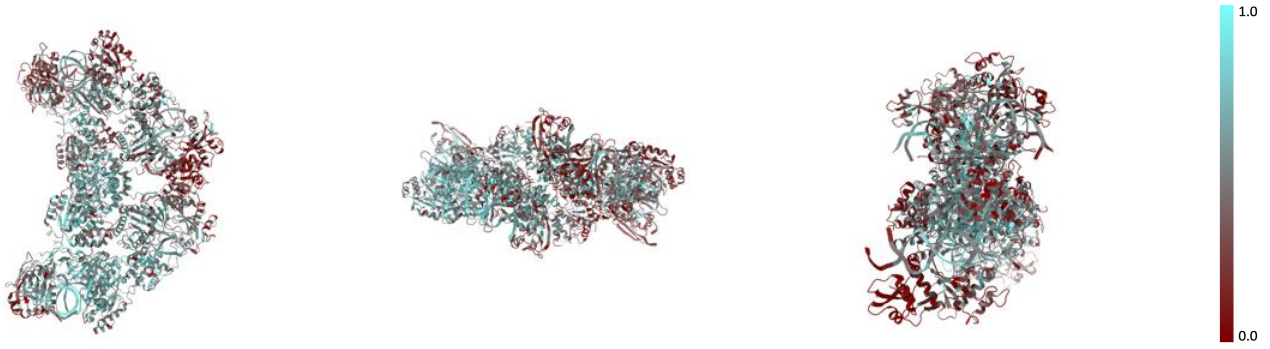
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

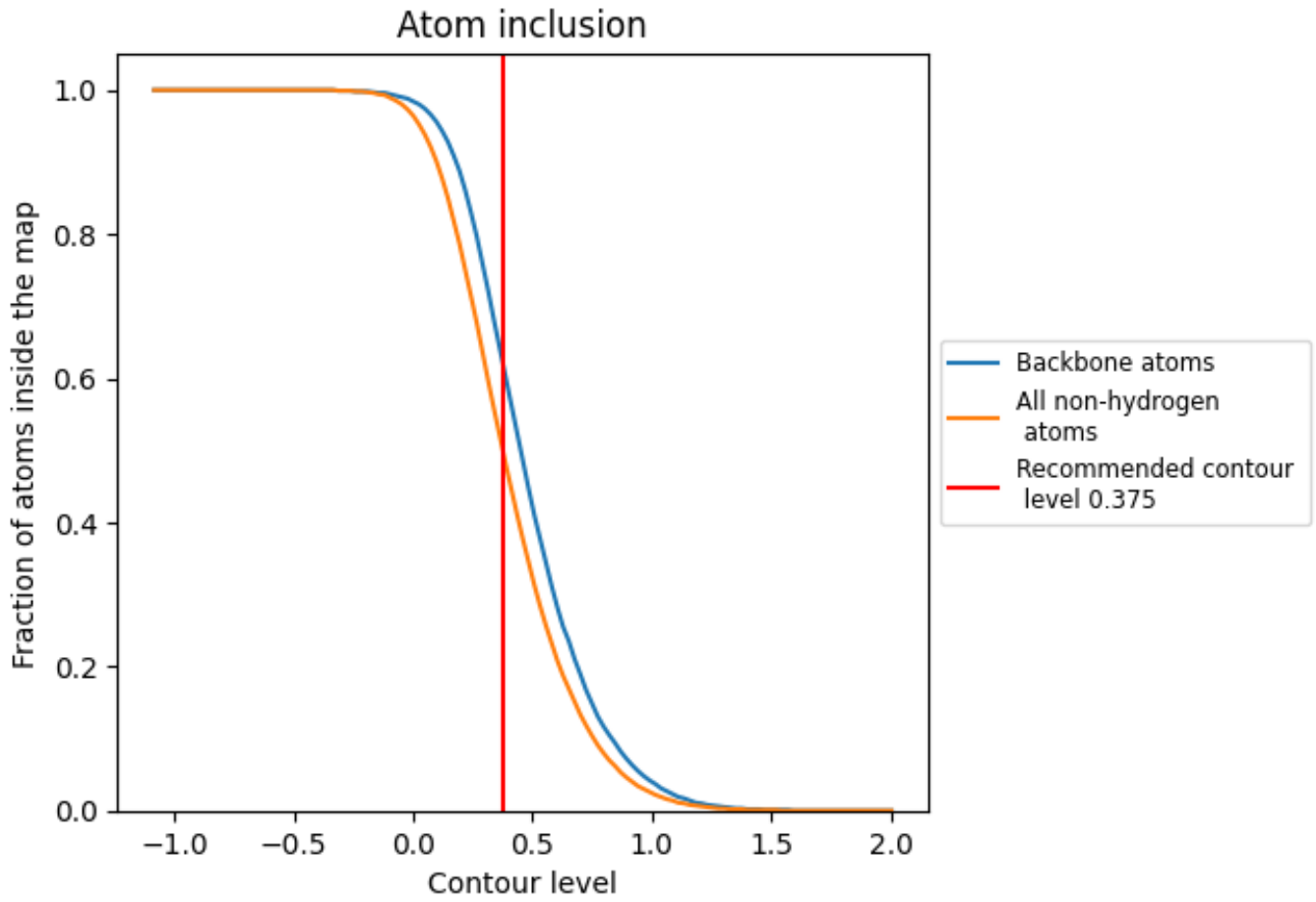
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.375).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 50% 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 (0.375) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5000	0.3310
A	0.5130	0.3510
B	0.6620	0.4180
C	0.7130	0.3200
D	0.7450	0.3530
E	0.5390	0.3370
F	0.5890	0.3720
G	0.7040	0.3300
H	0.7010	0.3210
I	0.2830	0.2840
J	0.4500	0.3430
K	0.5330	0.2810
L	0.4940	0.2810
M	0.4420	0.2900
N	0.4200	0.3030
O	0.5410	0.2350
P	0.4960	0.2090